

Electronic Supplementary Information

Deactivation of Ti and Zr Half-Metallocene Complexes Activated with B(C₆F₅)₃: A Case Study in Constructing DFT-Based QSARs to Predict Unimolecular Rate Constants

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The total SCF energies (in Hartrees) reported here can only be compared to total SCF energies computed using Gaussian software with the same exchange-correlation functional, basis sets, grids, and solvation model (where applicable). On the other hand, it is possible to compare relative energy differences (such as barrier heights, heats of reaction, solvation energies, etc.) for different computational methods.

DFT-optimized geometries are reported as XYZ coordinates in angstroms. The methyl ion pair and bare cation geometries for catalysts **1a-18a** were reported in the Supporting Information of T.A. Manz, S. Sharma, K. Phomphrai, K.A. Novstrup, A.E. Fenwick, P.E. Fanwick, G.A. Medvedev, M.M. Abu-Omar, W.N. Delgass, K.T. Thomson, and J.M. Caruthers, "Quantitative Effects of Ion Pairing and Sterics on Chain Propagation Kinetics for 1-Hexene Polymerization Catalyzed by Mixed Cp'/ArO Complexes," *Organometallics* **27** (2008) 5504-5520.

The computational tolerance for frequencies was approximately 30 cm⁻¹. Consequently, some ground states have imaginary frequencies with magnitudes less than or equal to approximately 30 cm⁻¹. These small magnitude frequencies are not significant and should be ignored.

1. List of Catalyst Structures and Summary Tables
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Table S1: List of catalyst structures

Catalyst	m	Ligand 1	Ligand 2 Aryloxy Substituents				
			R2	R3	R4	R5	R6
1	Ti	Cp	Me	H	Br	H	Me
2	Ti	Cp	Et	H	H	H	Et
3	Ti	Cp	ⁱ Pr	H	H	H	ⁱ Pr
4	Ti	Cp	H	H	H	H	H
5	Ti	Cp*	H	H	F	H	H
6	Ti	Cp*	H	H	Cl	H	H
7	Ti	Cp*	H	H	Br	H	H
8	Ti	Cp*	H	H	Ph	H	H
9	Ti	Cp*	H	H	^t Bu	H	H
10	Ti	Cp*	Me	H	H	H	Me
11	Ti	Cp*	Et	H	H	H	Et
12	Ti	Cp*	ⁱ Pr	H	H	H	ⁱ Pr
13	Ti	Cp*	Cyclo- hexyl (chair)	H	H	H	H
14	Ti	Cp*	Me	H	Br	H	Me
15	Ti	Cp*	CH ₂ Ph	H	H	H	H
16	Ti	Cp*	Ph	Ph	H	Ph	Ph
17	Ti	Cp*	H	OMe	H	H	H
18	Ti	Cp*	H	H	OMe	H	H
19	Ti	Cp	Ph	Ph	H	Ph	Ph
20	Ti	Cp*	Br	H	H	H	H
21	Ti	Cp*	Ph	H	H	H	H
22	Ti	Ind	Ph	Ph	H	Ph	Ph
23	Ti	Ind	ⁱ Pr	H	H	H	ⁱ Pr
24	Zr	Cp*	Ph	Ph	H	Ph	Ph
30	Ti	Cp*	OMe	H	H	H	OMe
31	Ti	Cp*	ⁱ Pr	H	Br	H	ⁱ Pr
33	Ti	Cp	Me	H	H	H	Me

Cp = C₅H₅; Cp* = C₅Me₅; Ind = C₅H₃C₆H₄

Table S2: Computed barrier heights and reaction energies in toluene solvent (SCF energies without zero-point and thermal vibrational corrections and without dispersion corrections)

cat. #	$\Theta_{\text{Cp}^{\cdot}}$ (°)	Θ_{OAr} (°)	H transfer (in kcal/mol)			C ₆ F ₅ transfer (in kcal/mol)		
			ΔV_0 toluene	E_{rxn} vac.	E_{rxn} toluene	ΔV_0 toluene	E_{rxn} vac.	E_{rxn} toluene
1	128	129	28.4	-3.5	-3.2	34.7	-8.6	-8.5
2	129	132	28.8	-4.0	-3.8	34.9	-9.9	-9.8
3	130	136	27.7	-5.1	-5.2	35.4	-10.5	-10.6
4	155	96	30.9	-5.5	-6.0	38.3	-9.2	-9.3
5	156	96	35.9	-5.6	-5.4	38.8	-10.1	-9.5
6	156	96	31.3	-5.6	-5.7	38.7	-10.3	-9.9
7	156	96	30.3	-5.6	-5.8	38.4	-10.2	-10.0
8	156	96	31.0	-5.4	-5.6	38.6	-9.1	-9.0
9	156	96	31.9	-5.5	-5.5	38.5	-8.4	-8.2
10	154	127	29.1	-3.4	-3.4	42.1	-4.8	-4.7
11	155	132	30.9	-3.4	-3.7	42.4	-3.8	-4.3
12	154	136	29.0	-5.2	-0.9	44.8	-5.1	-5.1
13d	155	125	29.3	-3.0	-2.9	41.8	-7.5	-7.4
13p	156	127	31.0	-2.9	-2.7	42.4	-7.2	-7.1
14	155	127	28.9	-3.8	-3.8	42.0	-1.6	-1.6
15d	155	113	29.4	-3.5	-3.3	41.5	-8.0	-8.3
15p	156	111	31.1	-3.6	-3.2	40.8	-7.3	-7.4
16	154	163	27.0	-7.3	-7.0	41.0	-2.7	-3.6
17d	156	96	30.0	-5.8	-6.2	38.5	-8.7	-8.9
17p	155	96	30.5	-5.7	-5.3	39.2	-8.7	-8.4
18	156	96	31.2	-5.4	-5.1	39.1	-8.4	-8.1
19	130	167	26.9	-4.6	-4.5	39.7	-9.1	-9.4
20d	154	118	29.8	-2.7	-2.4	41.8	-7.1	-6.9
20p	155	117	29.5	-5.5	-5.4	40.4	-9.1	-8.7
21d	154	127	n.a.	-3.5	-3.4	42.2	-6.2	-6.5
21p	154	128	29.5	-4.2	-3.9	41.7	-6.8	-6.9
22	136	169	32.1	-5.2	-4.9	41.2	-8.9	-9.5
23	136	138	28.8	-5.8	-5.6	37.4	-10.7	-10.7
24	149	155	28.4	-3.0	-4.6	43.7	-4.5	-6.9
30	155	135	29.3	-6.9	-7.0	42.6	-2.5	-2.7
31	154	135	29.0	-5.2	-4.6	45.7	-5.9	-5.9
33	128	129	29.9	-3.9	-3.4	35.4	-7.8	-7.2

d = ortho aryloxy substituent distal to chain, p = ortho aryloxy substituent proximal to chain

2. Computational Methods

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All DFT computations were performed in the Gaussian 03 software program. The reported SCF energies are those obtained using the OLYP exchange-correlation functional and LANL2DZ basis sets on all atoms. Auto electron density fitting basis sets were used by specifying olyp/lanl2dz/auto in the Gaussian 03 route line. The SCF energies in solution were generated using the PCM model as described below. SCF energies were usually converged to 10^{-8} Hartree or better. In all cases, the default set of DFT grids was used. (“The default grid is a pruned (75,302) grid, having 75 radial shells and 302 angular points per shell, resulting in about 7000 points per atom.”¹) Fermi damping was used to improve SCF convergence performance by specifying scf=(fermi, tight, maxcycle=400) or similar. If this failed, the SCF algorithm was modified to scf=(SSD, maxcycle=400, conver=6), scf=(maxcycle=400,conver=6), or similar.

Except where otherwise specified, all geometries were optimized in vacuum to better than 0.005 Å on atom displacements and 0.0025 AU on forces. Ground state geometries were optimized using the GDIIS method. Transition state geometries were optimized using the QST3 (quadratic synchronous transit) or TS method. The initial transition state guess was obtained by performing a series of constrained geometry optimizations or by modifying ligand substituents on a converged transition state geometry for a similar catalyst. Using this initial guess, the transition state was found using the QST3 or TS method with estimated Hessians. Using this transition state as input, the final transition state geometry was obtained using the QST3 or TS method with either (a) CALCALL or (b) CALCFC and FREQ. Analytic frequency analysis was performed to verify transition states, and the imaginary frequency corresponding to the reaction coordinate is given for each of the optimized transition states.

Once the geometries were converged in vacuum, the following parameters (Gaussian 03 defaults for the PCM model) were used to perform the solvation energy calculations in an implicit toluene-like solvent:

```

Model                : PCM.
Atomic radii         : UA0 (Simple United Atom Topological Model).
Polarization charges : Total charges.
Charge compensation  : None.
Solution method      : Matrix inversion.
Cavity               : GePol (RMin= .200 OFac= .890).
                    : Default sphere list used.
                    : Tesserae with average area of .200 Ang**2.
Solvent              : Toluene, Eps      = 2.379000
                    : Eps(inf)= 2.232000
                    : RSolv  = 2.820000 Ang.

```

These parameters were chosen by specifying scrf=(pcm,solvent=toluene) in the route line. In the case of bromobenzene-like and 1,2-dichlorobenzene-like solvents, the parameters had to be specified manually. This was done by using scrf=(pcm,read) together with the following PCM keywords:

```

(a) for bromobenzene
EPS = 5.40
EPSINF = 5.40
RSolv=2.82

```

DENSITY=0.00539

(b) for 1,2-dichlorobenzene

EPS=9.93

EPSINF=9.93

RSolv=2.82

DENSITY=0.00534

The above parameter set assumes the solvent radius is approximately the same for toluene, bromobenzene, and 1,2-dichlorobenzene. (A reasonable assumption due to the similar sizes and shapes of these molecules.)

The program alerted the user when one or more hydrogen atoms was not bonded to a single heavy atom. In such cases, an individual sphere was placed around that particular hydrogen atom rather than grouping it with a heavier atom. This was done by specifying `sphereonh=X` where X was the number of the hydrogen atom.

Where the program had difficulty with PCM convergence and returned the error “Inv2 failed in DMIVCL”, the following values were specified: `Rmin=0.5` and `OFac=0.8`. (The change in energy associated with this change in parameters is small enough to be neglected.) This suggestion was provided by Gaussian technical support.

Gaussian 03 Reference:

¹ Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; J. J. Dannenberg; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A.; Gaussian 03; Gaussian, Inc.: Pittsburgh PA, 2003.

3. Methyl Ion Pairs ([return to table of contents](#))

Geometries and energies of the methyl ion pairs for catalysts **1-18** were reported in T.A. Manz, S. Sharma, K. Phomphrai, K. A. Novstrup, A. E. Fenwick, P. E. Fanwick, G. A. Medvedev, M. M. Abu-Omar, W. N. Delgass, K. T. Thomson, and J. M. Caruthers, *Organometallics*, 27 (2008) 5504-5520.

Catalyst 1:

vacuum	toluene-like solvent	D3 dispersion
-2937.07916345	-2937.091722	-0.49768288

Frequencies --	-2.6382	8.0348	10.9429
Frequencies --	15.9487	19.3573	24.0573
Frequencies --	27.2232	30.9377	32.6093
Frequencies --	34.9954	41.7533	44.4095
Frequencies --	49.8131	71.2756	75.2276
Frequencies --	95.2457	101.4752	107.0002
Frequencies --	107.7845	115.7530	118.6533
Frequencies --	119.7685	125.4493	130.7109
Frequencies --	141.1742	149.3343	152.4272
Frequencies --	152.8542	153.2844	157.3586
Frequencies --	161.0517	161.8299	167.2024
Frequencies --	184.2984	194.7208	212.6272
Frequencies --	218.4472	219.0625	220.1642
Frequencies --	224.6661	235.3721	238.0064
Frequencies --	246.4970	249.4542	261.7954
Frequencies --	264.7743	264.8535	265.8323
Frequencies --	269.9944	272.6848	273.3692
Frequencies --	282.1208	290.5344	292.8589
Frequencies --	308.9396	317.6773	320.6967
Frequencies --	333.3003	336.9078	337.8158
Frequencies --	347.8541	357.5292	362.5031
Frequencies --	379.3782	380.1840	380.3239
Frequencies --	389.0646	391.2395	401.8081
Frequencies --	431.9069	431.9695	432.4087
Frequencies --	433.3223	456.9793	457.4179
Frequencies --	459.6730	479.2288	501.6076
Frequencies --	509.5751	513.5717	541.1497
Frequencies --	541.8482	547.6642	560.4526
Frequencies --	563.4916	569.1415	569.6773
Frequencies --	573.5720	595.3040	596.8225
Frequencies --	599.9694	632.0503	639.1978
Frequencies --	639.7316	642.7692	661.7248
Frequencies --	663.1851	682.2074	692.8898
Frequencies --	728.6853	730.4308	730.6695
Frequencies --	741.9752	759.5357	760.3606
Frequencies --	771.0042	790.7380	801.5757
Frequencies --	806.5409	815.7092	831.2055
Frequencies --	840.4983	840.7659	867.3843
Frequencies --	869.6145	871.3868	887.0620
Frequencies --	891.0419	895.2405	906.0748
Frequencies --	909.5396	912.6339	933.2209
Frequencies --	950.5509	1011.9560	1021.1087
Frequencies --	1022.9101	1026.3621	1028.3037
Frequencies --	1034.6698	1048.4716	1050.3873
Frequencies --	1052.0702	1052.6817	1053.0369

Frequencies --	1059.0343	1075.5384	1089.0893
Frequencies --	1090.6997	1094.9028	1110.5437
Frequencies --	1122.3723	1127.3044	1188.2187
Frequencies --	1206.0469	1216.0494	1217.3727
Frequencies --	1217.7969	1264.8217	1285.5338
Frequencies --	1286.1968	1320.0426	1321.1373
Frequencies --	1326.1283	1339.0047	1342.2843
Frequencies --	1343.9778	1354.7784	1389.3837
Frequencies --	1396.6387	1413.7670	1417.9618
Frequencies --	1418.3194	1419.7128	1423.6329
Frequencies --	1425.7240	1426.9261	1427.9830
Frequencies --	1440.1524	1442.8570	1447.4986
Frequencies --	1449.4381	1457.4046	1470.2013
Frequencies --	1470.5002	1472.4190	1490.3560
Frequencies --	1493.0456	1501.5386	1503.2245
Frequencies --	1586.8399	1590.5427	1595.2952
Frequencies --	1596.4891	1597.0894	1620.3209
Frequencies --	1621.2222	1622.7697	2982.2637
Frequencies --	2993.8930	3022.1630	3029.6070
Frequencies --	3103.3338	3109.2915	3116.0802
Frequencies --	3131.6426	3139.3641	3140.3338
Frequencies --	3141.1794	3166.0761	3202.3397
Frequencies --	3204.6479	3241.3611	3243.8453
Frequencies --	3257.8942	3267.1659	3280.8710

Catalyst 2:

vacuum	toluene-like solvent	D3 dispersion
-3003.09497634	-3003.10696	-0.52495552

Frequencies --	2.2515	7.7241	12.7659
Frequencies --	14.5809	17.8025	21.8994
Frequencies --	27.2799	30.7410	32.3365
Frequencies --	32.5484	40.0318	41.4731
Frequencies --	44.9100	53.2249	68.7259
Frequencies --	73.9885	80.9341	102.7277
Frequencies --	105.4604	106.5233	111.7729
Frequencies --	116.2932	119.0545	120.1331
Frequencies --	126.1707	141.6821	147.3127
Frequencies --	152.1899	153.1229	157.7356
Frequencies --	161.5354	161.9998	172.5194
Frequencies --	187.7536	204.2461	213.8749
Frequencies --	218.0111	219.5602	220.2478
Frequencies --	224.1195	236.9823	240.1818
Frequencies --	264.2416	264.6916	265.1615
Frequencies --	265.2506	271.1433	272.1140
Frequencies --	273.5848	282.2749	286.7557
Frequencies --	290.4191	293.7651	294.2927
Frequencies --	309.4914	315.8279	319.2492
Frequencies --	321.8049	324.4470	333.6305
Frequencies --	338.5021	340.8289	343.3184
Frequencies --	359.5162	371.2903	379.8563
Frequencies --	380.2314	381.1593	389.5457
Frequencies --	391.0498	397.6054	432.0930
Frequencies --	432.3652	432.9311	457.0248
Frequencies --	457.5011	459.5537	478.5766
Frequencies --	505.5907	514.4608	528.9682
Frequencies --	541.5027	542.1543	547.2263
Frequencies --	548.1533	562.0914	569.8540
Frequencies --	575.1550	594.6597	595.5970
Frequencies --	597.8872	606.1287	632.2184

Frequencies --	639.6316	640.1250	643.0142
Frequencies --	661.7951	663.2385	686.7697
Frequencies --	694.6666	708.8952	729.0983
Frequencies --	729.8624	734.2598	742.6480
Frequencies --	759.1825	760.7777	771.4906
Frequencies --	773.4528	787.0257	796.3377
Frequencies --	801.9650	813.9915	827.7881
Frequencies --	834.1251	840.3164	841.3518
Frequencies --	852.1779	866.9487	870.1487
Frequencies --	871.5679	894.4541	906.3184
Frequencies --	909.8903	912.2586	924.6109
Frequencies --	935.5024	995.1402	996.2805
Frequencies --	1021.2681	1024.6655	1025.3665
Frequencies --	1027.4016	1027.9840	1035.7438
Frequencies --	1048.7229	1050.8813	1052.5452
Frequencies --	1058.6329	1080.1710	1090.7300
Frequencies --	1093.5909	1094.3166	1097.2558
Frequencies --	1099.1248	1102.7291	1108.5364
Frequencies --	1120.6290	1127.3263	1183.3899
Frequencies --	1190.1962	1205.2936	1215.8075
Frequencies --	1216.9474	1217.4254	1258.3004
Frequencies --	1278.7507	1285.7057	1288.0015
Frequencies --	1288.4717	1320.4082	1320.5268
Frequencies --	1325.9391	1326.5512	1338.8523
Frequencies --	1341.4051	1342.5559	1343.2364
Frequencies --	1379.5371	1389.5213	1397.0515
Frequencies --	1413.0582	1415.3561	1417.8669
Frequencies --	1418.5332	1419.3109	1430.8186
Frequencies --	1432.4057	1439.8295	1442.5043
Frequencies --	1448.0754	1449.8671	1462.6945
Frequencies --	1467.5418	1469.8818	1470.4380
Frequencies --	1472.3053	1478.6807	1492.9690
Frequencies --	1500.3257	1501.8671	1507.0060
Frequencies --	1507.5960	1595.4708	1596.7519
Frequencies --	1597.0192	1598.9764	1607.1875
Frequencies --	1620.1825	1620.9898	1622.5783
Frequencies --	2983.2321	2990.9087	3013.0273
Frequencies --	3015.8597	3017.2332	3021.8712
Frequencies --	3063.3908	3067.1847	3106.0026
Frequencies --	3116.0216	3120.5265	3121.6078
Frequencies --	3123.6595	3134.3607	3136.3293
Frequencies --	3160.9016	3172.5229	3206.8625
Frequencies --	3215.3281	3241.6281	3243.9373
Frequencies --	3257.0216	3265.1815	3279.9043

Catalyst 3:

vacuum	toluene-like solvent	D3 dispersion
-3081.6707187	-3081.681987	-0.56435934

Frequencies --	6.2261	11.3502	12.5093
Frequencies --	20.9982	27.2697	28.5361
Frequencies --	29.7361	32.0349	34.4961
Frequencies --	36.6000	39.1398	39.3913
Frequencies --	46.4851	50.7832	67.0888
Frequencies --	72.0007	74.6098	90.4595
Frequencies --	102.0314	107.8972	110.9781
Frequencies --	119.4638	119.8435	125.5050
Frequencies --	126.4798	130.7363	143.7035
Frequencies --	145.8713	147.9969	154.8409
Frequencies --	157.5842	160.2611	163.4684

Frequencies --	171.6820	184.5552	212.1293
Frequencies --	215.1953	217.5882	221.6053
Frequencies --	221.7631	230.3031	233.0174
Frequencies --	239.2399	244.0314	250.1969
Frequencies --	259.2651	263.2475	264.7813
Frequencies --	264.9562	265.6145	271.5299
Frequencies --	273.1278	275.4159	276.9528
Frequencies --	283.8149	289.0183	293.4526
Frequencies --	297.2079	308.1353	310.0973
Frequencies --	313.1465	315.3101	323.6760
Frequencies --	331.1533	334.6266	336.7877
Frequencies --	342.2940	365.7370	378.8255
Frequencies --	379.2469	380.8665	381.4527
Frequencies --	384.7300	396.8047	427.3927
Frequencies --	431.0272	431.6468	432.1963
Frequencies --	433.4613	436.4796	454.1802
Frequencies --	457.1363	457.6477	476.0474
Frequencies --	509.7034	538.0421	540.6751
Frequencies --	542.4704	544.6329	548.1316
Frequencies --	560.7954	570.1519	589.1018
Frequencies --	591.7335	600.7626	605.6172
Frequencies --	613.8340	630.5865	632.5897
Frequencies --	637.6636	639.1251	642.2115
Frequencies --	655.3747	668.0911	691.8094
Frequencies --	698.5827	722.7271	729.6474
Frequencies --	731.0375	742.5761	754.9678
Frequencies --	765.0429	765.3401	769.9679
Frequencies --	797.7026	805.3933	816.7378
Frequencies --	820.1468	820.8811	840.7419
Frequencies --	842.0524	844.6717	852.6260
Frequencies --	877.1680	878.8510	884.7914
Frequencies --	904.0074	909.8581	910.4016
Frequencies --	913.4000	928.1586	931.9136
Frequencies --	932.6427	937.5102	940.4958
Frequencies --	964.1106	965.3483	996.2745
Frequencies --	1013.2149	1023.8444	1029.8195
Frequencies --	1031.3564	1031.9773	1046.9323
Frequencies --	1050.5712	1053.6652	1055.8615
Frequencies --	1070.2713	1073.4300	1091.5902
Frequencies --	1092.5908	1103.2449	1115.9198
Frequencies --	1116.4622	1118.0991	1125.4034
Frequencies --	1127.7100	1166.3658	1182.2689
Frequencies --	1184.3040	1193.7591	1206.1992
Frequencies --	1215.1395	1215.5598	1217.2908
Frequencies --	1253.8142	1279.2857	1286.8415
Frequencies --	1310.1105	1318.4272	1321.0988
Frequencies --	1324.8796	1326.7903	1330.0514
Frequencies --	1335.4409	1338.5411	1341.3053
Frequencies --	1346.6693	1383.7426	1389.9750
Frequencies --	1397.1417	1400.7974	1402.5764
Frequencies --	1414.8618	1418.8963	1419.7055
Frequencies --	1420.5895	1421.7394	1430.2890
Frequencies --	1437.8724	1443.9290	1447.3451
Frequencies --	1449.2387	1451.6932	1466.3654
Frequencies --	1468.9339	1470.6733	1472.6665
Frequencies --	1475.2459	1487.0302	1488.4398
Frequencies --	1488.8273	1493.5990	1499.9919
Frequencies --	1505.4894	1506.9234	1507.9695
Frequencies --	1594.7547	1595.8463	1596.7797
Frequencies --	1597.4324	1605.4316	1619.1171
Frequencies --	1621.4161	1623.3783	2976.5873
Frequencies --	2990.3934	3006.8297	3008.9459
Frequencies --	3011.0487	3019.1629	3070.6057

Frequencies --	3105.8353	3109.8319	3110.9678
Frequencies --	3112.2160	3112.8435	3116.2503
Frequencies --	3117.6632	3118.1494	3125.8516
Frequencies --	3133.0243	3136.2987	3152.0201
Frequencies --	3167.7187	3168.4418	3188.3446
Frequencies --	3201.3402	3246.0233	3248.0936
Frequencies --	3262.1491	3269.8992	3284.1743

Catalyst 4:

vacuum	toluene-like solvent	D3 dispersion
-3042.40812302	-3042.418617	-0.54218856

Frequencies --	7.4575	10.9138	12.7937
Frequencies --	18.6396	23.9836	26.1311
Frequencies --	28.6468	31.1611	31.5757
Frequencies --	38.7946	40.4266	43.5687
Frequencies --	47.9659	70.0621	83.4815
Frequencies --	101.8387	104.7607	106.7026
Frequencies --	113.6867	116.2342	117.8985
Frequencies --	118.3148	123.7391	126.4256
Frequencies --	128.6095	137.8902	139.9630
Frequencies --	141.8719	146.2670	150.9300
Frequencies --	153.3307	154.0377	157.1098
Frequencies --	160.1033	161.3888	162.7197
Frequencies --	166.1207	170.1757	199.6058
Frequencies --	211.4490	216.6044	218.1137
Frequencies --	219.0294	228.7589	247.3685
Frequencies --	263.3391	264.4272	264.7570
Frequencies --	266.4115	270.0229	272.4465
Frequencies --	282.1782	285.3288	286.3316
Frequencies --	291.2188	291.8276	299.2396
Frequencies --	301.2863	308.8352	312.2730
Frequencies --	317.5207	321.0057	329.0404
Frequencies --	331.7023	333.5529	338.9463
Frequencies --	349.0299	378.4917	378.8383
Frequencies --	379.2991	384.0763	387.2431
Frequencies --	390.3028	396.2000	408.7797
Frequencies --	417.6359	432.1630	432.7202
Frequencies --	432.9636	447.3392	452.8966
Frequencies --	456.3364	457.5357	473.3632
Frequencies --	507.6576	516.7102	531.0547
Frequencies --	536.3640	541.3362	542.0276
Frequencies --	547.8614	554.7074	579.7443
Frequencies --	583.1250	592.4301	596.0538
Frequencies --	605.2648	606.6624	614.9284
Frequencies --	630.4993	638.3019	638.6365
Frequencies --	641.3417	654.8510	661.4687
Frequencies --	663.2072	690.0076	694.8296
Frequencies --	700.9178	726.8739	729.0796
Frequencies --	741.9823	757.3771	758.7547
Frequencies --	762.3295	770.3076	800.8835
Frequencies --	802.8625	837.6813	840.3699
Frequencies --	859.5512	868.7714	906.6758
Frequencies --	907.3164	910.4744	921.6818
Frequencies --	927.1365	968.8808	970.2284
Frequencies --	977.4049	1000.7981	1008.3074
Frequencies --	1010.2382	1023.8747	1025.8775
Frequencies --	1030.4945	1042.3680	1043.0363
Frequencies --	1046.4892	1047.3080	1048.0541
Frequencies --	1049.1017	1049.3537	1051.5283

Frequencies --	1074.7333	1088.4723	1089.7492
Frequencies --	1090.5498	1101.7998	1125.9873
Frequencies --	1140.7653	1171.3254	1175.9266
Frequencies --	1183.5488	1190.3825	1193.3694
Frequencies --	1213.8683	1214.9553	1215.8277
Frequencies --	1242.1489	1319.6503	1321.6948
Frequencies --	1326.4852	1326.5542	1338.8968
Frequencies --	1341.7924	1344.6127	1376.2358
Frequencies --	1409.8105	1415.4808	1417.5078
Frequencies --	1417.9840	1420.1458	1425.6053
Frequencies --	1426.2546	1427.5486	1430.1796
Frequencies --	1433.4927	1437.9000	1443.2491
Frequencies --	1447.2846	1455.0059	1455.3048
Frequencies --	1459.4921	1468.0337	1469.4076
Frequencies --	1469.8152	1471.6751	1481.5553
Frequencies --	1481.8518	1484.4916	1492.1426
Frequencies --	1496.0347	1498.8086	1501.0317
Frequencies --	1506.6307	1507.9780	1512.3770
Frequencies --	1516.4539	1517.3179	1595.7607
Frequencies --	1596.7834	1597.3979	1597.7064
Frequencies --	1607.3365	1620.3938	1620.6541
Frequencies --	1622.3728	2987.7061	3006.5559
Frequencies --	3010.3094	3010.9133	3012.4384
Frequencies --	3014.4340	3016.4811	3101.8285
Frequencies --	3102.8472	3104.2318	3105.4249
Frequencies --	3109.0786	3111.5557	3131.2007
Frequencies --	3140.9786	3141.1791	3145.8070
Frequencies --	3148.5771	3151.0642	3159.2693
Frequencies --	3167.8581	3176.6355	3192.6747
Frequencies --	3194.5816	3202.8280	3210.8206

Catalyst 5:

vacuum	toluene-like solvent	D3 dispersion
-3141.63255757	-3141.644913	-0.54295154

Frequencies --	9.1656	11.2329	13.4093
Frequencies --	16.5521	23.9196	25.7465
Frequencies --	27.2175	32.0072	32.8185
Frequencies --	38.3209	39.5242	43.3612
Frequencies --	44.1938	69.6271	79.3178
Frequencies --	98.0048	103.7608	104.8886
Frequencies --	105.8488	111.1352	112.9738
Frequencies --	117.8700	118.5789	123.3260
Frequencies --	125.4633	127.0913	137.2621
Frequencies --	139.5648	144.2661	146.8385
Frequencies --	151.5981	153.0002	157.2191
Frequencies --	160.1675	160.5810	161.3168
Frequencies --	163.8967	167.2028	191.7001
Frequencies --	207.2377	213.6002	216.3123
Frequencies --	218.7642	219.2235	248.6073
Frequencies --	259.2337	264.1393	264.6984
Frequencies --	264.9086	268.8735	270.6922
Frequencies --	273.5434	283.2566	284.8535
Frequencies --	287.1750	292.3740	292.7451
Frequencies --	298.6860	303.1161	308.8742
Frequencies --	310.6428	314.5136	321.2656
Frequencies --	331.2864	333.8249	339.7733
Frequencies --	355.1100	360.3806	372.5047
Frequencies --	379.3693	379.9266	380.3093
Frequencies --	387.9485	389.8807	392.5512

Frequencies --	405.9008	415.9341	417.4618
Frequencies --	432.5044	432.8223	433.2480
Frequencies --	454.0878	456.4490	457.5458
Frequencies --	461.1341	474.0143	511.6150
Frequencies --	516.9474	530.8679	535.9737
Frequencies --	541.3469	542.4384	548.0230
Frequencies --	555.1268	568.2514	580.2073
Frequencies --	582.8882	592.7773	596.5403
Frequencies --	604.4313	612.9116	630.8975
Frequencies --	633.2327	638.5445	639.1008
Frequencies --	642.0025	662.6083	662.6816
Frequencies --	694.4052	701.0401	705.9405
Frequencies --	727.6229	729.1895	742.4489
Frequencies --	758.5988	759.2064	770.6301
Frequencies --	793.1362	801.7404	804.3456
Frequencies --	810.0619	834.5569	840.5564
Frequencies --	859.6143	870.6996	906.9729
Frequencies --	907.7931	911.0930	926.4733
Frequencies --	950.0408	961.8481	969.5515
Frequencies --	972.8803	1012.1767	1014.4566
Frequencies --	1024.1684	1026.5546	1043.2162
Frequencies --	1043.4482	1046.4288	1047.9058
Frequencies --	1048.0912	1049.3925	1049.8712
Frequencies --	1052.1173	1076.7918	1089.7788
Frequencies --	1090.2011	1103.5903	1113.8825
Frequencies --	1127.3539	1130.6253	1169.5097
Frequencies --	1171.7354	1175.4412	1193.4495
Frequencies --	1205.0667	1214.4526	1215.7087
Frequencies --	1216.4046	1258.6630	1306.2700
Frequencies --	1320.3407	1321.3925	1326.5850
Frequencies --	1339.3481	1342.3053	1344.5174
Frequencies --	1361.3828	1412.1393	1415.6089
Frequencies --	1417.6544	1418.6739	1420.4001
Frequencies --	1423.2527	1425.6884	1426.9981
Frequencies --	1429.1199	1430.0084	1434.2371
Frequencies --	1437.7514	1446.2857	1447.1468
Frequencies --	1455.7822	1458.9053	1467.1806
Frequencies --	1469.7108	1469.9159	1471.8327
Frequencies --	1476.3354	1482.1234	1491.6015
Frequencies --	1494.6459	1496.5206	1499.6544
Frequencies --	1500.6322	1506.7914	1508.4245
Frequencies --	1512.8982	1516.1467	1517.8613
Frequencies --	1595.8620	1596.9733	1597.5665
Frequencies --	1599.0862	1616.4042	1620.3032
Frequencies --	1620.7260	1622.3796	2988.7629
Frequencies --	3006.5402	3010.9975	3011.8442
Frequencies --	3012.9626	3014.7881	3016.5604
Frequencies --	3102.5592	3103.4503	3104.9072
Frequencies --	3106.0846	3109.2574	3113.4741
Frequencies --	3134.5014	3141.3125	3141.9216
Frequencies --	3145.1603	3147.7770	3150.3646
Frequencies --	3160.6746	3190.7633	3200.7622
Frequencies --	3201.8524	3218.1632	3221.7794

Catalyst 6:

vacuum	toluene-like solvent	D3 dispersion
-3056.7624852	-3056.774044	-0.55014210

Frequencies --	7.4819	13.2981	13.7339
Frequencies --	16.8949	23.3456	25.3273

Frequencies --	26.0496	28.7215	32.1136
Frequencies --	36.9272	37.6812	42.1525
Frequencies --	43.0145	67.8085	75.6667
Frequencies --	86.9208	92.6410	100.6043
Frequencies --	103.0469	104.9650	106.3901
Frequencies --	110.7995	117.3213	118.4724
Frequencies --	119.6614	123.1229	130.3334
Frequencies --	134.8883	140.4912	145.3473
Frequencies --	152.1194	152.6861	157.2608
Frequencies --	159.2796	160.6184	160.9833
Frequencies --	165.8439	166.9798	179.0035
Frequencies --	195.3914	208.1511	210.0014
Frequencies --	218.1506	218.4453	230.5105
Frequencies --	241.4910	252.5362	263.7580
Frequencies --	264.5480	264.7653	265.4150
Frequencies --	271.2916	273.4032	279.5339
Frequencies --	281.8326	286.4732	290.1764
Frequencies --	293.4787	296.0643	299.4426
Frequencies --	305.1488	308.5676	314.9626
Frequencies --	319.1402	331.5710	333.4893
Frequencies --	337.5626	339.5987	345.7671
Frequencies --	378.5219	379.8974	380.1038
Frequencies --	380.7390	388.2335	389.1923
Frequencies --	395.2258	407.7970	409.2152
Frequencies --	432.3687	432.6604	432.9902
Frequencies --	451.4614	453.1189	456.6011
Frequencies --	457.3744	471.4009	473.3423
Frequencies --	487.2583	515.0729	530.9914
Frequencies --	536.3966	541.1238	542.1917
Frequencies --	547.8727	555.9772	577.3349
Frequencies --	581.7808	592.4573	596.5166
Frequencies --	603.6248	609.0074	628.5937
Frequencies --	630.1194	638.6423	639.1005
Frequencies --	641.7759	642.7966	661.5806
Frequencies --	662.8663	680.7411	693.9879
Frequencies --	710.9740	727.7788	729.1075
Frequencies --	741.5491	757.9102	759.1060
Frequencies --	770.5310	782.4270	788.5002
Frequencies --	801.8061	805.0587	838.5398
Frequencies --	858.5806	869.7079	906.4397
Frequencies --	907.6246	910.5694	922.3471
Frequencies --	932.9875	947.7680	969.9343
Frequencies --	972.2229	1010.0112	1012.9917
Frequencies --	1023.5213	1025.9312	1041.9506
Frequencies --	1042.7381	1046.0517	1046.8684
Frequencies --	1048.1310	1049.2391	1049.6918
Frequencies --	1051.9204	1074.6688	1076.2790
Frequencies --	1089.4492	1090.0284	1098.7250
Frequencies --	1117.8108	1127.0636	1129.7587
Frequencies --	1171.2740	1175.8507	1188.6982
Frequencies --	1191.8801	1214.1553	1215.6948
Frequencies --	1216.4556	1250.2491	1309.9842
Frequencies --	1319.2574	1321.5471	1326.6166
Frequencies --	1339.4976	1342.7144	1344.2333
Frequencies --	1353.9545	1411.6563	1415.7653
Frequencies --	1416.4247	1417.4471	1418.9420
Frequencies --	1420.4583	1425.2351	1426.8766
Frequencies --	1427.7190	1429.5257	1431.4943
Frequencies --	1435.8483	1442.9153	1447.1626
Frequencies --	1454.3732	1458.3176	1464.0662
Frequencies --	1469.1736	1469.7271	1471.6028
Frequencies --	1476.4594	1481.6100	1485.5966
Frequencies --	1491.7054	1495.2102	1498.0006

Frequencies --	1501.5877	1506.0847	1508.2318
Frequencies --	1510.8417	1515.3974	1517.6541
Frequencies --	1581.0372	1595.7321	1596.8485
Frequencies --	1597.5173	1603.5855	1620.0371
Frequencies --	1620.6671	1622.3309	2988.0417
Frequencies --	3009.6680	3011.3661	3011.9885
Frequencies --	3013.3647	3015.3187	3016.5756
Frequencies --	3101.6966	3102.6746	3105.3816
Frequencies --	3106.3363	3109.9721	3112.1302
Frequencies --	3133.8308	3141.3582	3146.2979
Frequencies --	3146.5880	3148.9164	3151.6381
Frequencies --	3159.8154	3197.1035	3199.4708
Frequencies --	3201.2929	3215.7655	3220.9132

Catalyst 7:

vacuum	toluene-like solvent	D3 dispersion
-3054.96633024	-3054.977669	-0.55122293

Frequencies --	-4.5362	8.4499	9.7312
Frequencies --	12.7005	22.9240	24.0436
Frequencies --	26.6315	30.6349	31.5702
Frequencies --	37.0188	39.0741	40.5414
Frequencies --	43.6621	66.3563	71.1801
Frequencies --	88.1461	95.0956	100.3853
Frequencies --	104.0714	105.1078	109.3928
Frequencies --	115.5040	117.8461	119.2343
Frequencies --	123.4603	128.2501	134.0841
Frequencies --	138.6268	144.1283	151.0729
Frequencies --	152.8628	156.9054	157.1059
Frequencies --	159.9428	161.3094	162.7705
Frequencies --	162.9515	168.7607	179.5432
Frequencies --	194.5150	202.6645	209.4295
Frequencies --	217.0185	219.1882	234.4782
Frequencies --	236.2920	243.9658	253.1287
Frequencies --	258.4472	264.4816	264.5543
Frequencies --	264.7790	270.1029	272.8601
Frequencies --	279.7873	285.3557	289.1302
Frequencies --	291.4665	292.3541	297.4693
Frequencies --	303.7150	308.1887	313.8574
Frequencies --	319.4136	331.3392	333.8190
Frequencies --	338.3300	348.3480	353.9142
Frequencies --	378.9134	379.0570	379.6055
Frequencies --	380.2562	388.4096	389.9713
Frequencies --	394.3872	402.3532	412.6566
Frequencies --	432.2991	432.7378	432.8775
Frequencies --	436.1520	452.9827	454.0477
Frequencies --	456.3745	457.6777	474.0651
Frequencies --	506.6018	513.3175	530.6809
Frequencies --	535.8262	541.0169	542.1176
Frequencies --	547.8836	555.1337	574.6144
Frequencies --	582.0703	592.0836	596.1602
Frequencies --	602.7532	610.1528	627.6896
Frequencies --	630.8407	638.9004	639.4230
Frequencies --	642.2140	661.7932	662.6127
Frequencies --	675.7966	694.8978	699.4661
Frequencies --	706.5309	727.2878	729.2357
Frequencies --	742.5856	758.4988	759.1324
Frequencies --	770.5198	802.0001	803.2412
Frequencies --	819.9466	833.2985	840.9037
Frequencies --	858.1323	868.0407	907.0205

Frequencies --	907.4201	910.7701	925.8772
Frequencies --	956.3135	967.3648	970.2513
Frequencies --	973.1278	1009.6526	1017.9044
Frequencies --	1023.8257	1025.3159	1041.7571
Frequencies --	1043.0326	1045.8449	1047.3129
Frequencies --	1048.4431	1048.7846	1049.3178
Frequencies --	1051.8799	1063.9280	1074.0707
Frequencies --	1089.4474	1089.6472	1099.2328
Frequencies --	1116.3462	1127.3191	1129.1561
Frequencies --	1171.6583	1175.3503	1190.0854
Frequencies --	1193.3118	1214.3019	1215.4213
Frequencies --	1216.0194	1253.0409	1308.2644
Frequencies --	1319.7345	1321.2385	1326.3097
Frequencies --	1338.8978	1341.7425	1344.6694
Frequencies --	1349.4627	1407.8003	1411.3647
Frequencies --	1415.2453	1417.1137	1418.2150
Frequencies --	1420.1495	1424.5855	1426.6136
Frequencies --	1428.9448	1429.3542	1432.3051
Frequencies --	1436.1637	1445.7729	1447.1577
Frequencies --	1455.4570	1458.4617	1464.7341
Frequencies --	1469.7063	1469.7149	1471.7243
Frequencies --	1474.0878	1479.7075	1482.2766
Frequencies --	1492.1949	1494.0597	1500.0947
Frequencies --	1500.6141	1506.5650	1508.4537
Frequencies --	1512.8211	1515.4146	1518.2022
Frequencies --	1576.9339	1595.6324	1596.4605
Frequencies --	1596.6475	1597.5813	1620.4515
Frequencies --	1620.6248	1622.3722	2987.2198
Frequencies --	3005.5984	3011.4695	3011.9381
Frequencies --	3013.3690	3015.1585	3016.7959
Frequencies --	3102.9624	3103.7995	3105.1127
Frequencies --	3105.7457	3108.5540	3114.4680
Frequencies --	3132.6309	3141.7060	3142.4216
Frequencies --	3145.5789	3149.4009	3151.3640
Frequencies --	3161.9564	3192.7242	3193.2588
Frequencies --	3194.7213	3210.1352	3214.0284

Catalyst 8:

vacuum	toluene-like solvent	D3 dispersion
-3273.35926321	-3273.371798	-0.61743878

Frequencies --	5.3452	7.7819	13.3511
Frequencies --	15.4487	23.4251	24.0635
Frequencies --	24.8110	26.6002	31.1792
Frequencies --	32.1932	37.9960	40.1856
Frequencies --	43.2498	56.4325	65.5027
Frequencies --	72.8355	76.2219	91.3249
Frequencies --	103.4530	104.1342	106.2935
Frequencies --	107.4256	116.7681	117.7637
Frequencies --	118.1445	119.5889	119.7930
Frequencies --	124.6854	136.1147	137.5995
Frequencies --	146.6395	151.6695	152.4193
Frequencies --	155.9034	156.4366	157.2048
Frequencies --	159.5887	160.7348	161.2734
Frequencies --	163.4542	176.4932	192.1722
Frequencies --	206.6409	211.3236	216.7829
Frequencies --	218.1605	218.5793	238.8502
Frequencies --	246.5398	260.5140	264.6752
Frequencies --	264.9797	265.1358	269.6802
Frequencies --	272.3294	274.7969	282.1071

Frequencies --	287.5345	289.5893	291.7790
Frequencies --	294.2082	299.9532	303.7706
Frequencies --	308.9199	314.4898	317.6811
Frequencies --	330.9120	332.7294	336.0735
Frequencies --	338.8927	349.2885	367.9604
Frequencies --	378.3510	379.3715	380.0174
Frequencies --	388.2494	388.9293	393.3229
Frequencies --	399.3568	407.6014	415.7507
Frequencies --	420.8392	432.4936	432.6879
Frequencies --	432.7847	438.6366	452.4575
Frequencies --	456.3514	457.3676	459.1191
Frequencies --	473.0712	508.5021	515.4485
Frequencies --	530.8535	536.6464	541.4763
Frequencies --	542.0076	547.9307	555.2596
Frequencies --	556.0272	576.8047	582.0336
Frequencies --	592.5651	596.1960	603.1689
Frequencies --	611.0368	621.6460	630.1629
Frequencies --	638.2250	638.6765	638.8776
Frequencies --	639.9711	641.4584	661.1902
Frequencies --	662.5994	690.9197	695.4724
Frequencies --	707.2536	724.4736	727.9294
Frequencies --	728.9211	741.5869	748.6333
Frequencies --	757.5984	758.5024	770.5789
Frequencies --	773.8810	802.2422	804.1819
Frequencies --	829.4457	839.6869	848.4499
Frequencies --	858.8128	859.2100	869.7824
Frequencies --	906.6593	907.6020	910.7254
Frequencies --	929.1144	932.9259	962.9739
Frequencies --	969.8222	971.4032	974.6600
Frequencies --	986.9084	999.9177	1006.3388
Frequencies --	1010.5958	1022.3991	1023.7149
Frequencies --	1025.9813	1042.2681	1043.4615
Frequencies --	1046.7469	1047.3737	1048.1749
Frequencies --	1049.1436	1049.2965	1049.8473
Frequencies --	1051.6488	1060.1963	1075.5693
Frequencies --	1088.3493	1089.9934	1095.4221
Frequencies --	1102.6646	1126.5207	1129.5726
Frequencies --	1135.3154	1171.5910	1176.1516
Frequencies --	1184.7773	1191.3351	1199.1064
Frequencies --	1211.9723	1213.9523	1215.1071
Frequencies --	1215.7956	1252.3576	1301.3696
Frequencies --	1316.3514	1319.6317	1321.2438
Frequencies --	1326.3774	1327.3070	1339.3326
Frequencies --	1342.5406	1344.3798	1358.7654
Frequencies --	1374.7609	1410.6756	1416.0163
Frequencies --	1417.6893	1418.8248	1419.8879
Frequencies --	1424.3715	1425.2733	1426.0007
Frequencies --	1427.3282	1430.8841	1431.6840
Frequencies --	1435.9275	1443.1412	1447.3509
Frequencies --	1451.8180	1455.0857	1459.1795
Frequencies --	1463.6849	1469.3604	1469.7219
Frequencies --	1471.6040	1481.9136	1483.2401
Frequencies --	1488.7260	1492.6146	1495.7454
Frequencies --	1499.1998	1500.3302	1507.3808
Frequencies --	1507.8714	1512.5991	1516.2094
Frequencies --	1517.0968	1517.4648	1571.2335
Frequencies --	1595.7472	1596.8947	1597.4368
Frequencies --	1598.8618	1617.2735	1620.4691
Frequencies --	1620.8824	1622.5645	1624.3473
Frequencies --	2988.2072	3004.7110	3010.5996
Frequencies --	3010.8969	3012.3221	3014.4810
Frequencies --	3015.7072	3100.4899	3102.1878
Frequencies --	3104.1952	3105.4444	3109.1176

Frequencies --	3110.7766	3131.6980	3139.3642
Frequencies --	3140.2976	3145.6269	3147.7159
Frequencies --	3150.7306	3155.7013	3157.3992
Frequencies --	3162.3980	3174.9835	3179.6198
Frequencies --	3182.9888	3185.3017	3196.0477
Frequencies --	3197.8172	3202.5461	3209.1140

Catalyst 9:

vacuum	toluene-like solvent	D3 dispersion
-3199.56519266	-3199.57559	-0.61377851

Frequencies --	5.7273	10.7811	11.2690
Frequencies --	16.6040	23.1404	23.5430
Frequencies --	25.5970	26.9690	31.5162
Frequencies --	34.6494	37.8757	40.8181
Frequencies --	43.3060	54.4273	66.7958
Frequencies --	70.2066	83.5661	96.5900
Frequencies --	98.9206	104.9837	106.0137
Frequencies --	107.1456	112.6408	117.8255
Frequencies --	118.5094	120.3157	124.5095
Frequencies --	127.6228	134.5643	139.6464
Frequencies --	140.9152	151.3639	153.3303
Frequencies --	157.0829	157.2784	159.8945
Frequencies --	160.4260	161.5484	167.6403
Frequencies --	170.0402	182.2734	199.1936
Frequencies --	207.1796	211.8522	216.4221
Frequencies --	218.9918	223.5628	226.9631
Frequencies --	246.2285	250.1952	263.5202
Frequencies --	264.4079	264.6643	266.2893
Frequencies --	268.9584	269.6397	273.3417
Frequencies --	283.4512	283.5972	289.4956
Frequencies --	291.7013	293.0372	299.4965
Frequencies --	302.4320	304.0197	309.3672
Frequencies --	313.9558	317.4071	320.5337
Frequencies --	328.1141	330.8783	333.9905
Frequencies --	339.3279	353.5820	360.1443
Frequencies --	375.5029	378.9827	379.2702
Frequencies --	379.6254	388.0900	389.9063
Frequencies --	391.8822	398.4943	411.7235
Frequencies --	425.4289	430.2105	432.4332
Frequencies --	432.6741	433.1792	452.1655
Frequencies --	453.4662	456.5534	457.6049
Frequencies --	473.7169	477.4200	509.5484
Frequencies --	531.1701	536.6085	541.0739
Frequencies --	542.2586	547.8105	554.1409
Frequencies --	555.0958	556.0767	576.9773
Frequencies --	581.9953	592.2389	597.1034
Frequencies --	603.8697	612.6132	630.7758
Frequencies --	638.4765	638.5636	638.9212
Frequencies --	641.8771	661.4976	662.9608
Frequencies --	686.7850	696.4814	719.7211
Frequencies --	727.3255	729.5472	736.7953
Frequencies --	742.9329	757.8121	759.1202
Frequencies --	770.6138	801.7527	803.7290
Frequencies --	827.5334	832.2592	840.9679
Frequencies --	843.5364	860.0230	869.9260
Frequencies --	907.3798	907.6800	911.3190
Frequencies --	924.3041	933.7034	935.1560
Frequencies --	956.6410	966.2064	967.2096
Frequencies --	972.3019	979.1243	1011.3390

Frequencies --	1022.3894	1023.8035	1026.7916
Frequencies --	1036.1939	1040.3296	1042.0170
Frequencies --	1043.3796	1046.3325	1047.9252
Frequencies --	1048.2563	1049.1329	1049.7775
Frequencies --	1051.6750	1076.3086	1088.6240
Frequencies --	1089.7223	1106.3009	1119.9946
Frequencies --	1127.0528	1131.5501	1138.5808
Frequencies --	1171.5578	1175.5307	1190.5832
Frequencies --	1203.6402	1214.0940	1215.0039
Frequencies --	1215.0404	1215.5760	1222.3964
Frequencies --	1252.3614	1275.0244	1319.5590
Frequencies --	1321.6068	1326.5051	1326.5494
Frequencies --	1339.3120	1341.9552	1345.3853
Frequencies --	1352.0809	1396.9864	1399.2729
Frequencies --	1410.7085	1415.5060	1417.1637
Frequencies --	1418.7842	1420.7527	1422.2516
Frequencies --	1424.7128	1425.6880	1426.2744
Frequencies --	1428.3141	1428.9808	1432.1697
Frequencies --	1435.1704	1446.7474	1449.1543
Frequencies --	1455.3977	1459.3417	1469.4473
Frequencies --	1469.7497	1471.6178	1472.1800
Frequencies --	1478.0172	1481.5865	1482.9979
Frequencies --	1487.3870	1489.9509	1491.2878
Frequencies --	1494.2677	1499.1573	1499.3137
Frequencies --	1500.5645	1506.0080	1507.3862
Frequencies --	1507.9793	1511.5517	1512.3025
Frequencies --	1515.3189	1517.2056	1520.2519
Frequencies --	1578.9627	1596.0941	1597.0430
Frequencies --	1598.2286	1616.9408	1620.3328
Frequencies --	1620.6778	1622.3697	2987.6655
Frequencies --	3004.9874	3007.7951	3009.7381
Frequencies --	3011.0754	3011.2026	3012.3362
Frequencies --	3014.3597	3016.0089	3016.2147
Frequencies --	3102.5213	3103.5230	3104.6324
Frequencies --	3104.9550	3107.6069	3109.1945
Frequencies --	3111.8272	3112.3567	3114.6821
Frequencies --	3121.8506	3125.0108	3126.7961
Frequencies --	3131.6633	3139.0578	3141.6381
Frequencies --	3144.5473	3147.8640	3149.9204
Frequencies --	3160.0169	3179.8095	3187.4508
Frequencies --	3192.9448	3201.5936	3218.1720

Catalyst 10:

vacuum	toluene-like solvent	D3 dispersion
-3120.99058502	-3121.001069	-0.58557006

Frequencies --	6.2827	12.7817	14.0349
Frequencies --	20.9472	22.2362	25.2243
Frequencies --	29.7924	32.8217	35.1195
Frequencies --	38.4545	42.8996	45.0540
Frequencies --	48.5297	63.7058	71.1236
Frequencies --	78.9284	94.8004	98.2104
Frequencies --	103.4085	105.7295	107.4674
Frequencies --	109.3608	115.5666	118.3984
Frequencies --	119.3044	122.9605	125.1756
Frequencies --	126.4990	131.5357	133.9748
Frequencies --	138.7818	149.0804	152.3013
Frequencies --	152.7921	157.5207	160.9521
Frequencies --	161.4491	162.3738	165.0555
Frequencies --	168.6269	179.1235	195.1921

Frequencies --	207.4753	218.0482	218.7104
Frequencies --	219.3618	220.2567	232.1198
Frequencies --	241.1394	243.9663	261.1626
Frequencies --	264.5546	264.7010	265.0914
Frequencies --	270.0564	274.1564	278.4995
Frequencies --	286.7455	289.6405	292.2717
Frequencies --	295.3685	300.5613	306.1429
Frequencies --	307.5498	316.2465	320.5073
Frequencies --	332.2337	333.1349	338.2524
Frequencies --	339.6855	347.5640	348.6814
Frequencies --	355.6747	378.8787	380.3003
Frequencies --	380.7209	385.8941	389.1894
Frequencies --	390.3351	393.2271	411.0108
Frequencies --	432.4955	432.7649	433.0341
Frequencies --	452.7834	456.6689	457.3373
Frequencies --	472.8524	492.3949	505.2550
Frequencies --	512.4576	530.1112	535.9162
Frequencies --	541.4876	542.4352	548.0169
Frequencies --	550.8012	551.9185	554.5951
Frequencies --	561.5334	583.2233	587.3620
Frequencies --	593.1404	596.5852	600.4154
Frequencies --	619.8883	630.9155	638.8511
Frequencies --	640.0296	642.5555	659.8882
Frequencies --	662.1595	689.0470	696.7554
Frequencies --	727.7907	729.1987	738.0390
Frequencies --	742.7112	745.5467	757.8445
Frequencies --	758.1776	771.0312	786.4873
Frequencies --	802.2906	804.3919	844.3278
Frequencies --	858.6289	869.2767	907.1050
Frequencies --	908.3017	910.4939	911.3228
Frequencies --	922.7958	928.4167	968.8773
Frequencies --	973.5408	989.2330	1004.2180
Frequencies --	1013.3148	1022.4327	1025.7761
Frequencies --	1041.0949	1042.8483	1045.6704
Frequencies --	1047.0309	1048.2675	1049.0898
Frequencies --	1050.1674	1050.4984	1051.8131
Frequencies --	1054.2172	1058.1329	1075.4555
Frequencies --	1088.5512	1089.5426	1092.1729
Frequencies --	1110.2463	1126.8962	1148.2829
Frequencies --	1171.4877	1175.1254	1191.7871
Frequencies --	1193.5922	1200.5917	1214.2832
Frequencies --	1215.5983	1215.8899	1278.5998
Frequencies --	1281.5718	1319.5144	1320.7564
Frequencies --	1326.0202	1338.1385	1342.0395
Frequencies --	1342.7547	1360.8635	1411.2912
Frequencies --	1415.9199	1416.8059	1418.1569
Frequencies --	1418.6751	1421.1636	1422.9797
Frequencies --	1425.9277	1426.4322	1427.3984
Frequencies --	1428.8192	1429.5661	1434.4981
Frequencies --	1436.7598	1448.0232	1451.2212
Frequencies --	1455.1144	1461.7165	1469.1926
Frequencies --	1469.4000	1470.7916	1471.5547
Frequencies --	1472.7873	1473.5263	1481.3669
Frequencies --	1489.7734	1490.2679	1492.3142
Frequencies --	1495.6788	1498.7733	1500.6840
Frequencies --	1505.2975	1506.0361	1507.8509
Frequencies --	1508.4551	1513.6110	1515.4027
Frequencies --	1519.3575	1595.5550	1596.8560
Frequencies --	1597.3997	1604.4879	1607.4560
Frequencies --	1619.9025	1620.5217	1622.1434
Frequencies --	2995.7360	3008.4839	3011.2991
Frequencies --	3012.3642	3013.3813	3015.7735
Frequencies --	3016.5434	3026.5733	3034.8366

Frequencies --	3101.8487	3104.0466	3105.9420
Frequencies --	3110.4269	3111.3292	3112.6156
Frequencies --	3116.2580	3124.5778	3135.0467
Frequencies --	3141.1125	3142.9807	3145.3980
Frequencies --	3147.2822	3149.6892	3151.1063
Frequencies --	3152.8067	3163.3924	3164.7664
Frequencies --	3174.6347	3175.5200	3196.2041

Catalyst 11:

vacuum	toluene-like solvent	D3 dispersion
-3199.56485611	-3199.574155	-0.62184451

Frequencies --	10.0338	12.2064	14.6136
Frequencies --	19.2370	21.5338	24.1837
Frequencies --	28.9116	31.7619	32.9343
Frequencies --	39.2698	39.9345	44.6208
Frequencies --	46.0954	54.8471	62.0576
Frequencies --	69.8017	72.3200	83.7404
Frequencies --	99.1206	105.3826	106.0007
Frequencies --	108.4758	118.3235	119.1310
Frequencies --	120.6541	121.7977	126.7837
Frequencies --	134.7153	139.2799	142.0112
Frequencies --	151.6726	153.2933	156.4316
Frequencies --	157.4170	160.4586	161.3490
Frequencies --	162.4973	163.4297	166.9484
Frequencies --	172.7400	177.3285	185.5545
Frequencies --	191.7057	196.4584	213.3958
Frequencies --	216.5915	218.3283	219.5089
Frequencies --	229.3377	243.4358	263.4707
Frequencies --	264.4103	264.8193	265.0679
Frequencies --	269.6992	271.1522	274.4541
Frequencies --	282.5533	284.1862	286.8106
Frequencies --	287.7099	291.3932	292.1568
Frequencies --	295.4165	299.1571	299.9088
Frequencies --	309.1471	315.0887	318.6126
Frequencies --	322.1322	328.5794	331.9873
Frequencies --	335.1178	341.9792	349.0410
Frequencies --	355.1642	369.8333	378.6345
Frequencies --	379.9576	380.3973	384.3203
Frequencies --	388.0993	391.1489	395.6694
Frequencies --	412.5665	432.2590	433.2535
Frequencies --	433.3521	451.9745	456.4899
Frequencies --	457.5456	472.5567	500.7574
Frequencies --	505.3968	529.9107	534.1866
Frequencies --	535.7510	541.5396	542.4235
Frequencies --	548.1176	549.5461	553.9318
Frequencies --	572.7906	583.2601	586.8651
Frequencies --	592.6106	595.9996	597.0728
Frequencies --	604.1635	617.6195	630.2591
Frequencies --	638.4486	639.5480	642.2337
Frequencies --	659.2007	661.4600	682.6635
Frequencies --	696.5122	714.2095	727.4230
Frequencies --	729.3393	733.8869	742.0165
Frequencies --	756.0792	758.1961	770.6409
Frequencies --	771.4690	789.0221	800.4279
Frequencies --	803.2527	827.8763	842.6928
Frequencies --	853.9875	861.1539	865.6508
Frequencies --	907.2331	908.4087	911.3302
Frequencies --	921.4797	928.8824	966.5386
Frequencies --	972.1611	992.7765	995.4323

Frequencies --	1017.9558	1022.0787	1024.8267
Frequencies --	1027.7508	1042.3353	1043.7179
Frequencies --	1046.2874	1048.0554	1049.3697
Frequencies --	1049.8115	1051.3872	1051.8549
Frequencies --	1057.5096	1083.2184	1087.5505
Frequencies --	1089.9359	1090.4447	1092.3934
Frequencies --	1097.9131	1101.0333	1124.3167
Frequencies --	1126.2364	1139.8700	1171.6034
Frequencies --	1176.0170	1185.1526	1190.3959
Frequencies --	1204.9476	1214.2571	1215.0441
Frequencies --	1215.7319	1260.1042	1276.1872
Frequencies --	1289.3601	1292.2444	1318.7112
Frequencies --	1320.7662	1325.8976	1326.6933
Frequencies --	1338.3086	1341.4751	1343.6326
Frequencies --	1344.8517	1382.5964	1410.2032
Frequencies --	1414.2749	1415.6705	1416.3098
Frequencies --	1417.1123	1417.8956	1419.4194
Frequencies --	1424.8018	1427.6881	1428.4702
Frequencies --	1431.7073	1434.2925	1434.7383
Frequencies --	1436.6046	1447.8660	1450.7033
Frequencies --	1456.4456	1461.4666	1469.1518
Frequencies --	1470.0910	1471.1396	1471.9174
Frequencies --	1474.0333	1477.2814	1482.5674
Frequencies --	1486.7734	1492.2495	1494.6539
Frequencies --	1497.4510	1499.7285	1500.8574
Frequencies --	1501.1054	1501.3181	1507.6327
Frequencies --	1508.6259	1509.5689	1512.3137
Frequencies --	1513.9116	1516.3832	1517.2930
Frequencies --	1595.6874	1597.1184	1597.1548
Frequencies --	1600.3302	1609.1507	1619.9308
Frequencies --	1620.8055	1622.4197	2997.0118
Frequencies --	3011.3143	3011.5327	3012.3114
Frequencies --	3012.6997	3014.2697	3014.9009
Frequencies --	3015.4342	3015.9500	3027.0848
Frequencies --	3034.8824	3072.8767	3095.1209
Frequencies --	3103.3120	3104.0701	3105.4001
Frequencies --	3107.1655	3112.9543	3113.4684
Frequencies --	3113.9629	3119.5526	3121.0147
Frequencies --	3126.2921	3141.5479	3146.5232
Frequencies --	3147.9694	3148.9003	3151.4924
Frequencies --	3152.6115	3161.7179	3171.3361
Frequencies --	3183.0426	3204.8644	3213.6514

Catalyst 12:

vacuum	toluene-like solvent	D3 dispersion
-3278.13941821	-3278.149362	-0.66207898

Frequencies --	5.5866	13.4200	14.6747
Frequencies --	20.7586	23.9775	26.2375
Frequencies --	27.8969	30.6806	34.5887
Frequencies --	36.9730	40.5838	45.0541
Frequencies --	50.1256	56.1555	59.8539
Frequencies --	62.5110	69.3475	78.7726
Frequencies --	81.3793	85.2770	95.4297
Frequencies --	101.6638	107.0485	108.3387
Frequencies --	117.2425	119.2415	119.7374
Frequencies --	121.0487	128.5344	130.3408
Frequencies --	130.5002	138.8265	142.6186
Frequencies --	147.6043	153.8823	155.1460
Frequencies --	156.9632	158.2870	160.5094

Frequencies --	163.2301	165.9403	171.5879
Frequencies --	172.4263	185.3891	200.4960
Frequencies --	215.6321	216.8162	221.0752
Frequencies --	223.7156	224.4480	229.2454
Frequencies --	245.5015	250.1619	257.0789
Frequencies --	263.2966	264.2744	264.4115
Frequencies --	264.7963	265.6253	272.5465
Frequencies --	274.5859	278.6696	281.3564
Frequencies --	284.3790	286.8931	289.9730
Frequencies --	294.7457	296.5776	299.7389
Frequencies --	300.9902	302.9305	307.4596
Frequencies --	317.2692	319.9265	323.2955
Frequencies --	328.8820	334.5396	335.8752
Frequencies --	336.4594	354.9921	369.4841
Frequencies --	377.3407	378.2033	379.6613
Frequencies --	382.0904	395.9974	397.6107
Frequencies --	412.3512	425.1634	428.7909
Frequencies --	432.3888	432.8629	433.8554
Frequencies --	442.0606	445.3891	456.4445
Frequencies --	457.4969	471.7240	506.4539
Frequencies --	529.8195	535.2553	537.0554
Frequencies --	541.2088	542.7809	547.2846
Frequencies --	548.7031	552.6949	583.3759
Frequencies --	585.3883	588.2504	594.4455
Frequencies --	597.3238	600.2707	608.6970
Frequencies --	612.9454	629.7089	630.4871
Frequencies --	637.1605	638.1516	641.1262
Frequencies --	654.0339	666.7531	689.1844
Frequencies --	697.7146	721.8161	727.4408
Frequencies --	729.6191	739.9910	752.2003
Frequencies --	761.3902	764.7002	768.9991
Frequencies --	797.2365	801.1607	801.7170
Frequencies --	816.7100	843.8299	849.7375
Frequencies --	873.6747	877.8478	904.1033
Frequencies --	910.3228	911.3189	923.5766
Frequencies --	928.2958	931.4453	934.5764
Frequencies --	942.8273	963.7124	965.2186
Frequencies --	967.3258	969.0071	992.7589
Frequencies --	1011.7554	1021.7181	1025.7737
Frequencies --	1038.7515	1040.6327	1042.9209
Frequencies --	1046.9068	1046.9331	1048.5912
Frequencies --	1050.3115	1052.4689	1055.4489
Frequencies --	1070.1826	1072.9285	1086.4823
Frequencies --	1088.7189	1095.2006	1110.7662
Frequencies --	1116.6376	1120.0462	1124.7521
Frequencies --	1151.0126	1166.0407	1172.2813
Frequencies --	1175.3057	1182.6328	1184.3104
Frequencies --	1195.2532	1205.3848	1213.4946
Frequencies --	1214.3953	1215.5857	1254.8190
Frequencies --	1276.8673	1306.1660	1318.0276
Frequencies --	1321.0177	1322.0920	1325.8486
Frequencies --	1330.1364	1338.7013	1339.4104
Frequencies --	1340.6787	1346.2684	1382.5358
Frequencies --	1402.4994	1403.1227	1409.5359
Frequencies --	1414.6420	1415.8804	1417.6557
Frequencies --	1420.1398	1420.9860	1422.1448
Frequencies --	1424.6295	1426.8928	1428.1904
Frequencies --	1429.8420	1434.2199	1436.1205
Frequencies --	1444.4974	1448.0702	1448.9138
Frequencies --	1454.9514	1461.0059	1468.6669
Frequencies --	1469.1931	1471.4737	1474.4112
Frequencies --	1477.0056	1480.0183	1483.7766
Frequencies --	1487.2253	1489.3758	1489.9097

Frequencies --	1491.9098	1492.4499	1494.5682
Frequencies --	1497.6864	1500.5125	1503.2482
Frequencies --	1504.0882	1506.4549	1507.6017
Frequencies --	1509.3685	1510.5275	1511.9459
Frequencies --	1514.6959	1516.3561	1595.6124
Frequencies --	1595.6863	1596.6527	1597.3578
Frequencies --	1605.5154	1619.4917	1620.1640
Frequencies --	1621.8977	3000.5844	3007.8537
Frequencies --	3008.1657	3011.0893	3011.7786
Frequencies --	3012.4099	3012.7543	3013.1078
Frequencies --	3015.2309	3016.3986	3019.6387
Frequencies --	3069.6390	3103.0682	3104.5177
Frequencies --	3105.0905	3106.3809	3110.2776
Frequencies --	3110.8865	3112.5744	3112.9980
Frequencies --	3113.5555	3119.6850	3121.8340
Frequencies --	3123.8438	3126.5735	3133.3307
Frequencies --	3138.5668	3142.6704	3145.2306
Frequencies --	3146.9964	3150.3970	3154.4699
Frequencies --	3158.3527	3161.6482	3167.1164
Frequencies --	3187.5062	3189.7708	3202.0212

Catalyst 13:**distal conformation**

vacuum	toluene-like solvent	D3 dispersion
-3276.9466281	-3276.9570253	-0.65225182

Frequencies --	8.1042	12.1449	16.2281
Frequencies --	20.9566	23.0065	26.1409
Frequencies --	28.6386	29.1718	33.1764
Frequencies --	38.7392	41.8370	43.1375
Frequencies --	46.5418	56.8998	67.1601
Frequencies --	68.8333	83.1074	85.8353
Frequencies --	102.0291	103.4419	106.5231
Frequencies --	108.5488	111.8124	114.9845
Frequencies --	118.0476	119.4577	123.3792
Frequencies --	124.8694	127.4467	137.9021
Frequencies --	139.7776	145.5513	146.5987
Frequencies --	149.4379	153.6436	153.9666
Frequencies --	157.3940	159.9626	162.1432
Frequencies --	164.9766	169.1541	178.7886
Frequencies --	200.8586	212.0856	215.7828
Frequencies --	217.2263	219.7879	232.5422
Frequencies --	235.2546	251.4135	262.1989
Frequencies --	263.9478	264.7658	265.3792
Frequencies --	266.8084	270.6709	273.4949
Frequencies --	280.9985	283.4003	284.3243
Frequencies --	290.7419	291.6856	292.7186
Frequencies --	298.8128	302.4324	309.1846
Frequencies --	310.4468	315.4314	320.0846
Frequencies --	329.8090	334.3679	336.2485
Frequencies --	339.5583	349.3918	359.1479
Frequencies --	378.3010	378.6402	380.7260
Frequencies --	383.0550	384.6990	392.1827
Frequencies --	394.3298	416.2180	432.0744
Frequencies --	432.6650	433.3459	437.6725
Frequencies --	443.1476	450.9059	456.0695
Frequencies --	457.7758	472.9727	495.0182
Frequencies --	500.3325	506.5214	520.0793

Frequencies --	530.0301	536.2864	541.1174
Frequencies --	542.4570	548.2413	553.9351
Frequencies --	555.2813	578.9336	583.6863
Frequencies --	590.4799	595.6292	604.0101
Frequencies --	615.0996	618.5548	630.6316
Frequencies --	637.8658	639.0019	641.9268
Frequencies --	658.4304	662.6679	664.1545
Frequencies --	695.4962	703.3394	724.5535
Frequencies --	729.2825	742.0471	742.1552
Frequencies --	755.6947	760.1448	767.3258
Frequencies --	769.3465	770.0246	793.7088
Frequencies --	802.3980	803.4774	820.6765
Frequencies --	841.9275	859.7308	862.6877
Frequencies --	866.4029	867.7338	889.1737
Frequencies --	902.3308	905.6972	908.1124
Frequencies --	910.6661	926.8087	937.3239
Frequencies --	959.4461	968.0514	972.8935
Frequencies --	995.5781	999.3092	1008.0765
Frequencies --	1021.2557	1024.4060	1041.6222
Frequencies --	1042.6763	1046.0701	1047.4299
Frequencies --	1047.6108	1048.6620	1049.7404
Frequencies --	1051.6100	1052.5276	1055.7517
Frequencies --	1058.2618	1074.2326	1087.3657
Frequencies --	1088.5129	1088.9579	1090.6458
Frequencies --	1096.2336	1115.2557	1127.0440
Frequencies --	1138.8763	1153.2542	1172.3921
Frequencies --	1175.7222	1182.5980	1193.1520
Frequencies --	1194.1643	1199.3704	1214.0954
Frequencies --	1214.3909	1215.6341	1219.3362
Frequencies --	1251.7558	1279.0282	1281.5664
Frequencies --	1296.8626	1318.4777	1319.8829
Frequencies --	1322.5167	1326.9027	1328.6696
Frequencies --	1338.8205	1340.9697	1346.0095
Frequencies --	1352.5225	1358.3003	1361.2632
Frequencies --	1363.6895	1371.1594	1387.7216
Frequencies --	1411.1335	1416.3189	1416.3971
Frequencies --	1417.5688	1420.0438	1425.4205
Frequencies --	1426.0651	1428.5572	1430.4336
Frequencies --	1433.7288	1436.4678	1446.0165
Frequencies --	1447.7174	1450.0132	1455.4135
Frequencies --	1459.5309	1468.8967	1469.5999
Frequencies --	1470.7274	1471.8147	1479.4413
Frequencies --	1481.3970	1482.1735	1483.3400
Frequencies --	1485.2520	1487.2270	1491.9674
Frequencies --	1493.7134	1495.2651	1498.3763
Frequencies --	1499.8798	1501.1211	1506.6931
Frequencies --	1507.9945	1512.1766	1517.3699
Frequencies --	1517.8364	1585.5196	1595.5738
Frequencies --	1596.6007	1597.2547	1614.2185
Frequencies --	1620.1689	1620.5133	1622.3026
Frequencies --	2989.9769	3002.6811	3003.1256
Frequencies --	3005.1548	3010.7436	3011.4930
Frequencies --	3012.3264	3013.9635	3015.3460
Frequencies --	3017.0809	3017.2019	3024.5470
Frequencies --	3058.5436	3064.0698	3070.7058
Frequencies --	3080.7560	3082.0321	3098.4193
Frequencies --	3103.0679	3104.3313	3105.1291
Frequencies --	3107.2909	3109.0001	3117.0339
Frequencies --	3136.5168	3140.0446	3143.0445
Frequencies --	3147.4700	3152.6505	3154.8281
Frequencies --	3166.5035	3166.5323	3175.8392
Frequencies --	3180.6894	3196.6464	3213.7415

proximal conformation

vacuum	toluene-like solvent	D3 dispersion
-3276.9488587	-3276.9596011	-0.64966142

Frequencies --	4.0307	11.0094	14.2296
Frequencies --	18.9944	21.7009	23.0359
Frequencies --	26.0669	29.0656	30.2903
Frequencies --	34.4725	37.2518	39.9584
Frequencies --	41.8494	45.0838	57.7191
Frequencies --	69.0567	85.9939	91.1374
Frequencies --	102.5787	104.0534	105.3140
Frequencies --	106.2761	112.0276	116.7772
Frequencies --	118.0650	119.1016	121.3751
Frequencies --	124.2828	130.1947	132.9600
Frequencies --	137.1538	142.7875	149.5131
Frequencies --	151.7623	153.4304	157.3234
Frequencies --	160.4633	161.4977	162.8452
Frequencies --	164.0806	169.3918	185.9681
Frequencies --	202.8226	206.3506	210.6850
Frequencies --	217.1805	218.4141	222.0151
Frequencies --	223.4752	239.6336	257.5958
Frequencies --	260.4410	264.5832	264.8380
Frequencies --	265.1487	269.1178	273.2264
Frequencies --	279.8099	280.7102	285.7193
Frequencies --	288.6562	292.2665	294.0078
Frequencies --	299.9749	302.3898	308.5612
Frequencies --	312.5700	314.6700	320.7099
Frequencies --	330.9900	333.7784	339.1347
Frequencies --	342.3815	351.2648	357.3314
Frequencies --	378.5592	379.2283	379.5474
Frequencies --	384.4753	388.8522	389.7633
Frequencies --	392.8683	415.2860	432.4157
Frequencies --	432.7639	433.3543	438.0161
Frequencies --	443.0355	452.1082	456.0559
Frequencies --	457.5890	472.8754	494.9248
Frequencies --	495.7246	506.5498	523.1018
Frequencies --	530.1936	536.6953	541.0657
Frequencies --	542.6033	548.0760	554.1746
Frequencies --	555.7283	580.8072	583.2394
Frequencies --	591.3000	596.6971	605.3816
Frequencies --	612.3065	617.1889	630.4311
Frequencies --	638.4780	638.9700	641.7192
Frequencies --	658.6341	660.3617	662.8059
Frequencies --	695.0236	701.8092	727.0823
Frequencies --	728.6551	742.4127	744.3666
Frequencies --	757.4232	758.1427	768.4040
Frequencies --	770.4260	770.8489	789.4518
Frequencies --	801.1423	803.2884	820.6862
Frequencies --	842.6489	853.9967	867.0769
Frequencies --	867.8893	874.0384	890.4255
Frequencies --	901.7340	906.8288	907.4266
Frequencies --	910.3825	924.7887	938.2797
Frequencies --	964.6495	967.7560	972.5025
Frequencies --	996.5020	997.7039	1005.2404
Frequencies --	1023.5174	1024.5564	1042.1046
Frequencies --	1043.5311	1046.2926	1046.7818
Frequencies --	1047.3714	1048.6468	1048.9905
Frequencies --	1050.8820	1052.5618	1055.0324
Frequencies --	1057.7086	1071.5181	1085.8657
Frequencies --	1088.8099	1089.8446	1095.5980

Frequencies --	1097.2957	1115.3752	1126.8729
Frequencies --	1132.1455	1152.8631	1171.2390
Frequencies --	1175.6899	1184.1451	1191.8754
Frequencies --	1192.0876	1199.1596	1213.7736
Frequencies --	1214.7131	1215.1448	1221.9834
Frequencies --	1248.4219	1277.8197	1282.7809
Frequencies --	1293.1755	1317.2010	1319.1139
Frequencies --	1321.0430	1326.1793	1329.3717
Frequencies --	1338.9210	1341.7484	1344.3766
Frequencies --	1351.8613	1354.2902	1359.9875
Frequencies --	1361.1722	1370.7620	1388.9045
Frequencies --	1410.2828	1415.0524	1416.7975
Frequencies --	1417.8155	1418.9463	1424.8814
Frequencies --	1425.5580	1427.6997	1429.5012
Frequencies --	1432.2142	1435.4134	1445.4385
Frequencies --	1446.8074	1447.5970	1454.7830
Frequencies --	1459.3970	1465.8971	1469.3920
Frequencies --	1469.7781	1471.7576	1477.4470
Frequencies --	1478.9907	1481.1549	1481.8839
Frequencies --	1484.1460	1484.7349	1488.2720
Frequencies --	1492.2783	1495.8124	1496.7522
Frequencies --	1499.0821	1500.5083	1506.7646
Frequencies --	1507.3827	1512.4699	1516.5417
Frequencies --	1517.1888	1586.0936	1595.7951
Frequencies --	1596.9496	1597.3361	1612.0482
Frequencies --	1620.3034	1620.6818	1622.4137
Frequencies --	2991.2089	2994.3854	3002.3229
Frequencies --	3004.6286	3005.3615	3010.8512
Frequencies --	3011.1164	3011.8495	3013.0938
Frequencies --	3013.9662	3015.6948	3021.7148
Frequencies --	3059.2688	3064.0760	3068.9601
Frequencies --	3076.6758	3082.2262	3100.6377
Frequencies --	3102.0554	3103.9541	3105.2247
Frequencies --	3106.4397	3111.1109	3112.0365
Frequencies --	3135.8411	3139.0103	3141.8539
Frequencies --	3145.5446	3148.3553	3150.6399
Frequencies --	3159.1170	3168.0692	3181.6756
Frequencies --	3196.7372	3198.0797	3215.8189

Catalyst 14:

vacuum	toluene-like solvent	D3 dispersion
-3133.54961423	-3133.560332	-0.59429348

Frequencies --	4.8773	8.7103	10.1140
Frequencies --	16.2606	20.6107	24.2991
Frequencies --	26.5309	30.8642	32.6743
Frequencies --	35.7097	40.9953	43.7722
Frequencies --	46.8762	65.4322	69.7809
Frequencies --	84.4179	89.3346	94.6231
Frequencies --	100.9592	105.0500	105.9463
Frequencies --	106.5145	116.4937	118.0747
Frequencies --	118.7522	122.1203	123.8344
Frequencies --	127.7595	136.4381	137.8099
Frequencies --	144.6584	146.7696	152.0860
Frequencies --	153.0667	154.7848	156.1050
Frequencies --	157.3438	160.8974	161.2902
Frequencies --	164.1930	168.5860	177.9024
Frequencies --	187.8014	195.8648	211.0693
Frequencies --	216.8012	218.9062	220.8070
Frequencies --	222.7602	233.9498	245.7109

Frequencies --	251.7248	253.3587	264.2788
Frequencies --	264.6316	264.8009	265.2071
Frequencies --	270.1456	273.9727	279.4171
Frequencies --	285.9712	289.7049	290.6055
Frequencies --	295.7467	299.1932	301.9825
Frequencies --	308.1467	315.4024	322.0196
Frequencies --	331.5104	334.4994	340.7913
Frequencies --	348.8238	357.3778	359.8856
Frequencies --	378.8670	379.5826	380.2402
Frequencies --	385.6848	389.1237	389.9246
Frequencies --	397.1459	403.2595	429.5907
Frequencies --	432.0454	432.7260	433.0625
Frequencies --	452.0612	456.5142	457.2972
Frequencies --	472.5462	500.8220	503.5873
Frequencies --	510.3429	529.8877	536.0215
Frequencies --	541.1205	542.1528	547.8043
Frequencies --	554.5435	561.9939	566.6600
Frequencies --	573.1959	583.1885	586.4379
Frequencies --	592.2235	596.9752	598.1057
Frequencies --	616.7984	630.4472	638.8244
Frequencies --	639.1787	642.0530	658.8649
Frequencies --	662.9067	689.9375	695.7600
Frequencies --	727.2255	729.2853	732.6153
Frequencies --	742.0870	756.9001	758.5316
Frequencies --	770.6224	799.5543	801.7902
Frequencies --	804.6471	841.4786	858.0535
Frequencies --	869.0215	885.5282	891.0054
Frequencies --	906.9140	907.7173	911.6218
Frequencies --	926.3706	951.1863	966.3024
Frequencies --	973.2266	1011.9143	1013.4941
Frequencies --	1022.4872	1025.1884	1040.0808
Frequencies --	1041.4795	1045.6522	1046.1748
Frequencies --	1047.3900	1049.1848	1050.0189
Frequencies --	1051.5062	1051.7824	1053.8890
Frequencies --	1058.7676	1077.1770	1087.6193
Frequencies --	1088.3769	1089.5123	1124.9430
Frequencies --	1125.9370	1134.7427	1171.1119
Frequencies --	1175.2411	1191.4335	1207.4262
Frequencies --	1214.4249	1215.5385	1216.0096
Frequencies --	1265.4622	1287.2744	1319.3062
Frequencies --	1320.3718	1325.6921	1337.8808
Frequencies --	1341.7306	1343.0343	1354.1933
Frequencies --	1409.3694	1414.0604	1416.0592
Frequencies --	1416.6206	1417.6821	1418.2175
Frequencies --	1422.9059	1424.8694	1426.1401
Frequencies --	1426.9959	1428.1747	1428.9724
Frequencies --	1429.5637	1434.7584	1437.4495
Frequencies --	1447.7964	1451.3924	1455.6543
Frequencies --	1461.7207	1465.5331	1469.1389
Frequencies --	1469.8620	1470.7749	1471.7953
Frequencies --	1481.2255	1489.6472	1490.4434
Frequencies --	1491.6575	1495.5998	1499.1112
Frequencies --	1501.3257	1503.5370	1505.1694
Frequencies --	1506.9001	1507.4179	1512.5545
Frequencies --	1516.5349	1518.8537	1587.3457
Frequencies --	1591.3440	1595.2172	1596.5877
Frequencies --	1596.7575	1619.7081	1620.5322
Frequencies --	1622.1221	2997.8445	3011.4436
Frequencies --	3011.6412	3013.0145	3014.4874
Frequencies --	3015.4909	3016.3926	3029.6695
Frequencies --	3037.4624	3102.4004	3105.0682
Frequencies --	3105.4572	3108.6448	3112.6376
Frequencies --	3113.5419	3119.9797	3128.4753

Frequencies --	3139.1427	3143.1620	3143.4606
Frequencies --	3146.6680	3148.1330	3150.1392
Frequencies --	3152.3555	3153.2440	3161.5997
Frequencies --	3179.9435	3201.1682	3203.1163

Catalyst 15:**distal conformation**

vacuum	toluene-like solvent	D3 dispersion
-3312.6410099	-3312.6528831	-0.63989531

Frequencies --	7.5039	9.2799	10.3058
Frequencies --	13.2965	16.9163	21.2971
Frequencies --	23.4875	26.3525	28.7348
Frequencies --	30.7127	35.4709	38.1513
Frequencies --	40.9706	43.7478	53.4429
Frequencies --	68.4216	75.0078	78.7931
Frequencies --	94.6140	97.9698	103.8482
Frequencies --	105.1768	105.9848	106.7496
Frequencies --	118.0002	118.4150	122.0492
Frequencies --	123.5281	126.0113	127.8357
Frequencies --	132.6868	138.8387	151.2502
Frequencies --	152.3871	152.6963	157.2088
Frequencies --	160.2980	160.5738	160.8288
Frequencies --	162.4133	168.4087	173.5566
Frequencies --	197.8991	203.7074	210.4694
Frequencies --	217.2033	218.0675	219.0543
Frequencies --	235.5451	247.9995	258.5038
Frequencies --	264.1027	264.8157	264.9232
Frequencies --	268.5375	273.2845	276.4324
Frequencies --	279.6040	283.3725	285.0456
Frequencies --	289.7161	293.0111	293.4419
Frequencies --	297.0020	302.7908	308.2043
Frequencies --	314.2447	319.7985	324.7945
Frequencies --	331.6734	334.4064	338.4477
Frequencies --	347.2043	356.3372	378.5166
Frequencies --	380.1064	380.6824	384.1708
Frequencies --	388.9034	389.5491	394.1637
Frequencies --	407.5070	420.3506	431.9497
Frequencies --	432.5643	433.4124	450.8736
Frequencies --	454.0780	456.5724	457.5138
Frequencies --	469.2808	473.9614	483.9957
Frequencies --	509.4651	528.9795	532.9852
Frequencies --	535.9192	541.2006	542.3628
Frequencies --	547.9478	553.1512	572.5555
Frequencies --	580.0017	584.5805	593.1758
Frequencies --	596.4151	605.1938	613.9691
Frequencies --	618.1453	624.6100	630.7864
Frequencies --	638.5093	639.7062	642.2677
Frequencies --	655.5732	661.1232	663.5291
Frequencies --	695.3671	702.1234	708.4817
Frequencies --	721.8328	728.0097	729.0086
Frequencies --	742.3285	743.7075	758.1340
Frequencies --	758.5874	768.4764	770.9696
Frequencies --	798.3486	802.5093	810.4297
Frequencies --	825.7916	842.9074	861.7253
Frequencies --	862.3538	869.4246	874.1214
Frequencies --	907.2696	907.9397	911.0970
Frequencies --	915.5060	940.6939	953.8792

Frequencies --	967.0241	968.5764	970.2849
Frequencies --	988.6090	999.5500	1006.3327
Frequencies --	1016.0863	1021.3363	1023.8736
Frequencies --	1025.4475	1041.8686	1042.4573
Frequencies --	1045.3644	1047.6027	1048.7516
Frequencies --	1049.0805	1050.1257	1050.6787
Frequencies --	1051.7262	1052.0311	1081.0951
Frequencies --	1087.4236	1089.0381	1091.8119
Frequencies --	1099.3399	1109.8819	1124.7869
Frequencies --	1139.0768	1171.4167	1175.4358
Frequencies --	1180.9707	1183.0570	1192.0571
Frequencies --	1194.6975	1204.0026	1214.4834
Frequencies --	1215.6050	1215.6425	1217.1487
Frequencies --	1218.3464	1237.7286	1292.9703
Frequencies --	1316.6041	1320.2182	1321.2273
Frequencies --	1326.4966	1339.1044	1342.6629
Frequencies --	1343.4678	1357.5966	1376.1826
Frequencies --	1380.9804	1409.0418	1414.5094
Frequencies --	1417.4378	1418.7361	1419.2141
Frequencies --	1423.9340	1427.1427	1428.4091
Frequencies --	1429.0250	1433.8994	1436.9285
Frequencies --	1444.9618	1446.6012	1450.0625
Frequencies --	1455.5369	1455.8647	1460.2775
Frequencies --	1468.0262	1468.7485	1469.9139
Frequencies --	1471.6388	1476.1452	1481.2225
Frequencies --	1484.1936	1489.8230	1491.4703
Frequencies --	1494.3083	1498.9336	1499.7808
Frequencies --	1502.7975	1505.2070	1508.7000
Frequencies --	1512.5687	1514.2748	1516.9387
Frequencies --	1585.8858	1595.3887	1596.7242
Frequencies --	1597.1652	1604.1122	1614.6163
Frequencies --	1619.7840	1620.6261	1622.2753
Frequencies --	1626.8748	2990.9500	3009.2927
Frequencies --	3010.5994	3011.4123	3012.8776
Frequencies --	3013.8504	3016.1008	3031.9949
Frequencies --	3101.1475	3103.6007	3104.0232
Frequencies --	3105.0528	3107.4503	3110.5676
Frequencies --	3111.8416	3135.2267	3139.6243
Frequencies --	3144.0206	3144.7235	3148.6096
Frequencies --	3149.0442	3153.4297	3154.2225
Frequencies --	3158.9938	3165.6832	3167.5267
Frequencies --	3175.2102	3179.4803	3189.0120
Frequencies --	3192.3121	3195.5661	3213.2780

proximal conformation

vacuum	toluene-like solvent	D3 dispersion
-3312.6437062	-3312.655988	-0.63958401

Frequencies --	4.4705	9.6368	12.7811
Frequencies --	16.6142	17.9256	21.7366
Frequencies --	24.3740	27.3225	29.6843
Frequencies --	30.2012	35.3075	38.4346
Frequencies --	40.2761	43.7283	49.0541
Frequencies --	62.3357	74.0959	74.9525
Frequencies --	95.8222	103.5172	104.6843
Frequencies --	107.3708	116.6897	117.7382
Frequencies --	118.6021	120.8307	121.5154
Frequencies --	125.3856	130.6862	137.1183
Frequencies --	141.6423	144.8140	151.4974
Frequencies --	152.4679	154.7651	157.4124

Frequencies --	160.4800	161.2186	163.5746
Frequencies --	166.4892	177.3295	184.5874
Frequencies --	194.3537	195.7896	203.1549
Frequencies --	208.3589	217.8516	218.5335
Frequencies --	225.6927	240.2765	242.4442
Frequencies --	259.4178	264.5408	264.8455
Frequencies --	265.2163	270.1029	273.3681
Frequencies --	278.7333	285.9729	288.1246
Frequencies --	291.7438	293.2387	302.3764
Frequencies --	304.7415	307.6054	310.6425
Frequencies --	315.3860	319.6751	330.0770
Frequencies --	331.9535	335.4324	337.4348
Frequencies --	348.5071	349.6369	378.7006
Frequencies --	379.1348	380.4060	387.0566
Frequencies --	389.5191	390.3622	392.2707
Frequencies --	406.1621	413.1802	432.5397
Frequencies --	432.7878	432.8931	450.7147
Frequencies --	454.0002	456.6412	457.1789
Frequencies --	467.5187	473.6999	483.0557
Frequencies --	512.4828	530.4424	536.0326
Frequencies --	536.9352	541.4594	542.1378
Frequencies --	548.0274	556.0215	568.8372
Frequencies --	579.1306	583.6930	592.0388
Frequencies --	595.9965	603.2016	613.4681
Frequencies --	617.8554	623.7466	630.7608
Frequencies --	638.5894	639.6215	642.4773
Frequencies --	651.5840	660.1959	662.5982
Frequencies --	691.5650	697.3178	709.8148
Frequencies --	722.9107	727.6438	728.6642
Frequencies --	742.5185	747.6381	757.9916
Frequencies --	758.6722	769.7409	770.5713
Frequencies --	801.8272	804.1217	812.1508
Frequencies --	827.2566	842.2506	855.8265
Frequencies --	865.1191	867.6573	877.4414
Frequencies --	906.5648	907.1705	909.9327
Frequencies --	924.6290	938.0116	950.5351
Frequencies --	969.4599	970.2730	974.0247
Frequencies --	990.6750	999.9090	1008.7289
Frequencies --	1010.9546	1021.8952	1023.3415
Frequencies --	1023.9986	1042.5339	1044.0158
Frequencies --	1047.0118	1047.6821	1048.2932
Frequencies --	1048.5833	1049.3510	1050.4732
Frequencies --	1051.6865	1053.0454	1074.9598
Frequencies --	1089.1787	1090.7609	1092.5681
Frequencies --	1094.2822	1110.3020	1127.1947
Frequencies --	1130.9642	1172.3168	1176.0380
Frequencies --	1182.0539	1183.3429	1191.8470
Frequencies --	1194.8218	1204.2139	1209.2643
Frequencies --	1213.9477	1214.7844	1215.3135
Frequencies --	1220.4660	1237.4164	1290.6715
Frequencies --	1319.5204	1320.2192	1320.9175
Frequencies --	1325.6835	1338.6706	1342.3463
Frequencies --	1343.2050	1354.8057	1376.3637
Frequencies --	1380.2369	1411.5924	1415.7200
Frequencies --	1417.0361	1417.9665	1418.4599
Frequencies --	1424.7359	1426.3383	1428.5777
Frequencies --	1428.8112	1431.4305	1435.3080
Frequencies --	1444.7533	1446.3154	1448.0132
Frequencies --	1455.9421	1456.4882	1458.8869
Frequencies --	1463.1338	1469.5274	1469.7507
Frequencies --	1471.7097	1474.2368	1482.9424
Frequencies --	1483.3867	1492.4590	1493.7112
Frequencies --	1495.8316	1500.6932	1501.9347

Frequencies --	1502.3397	1506.8927	1509.4750
Frequencies --	1512.6282	1517.9035	1519.7748
Frequencies --	1587.0926	1595.4619	1596.6591
Frequencies --	1597.1143	1605.0883	1612.9497
Frequencies --	1620.5298	1620.8160	1622.5420
Frequencies --	1626.6955	2988.3205	3004.5174
Frequencies --	3011.1535	3011.4036	3012.4892
Frequencies --	3014.4461	3015.2358	3016.3283
Frequencies --	3100.8930	3103.0854	3104.0435
Frequencies --	3105.4125	3107.8452	3110.7468
Frequencies --	3118.4112	3134.6735	3139.9097
Frequencies --	3140.9617	3145.2487	3145.4209
Frequencies --	3149.0356	3151.0012	3158.4746
Frequencies --	3159.1166	3168.2315	3170.1799
Frequencies --	3181.3448	3182.8882	3187.7922
Frequencies --	3195.6263	3195.7220	3210.6911

Catalyst 16:

vacuum	toluene-like solvent	D3 dispersion
-3966.17046713	-3966.18495693	-0.87892812

Frequencies --	7.3239	9.3097	10.2288
Frequencies --	13.5591	17.3815	19.8921
Frequencies --	26.0852	28.2556	28.8740
Frequencies --	33.2364	35.5023	37.7438
Frequencies --	41.5367	41.7054	46.6221
Frequencies --	47.9868	49.9393	51.0801
Frequencies --	54.8544	57.8565	68.0939
Frequencies --	73.6113	75.4059	80.0658
Frequencies --	84.4410	90.3374	103.3719
Frequencies --	105.5720	106.8578	117.6402
Frequencies --	118.9327	119.1974	120.3593
Frequencies --	121.6752	123.8105	128.2877
Frequencies --	132.3633	135.7427	137.0302
Frequencies --	138.9810	140.8121	144.1179
Frequencies --	151.5675	152.2407	157.8043
Frequencies --	160.5179	161.2829	163.7739
Frequencies --	167.7478	175.7123	181.0094
Frequencies --	194.0242	197.1980	207.9773
Frequencies --	209.5852	211.3605	218.1649
Frequencies --	220.2770	226.1757	232.1588
Frequencies --	245.3895	252.7195	256.0471
Frequencies --	261.5196	264.5105	264.9254
Frequencies --	265.0344	269.9102	272.6037
Frequencies --	278.1266	278.4553	285.3721
Frequencies --	290.4041	291.2089	294.6165
Frequencies --	297.7386	302.8225	305.2395
Frequencies --	309.4755	315.4595	317.9982
Frequencies --	319.9141	329.1207	332.5094
Frequencies --	335.8445	337.6000	343.9134
Frequencies --	361.8232	378.6346	379.1714
Frequencies --	381.3212	385.8565	389.4402
Frequencies --	392.2456	394.3293	405.4208
Frequencies --	405.5623	408.2849	411.7744
Frequencies --	414.8359	423.0625	432.4226
Frequencies --	433.0572	434.1832	436.5283
Frequencies --	442.6555	456.0725	457.0329
Frequencies --	470.0071	497.1114	511.1846
Frequencies --	518.2070	528.4862	530.0605
Frequencies --	536.6323	541.8418	542.7704

Frequencies --	543.0102	548.6030	551.7840
Frequencies --	555.6834	584.1257	586.0743
Frequencies --	591.4455	593.7763	593.9431
Frequencies --	612.5003	615.3266	616.5754
Frequencies --	617.5904	620.5740	625.1540
Frequencies --	627.4370	634.6402	638.8636
Frequencies --	639.7577	639.9653	641.9478
Frequencies --	654.7861	658.4977	660.1701
Frequencies --	683.5884	689.7624	693.8309
Frequencies --	700.8700	710.6333	711.3840
Frequencies --	717.9324	718.9525	726.6217
Frequencies --	727.4498	740.6883	741.8423
Frequencies --	745.3868	756.6485	757.2689
Frequencies --	769.8266	774.0299	776.0069
Frequencies --	777.9794	794.1401	803.7531
Frequencies --	806.9356	807.1645	842.9238
Frequencies --	848.6371	857.8339	859.3999
Frequencies --	860.4186	863.6537	870.5629
Frequencies --	871.6398	907.4514	907.8854
Frequencies --	909.2249	917.9451	931.7552
Frequencies --	939.5503	944.4165	947.9807
Frequencies --	961.3853	971.0566	975.0460
Frequencies --	986.3000	986.5086	994.7045
Frequencies --	995.9218	997.8056	1001.7166
Frequencies --	1004.5178	1005.2640	1008.5395
Frequencies --	1010.9758	1015.9490	1020.3324
Frequencies --	1022.7562	1023.4811	1025.9429
Frequencies --	1039.6119	1040.7773	1042.2935
Frequencies --	1046.0549	1047.0068	1047.6587
Frequencies --	1048.9407	1049.9106	1050.2764
Frequencies --	1051.3029	1052.4252	1054.7801
Frequencies --	1055.5709	1066.9552	1089.3731
Frequencies --	1089.6765	1090.2043	1091.0294
Frequencies --	1091.5374	1093.0028	1093.8538
Frequencies --	1122.1973	1128.4773	1128.7864
Frequencies --	1170.7996	1174.4597	1177.8996
Frequencies --	1183.0876	1183.1333	1183.8423
Frequencies --	1185.0937	1201.6733	1204.0815
Frequencies --	1205.2672	1206.8358	1207.5426
Frequencies --	1212.3391	1213.3519	1214.0191
Frequencies --	1226.6879	1254.6138	1280.5241
Frequencies --	1304.6486	1318.3483	1320.4642
Frequencies --	1321.2453	1325.6993	1328.8989
Frequencies --	1331.1468	1331.7886	1333.6670
Frequencies --	1338.1102	1341.4222	1343.7889
Frequencies --	1368.0050	1368.4119	1368.9889
Frequencies --	1370.1087	1378.3028	1412.6197
Frequencies --	1416.1345	1416.8796	1417.4667
Frequencies --	1418.7414	1426.7886	1428.0582
Frequencies --	1428.5367	1431.3492	1436.2620
Frequencies --	1440.4198	1441.0347	1443.8652
Frequencies --	1445.7819	1447.0165	1448.3114
Frequencies --	1450.6835	1453.4696	1455.9827
Frequencies --	1461.9890	1468.0493	1468.7950
Frequencies --	1471.2397	1480.1287	1481.6263
Frequencies --	1488.8921	1494.2862	1496.7337
Frequencies --	1497.4098	1497.9873	1501.6735
Frequencies --	1503.0388	1503.3169	1507.0775
Frequencies --	1508.7045	1509.1004	1512.5075
Frequencies --	1517.5242	1521.2915	1525.2206
Frequencies --	1592.0896	1594.9489	1595.6986
Frequencies --	1596.5823	1597.1195	1597.2905
Frequencies --	1597.4714	1599.7963	1619.7075

Frequencies --	1620.0575	1621.8096	1623.5703
Frequencies --	1623.9846	1624.3040	1624.7433
Frequencies --	3010.2173	3010.4722	3011.2954
Frequencies --	3012.3583	3013.7279	3014.3767
Frequencies --	3019.9690	3101.0979	3105.3845
Frequencies --	3107.2614	3109.0051	3112.9491
Frequencies --	3141.3791	3146.1861	3148.2934
Frequencies --	3149.9445	3152.2837	3153.3032
Frequencies --	3154.0415	3155.8849	3160.0993
Frequencies --	3160.4979	3161.7624	3161.8539
Frequencies --	3167.8456	3169.4396	3171.8537
Frequencies --	3171.9583	3172.6059	3173.4740
Frequencies --	3178.1053	3183.8432	3185.2687
Frequencies --	3186.0310	3186.1694	3191.1291
Frequencies --	3194.4639	3194.8699	3197.2778
Frequencies --	3199.5921	3204.3852	3217.5678

Catalyst 17:**distal conformation**

vacuum	toluene-like solvent	D3 dispersion
-3156.880895	-3156.8919365	-0.56228723

Frequencies --	6.7928	10.4348	12.6404
Frequencies --	17.2972	20.0510	24.6223
Frequencies --	26.3256	28.7343	31.5993
Frequencies --	35.7626	38.9324	41.7943
Frequencies --	43.0403	69.0706	75.0159
Frequencies --	78.5781	85.4642	98.9669
Frequencies --	104.9412	105.7747	109.0730
Frequencies --	117.8152	118.2631	120.8283
Frequencies --	125.5847	126.2578	134.4423
Frequencies --	137.2890	141.4627	143.5395
Frequencies --	150.5358	152.5949	153.6711
Frequencies --	157.2847	160.0270	161.6566
Frequencies --	162.9045	163.9211	168.8642
Frequencies --	185.6322	192.3476	205.5908
Frequencies --	211.9900	216.8113	218.8921
Frequencies --	219.6076	238.6669	248.9692
Frequencies --	253.4732	263.9873	264.4412
Frequencies --	264.6418	268.5208	269.2786
Frequencies --	273.1943	283.0175	285.5166
Frequencies --	286.4424	291.5436	293.3769
Frequencies --	299.6349	306.3000	307.9200
Frequencies --	310.7318	314.9213	319.4449
Frequencies --	327.3135	331.3942	334.6120
Frequencies --	339.6910	358.9087	378.6426
Frequencies --	378.9381	379.1356	380.9686
Frequencies --	387.4168	390.7411	396.3368
Frequencies --	397.9905	421.4520	432.4000
Frequencies --	432.7252	433.1761	452.6335
Frequencies --	454.0087	456.4170	457.5495
Frequencies --	473.2331	474.3666	510.4040
Frequencies --	530.9206	536.8470	541.3167
Frequencies --	542.2585	548.0258	555.8106
Frequencies --	559.1006	573.6475	581.7500
Frequencies --	591.7780	596.7200	602.9499
Frequencies --	604.4910	612.3757	630.3786
Frequencies --	638.3379	639.0026	641.9280

Frequencies --	650.2978	660.1134	662.9984
Frequencies --	676.4394	694.1589	697.3892
Frequencies --	726.4759	729.6706	742.6069
Frequencies --	756.9624	759.7890	760.1991
Frequencies --	770.4219	785.5634	802.4841
Frequencies --	804.9385	829.4264	842.5886
Frequencies --	860.1404	867.0738	868.4518
Frequencies --	906.5842	908.1086	911.0424
Frequencies --	952.7405	963.7375	970.6021
Frequencies --	972.7942	987.4389	1009.7184
Frequencies --	1022.7449	1024.5377	1026.5253
Frequencies --	1042.3596	1043.5756	1046.8160
Frequencies --	1047.7138	1048.3141	1048.9936
Frequencies --	1050.5035	1051.8726	1075.5324
Frequencies --	1089.2425	1090.4505	1098.5138
Frequencies --	1102.6154	1126.8811	1127.0880
Frequencies --	1134.2407	1165.5172	1171.4614
Frequencies --	1173.0644	1176.0862	1190.0379
Frequencies --	1201.7025	1214.0493	1215.1419
Frequencies --	1215.3495	1273.3120	1300.6555
Frequencies --	1318.9686	1322.0097	1326.9187
Frequencies --	1339.0153	1341.5525	1345.7646
Frequencies --	1385.8422	1411.0922	1415.7755
Frequencies --	1417.5280	1418.1333	1420.6177
Frequencies --	1424.6745	1426.3618	1428.2217
Frequencies --	1430.1386	1433.3977	1436.5774
Frequencies --	1444.5928	1446.4737	1447.7313
Frequencies --	1455.3774	1456.3803	1459.4734
Frequencies --	1466.3653	1469.2795	1469.5985
Frequencies --	1471.5603	1476.8031	1481.6793
Frequencies --	1483.9515	1484.7672	1488.0051
Frequencies --	1492.9771	1494.2660	1499.0720
Frequencies --	1501.1453	1507.1699	1508.4696
Frequencies --	1512.1779	1514.7389	1518.9926
Frequencies --	1589.1223	1596.2313	1597.1856
Frequencies --	1598.2886	1617.2873	1620.1779
Frequencies --	1620.4596	1622.2388	2989.9581
Frequencies --	2999.1927	3000.7469	3011.0191
Frequencies --	3011.3303	3012.6030	3014.6234
Frequencies --	3015.8510	3100.1123	3101.9756
Frequencies --	3103.4690	3105.1311	3106.2763
Frequencies --	3109.8433	3111.4609	3131.2473
Frequencies --	3134.6786	3141.5389	3145.4881
Frequencies --	3148.0744	3150.4617	3159.9855
Frequencies --	3163.2398	3176.9675	3194.4367
Frequencies --	3214.0659	3220.6658	3223.5325

proximal conformation

vacuum	toluene-like solvent	D3 dispersion
-3156.8812101	-3156.8932735	-0.56233843

Frequencies --	-0.4387	9.6515	13.5008
Frequencies --	14.5643	20.6778	25.0596
Frequencies --	25.6656	27.9948	31.2709
Frequencies --	37.6854	39.9090	42.1747
Frequencies --	44.2112	66.7495	73.7532
Frequencies --	85.1269	96.3349	105.2622
Frequencies --	105.6559	108.6076	115.9838
Frequencies --	118.2858	118.5550	120.9175
Frequencies --	124.3888	126.4759	134.3113

Frequencies --	137.4797	142.7052	147.2442
Frequencies --	148.6278	151.7319	153.5371
Frequencies --	157.3524	160.1347	161.3300
Frequencies --	162.6875	164.6653	169.5027
Frequencies --	186.9079	192.2060	205.0971
Frequencies --	211.0522	216.9720	218.1296
Frequencies --	219.2729	238.1847	244.1524
Frequencies --	253.4349	263.4843	264.9006
Frequencies --	265.0862	267.1023	269.0845
Frequencies --	272.4536	282.1871	283.2924
Frequencies --	285.2886	290.5519	293.1082
Frequencies --	298.6834	304.7795	306.8223
Frequencies --	309.3446	315.3309	319.9102
Frequencies --	327.8896	331.2589	334.2949
Frequencies --	339.2026	354.0576	378.7979
Frequencies --	379.2775	379.3659	380.1855
Frequencies --	389.0671	389.8092	394.8993
Frequencies --	401.3945	421.3357	432.3847
Frequencies --	432.6435	433.0117	453.1671
Frequencies --	454.8316	456.4570	457.4733
Frequencies --	473.2515	475.4103	514.3099
Frequencies --	530.7695	536.5801	541.2869
Frequencies --	542.1339	547.8858	556.1990
Frequencies --	559.5612	575.7243	581.9920
Frequencies --	592.7062	596.3482	603.0030
Frequencies --	604.8400	611.0277	630.0138
Frequencies --	638.5038	639.5450	642.3249
Frequencies --	649.8058	661.2499	661.7886
Frequencies --	676.8700	694.1282	697.4084
Frequencies --	727.8246	728.8549	742.1755
Frequencies --	758.2088	758.3067	763.1536
Frequencies --	770.7118	783.8975	802.5055
Frequencies --	804.5642	840.2064	840.7899
Frequencies --	857.8313	870.2014	870.2698
Frequencies --	906.7398	907.6227	910.8759
Frequencies --	952.9082	965.6291	969.9671
Frequencies --	971.7215	987.3131	1008.6492
Frequencies --	1023.0078	1024.7423	1026.2446
Frequencies --	1042.7238	1044.0959	1047.1460
Frequencies --	1047.6092	1048.6035	1049.0796
Frequencies --	1049.7153	1051.5535	1073.9210
Frequencies --	1089.5551	1089.7668	1101.4074
Frequencies --	1103.0524	1126.9196	1127.4057
Frequencies --	1133.1634	1164.0910	1171.8135
Frequencies --	1174.6143	1175.9257	1190.2040
Frequencies --	1202.9278	1213.8991	1214.9419
Frequencies --	1215.6707	1273.3345	1302.4978
Frequencies --	1319.7038	1320.9486	1326.1250
Frequencies --	1339.3779	1342.4902	1344.6401
Frequencies --	1385.7632	1412.0566	1415.1177
Frequencies --	1417.7873	1418.3781	1419.8949
Frequencies --	1425.2026	1427.1604	1428.0141
Frequencies --	1430.1769	1431.9509	1435.6527
Frequencies --	1443.6640	1446.4673	1447.2076
Frequencies --	1455.0377	1456.3392	1459.5274
Frequencies --	1467.3078	1469.4321	1469.6711
Frequencies --	1471.5756	1478.8366	1482.0684
Frequencies --	1482.7480	1484.4407	1487.9707
Frequencies --	1492.5433	1494.5926	1498.5611
Frequencies --	1501.3069	1506.8731	1508.2351
Frequencies --	1512.3328	1515.4333	1517.9784
Frequencies --	1587.9903	1596.0250	1597.1780
Frequencies --	1598.0166	1617.8453	1620.3661

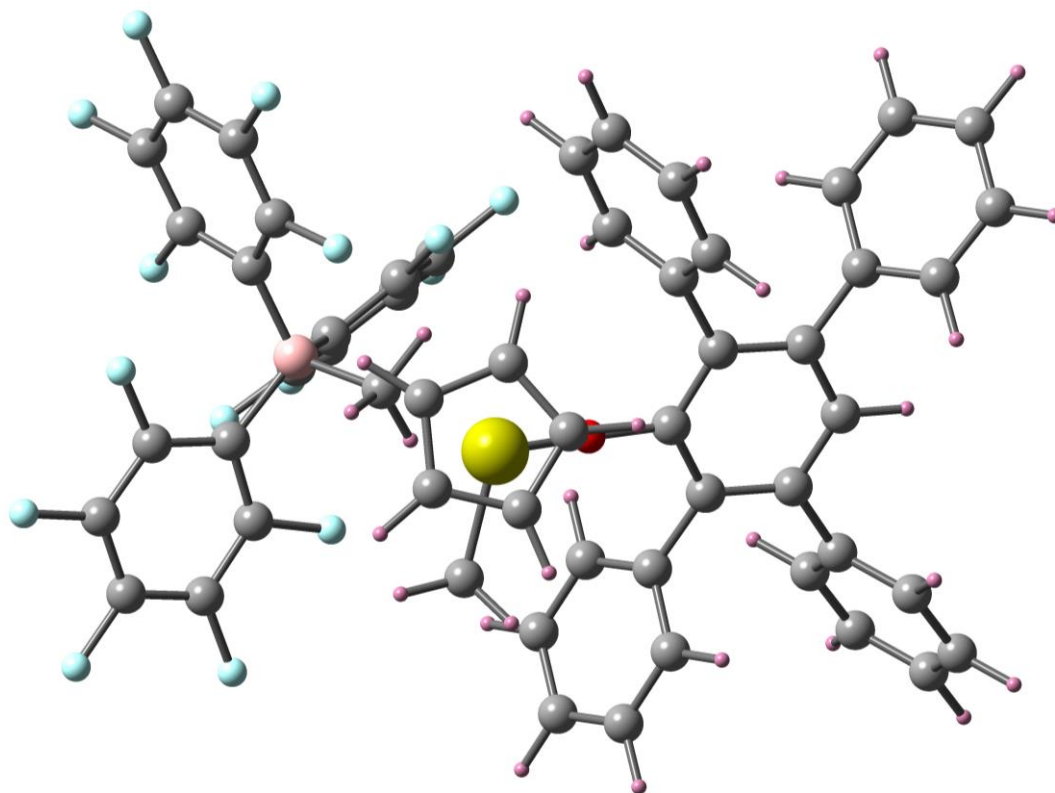
Frequencies --	1620.6080	1622.3306	2987.1543
Frequencies --	2997.8166	3003.8909	3010.9134
Frequencies --	3010.9993	3012.8757	3014.4645
Frequencies --	3016.0861	3098.2097	3102.2393
Frequencies --	3103.9506	3105.1870	3105.5191
Frequencies --	3108.5529	3112.3988	3132.5801
Frequencies --	3138.1500	3141.4175	3145.8111
Frequencies --	3148.9965	3151.4224	3159.8224
Frequencies --	3161.6816	3176.2899	3196.8267
Frequencies --	3210.6215	3219.1251	3222.7856

Catalyst 18:

vacuum	toluene-like solvent	D3 dispersion
-3156.88123797	-3156.89332624	-0.56175247

Frequencies --	1.9503	8.0862	14.8136
Frequencies --	16.0895	22.0549	23.9277
Frequencies --	25.7503	27.7772	31.1112
Frequencies --	36.6601	36.9474	41.2078
Frequencies --	43.5534	66.4142	71.6169
Frequencies --	82.8486	98.3890	104.9518
Frequencies --	106.1645	107.0834	108.5670
Frequencies --	116.9009	118.2905	119.3998
Frequencies --	124.1222	125.0713	125.7570
Frequencies --	132.7227	140.2813	148.3574
Frequencies --	151.8374	152.9085	154.8521
Frequencies --	157.1113	159.1186	160.3111
Frequencies --	160.8445	161.8482	166.9383
Frequencies --	183.2727	193.5764	199.7473
Frequencies --	212.6235	217.5756	217.7816
Frequencies --	218.9340	233.8894	242.3537
Frequencies --	262.9819	263.5753	264.6743
Frequencies --	265.1843	266.6535	271.4430
Frequencies --	273.5315	281.7697	283.0658
Frequencies --	288.0603	292.3649	293.5458
Frequencies --	299.4682	302.7141	305.3414
Frequencies --	310.2144	315.3021	320.0364
Frequencies --	331.1262	334.2371	338.7951
Frequencies --	353.3578	370.5922	378.8590
Frequencies --	378.9810	380.2792	388.1021
Frequencies --	390.1604	393.0622	406.1356
Frequencies --	411.5768	417.3961	431.0432
Frequencies --	432.2622	432.5068	432.8361
Frequencies --	453.4341	456.4541	457.4084
Frequencies --	473.3929	482.6956	510.4511
Frequencies --	517.9659	530.8746	537.0359
Frequencies --	541.1537	542.0923	547.7794
Frequencies --	554.8405	568.0793	580.2247
Frequencies --	582.0481	592.8067	595.9267
Frequencies --	603.2961	612.5028	630.6657
Frequencies --	635.9753	638.5585	639.8093
Frequencies --	642.5831	661.1910	662.0349
Frequencies --	690.8022	697.1023	714.4308
Frequencies --	727.9357	728.4397	742.8914
Frequencies --	758.3871	758.8897	768.5463
Frequencies --	770.8159	801.7267	802.1922
Frequencies --	804.2397	826.4331	843.1308
Frequencies --	857.9413	869.8225	907.0388
Frequencies --	907.9721	910.7158	927.8294
Frequencies --	945.1647	968.4151	969.1873

Frequencies --	972.4159	990.4606	1010.2472
Frequencies --	1012.3416	1023.5739	1025.5499
Frequencies --	1042.1124	1044.8455	1046.9806
Frequencies --	1048.2822	1048.8137	1049.3188
Frequencies --	1050.2851	1051.6068	1077.0343
Frequencies --	1088.7487	1089.8808	1102.1459
Frequencies --	1121.8271	1126.2280	1126.5728
Frequencies --	1144.1723	1171.3491	1171.5690
Frequencies --	1176.0768	1186.3420	1188.5062
Frequencies --	1214.0033	1214.8777	1215.5182
Frequencies --	1232.3234	1262.9219	1315.4892
Frequencies --	1320.4326	1320.8632	1326.3301
Frequencies --	1339.0699	1342.6470	1343.4560
Frequencies --	1362.5851	1411.6424	1416.2170
Frequencies --	1417.5180	1418.4727	1419.1470
Frequencies --	1425.6792	1426.3183	1427.1679
Frequencies --	1430.1667	1432.0569	1435.6920
Frequencies --	1438.7890	1443.6590	1447.1192
Frequencies --	1455.0949	1455.3536	1461.1459
Frequencies --	1469.2533	1469.2552	1471.2535
Frequencies --	1472.2052	1475.7509	1482.7451
Frequencies --	1483.8621	1485.5321	1491.5237
Frequencies --	1495.2526	1498.5538	1501.1277
Frequencies --	1501.2654	1506.6114	1508.4723
Frequencies --	1512.1904	1515.4276	1517.3285
Frequencies --	1580.3087	1595.9133	1597.3151
Frequencies --	1597.4432	1620.0303	1620.2451
Frequencies --	1621.9463	1623.8638	2987.8598
Frequencies --	2998.3815	3005.3252	3010.5536
Frequencies --	3010.8829	3012.3150	3014.2011
Frequencies --	3015.7129	3099.0300	3100.5849
Frequencies --	3102.8405	3103.9981	3105.1721
Frequencies --	3108.3090	3110.6595	3132.8769
Frequencies --	3138.6931	3139.1309	3144.1366
Frequencies --	3145.9507	3149.4501	3159.6600
Frequencies --	3163.5237	3192.5436	3192.9164
Frequencies --	3195.0941	3214.1126	3217.6944

Catalyst 19:

vacuum	toluene-like solvent	D3 dispersion
-3769.708235	-3769.7250185	-0.78125342

Ti	-0.39067700	-0.09488400	-2.29715400
C	-0.14459900	-2.10885300	-2.75586200
H	-0.13022500	-2.61776500	-1.78156700
H	-0.97088200	-2.51562300	-3.35558400
H	0.80292500	-2.27656500	-3.29125200
O	-1.80147000	-0.13054300	-1.21241400
C	-3.05432700	-0.03855700	-0.59759300
C	-3.64424400	1.25017900	-0.38878200
C	-3.71008100	-1.26421800	-0.25592300
C	-4.97913000	1.29234800	0.11742400
C	-5.04728800	-1.19033700	0.23601900
C	-5.65320300	0.07844300	0.38138900
H	-6.66220600	0.12556400	0.78866800
H	-0.54892600	2.85299000	-2.89322600
C	-0.44515300	1.93978300	-3.46611900
C	0.79426000	1.35147200	-3.89927600
C	-1.51943700	1.11771100	-3.95479200
H	1.78307900	1.74520400	-3.69062700
C	0.48779600	0.16897600	-4.64451500
H	-2.57810400	1.30384600	-3.81487300
C	-0.93897000	0.01766200	-4.67440600
H	1.20835100	-0.51120600	-5.08891400
H	-1.48360000	-0.78641700	-5.15920700

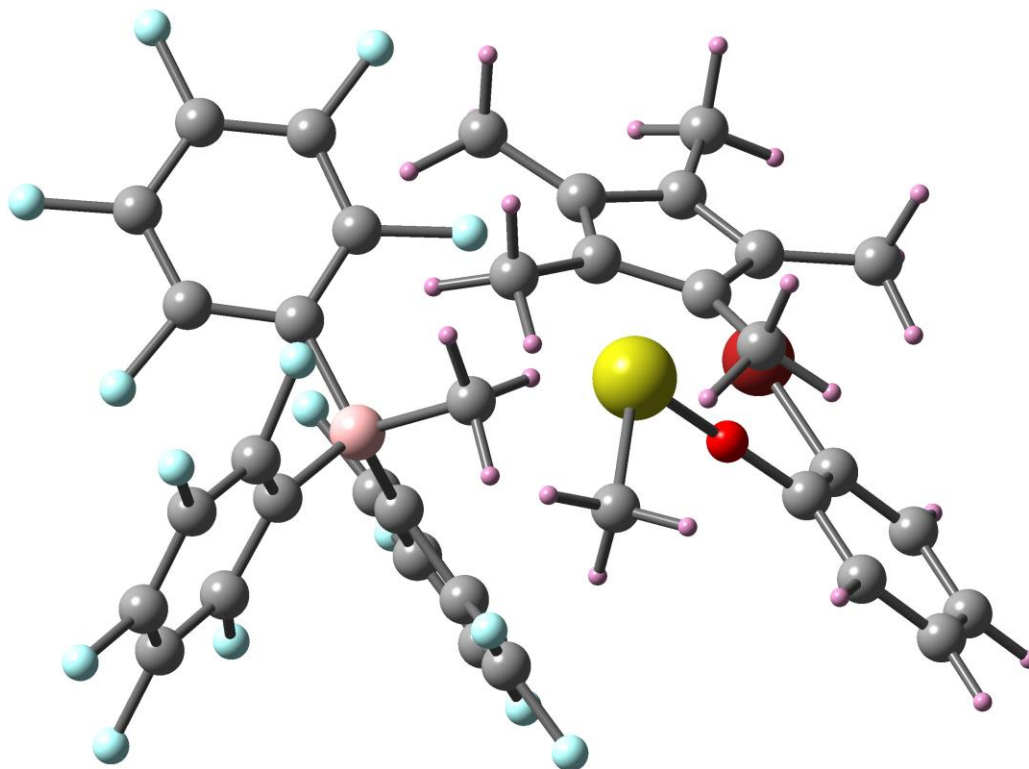
F	5.72161600	-4.61430100	-2.31960500
C	5.08686000	-3.53829000	-1.71600000
C	5.62904700	-2.24658300	-1.79990600
C	3.87629600	-3.71734200	-1.02502900
C	4.96372100	-1.16531800	-1.18233400
F	6.81206000	-2.04136900	-2.50062100
C	3.25854300	-2.60626300	-0.42732100
F	3.30289500	-4.98252500	-0.94596400
C	3.76382500	-1.28366500	-0.44345700
F	5.57583100	0.08168700	-1.37031100
F	2.03998200	-2.87518000	0.22420900
B	2.90909900	-0.02178200	0.23052000
C	3.76082100	1.40975300	0.27321700
C	3.48207800	2.58528900	-0.45349400
C	4.86492200	1.55563200	1.14963900
C	4.19079900	3.79686200	-0.32740600
F	2.43699500	2.61851900	-1.40068200
C	5.61153300	2.73627600	1.31258500
F	5.29430500	0.45670100	1.90058700
C	5.26796700	3.87774700	0.56767000
F	3.83095200	4.90948200	-1.08364000
F	6.68416900	2.78530000	2.19425900
F	5.98191800	5.05850500	0.71091700
C	2.41582300	-0.28660300	1.80791900
C	1.45059000	0.55387400	2.40848100
C	2.91402200	-1.27075200	2.69658100
C	0.97158600	0.43207500	3.72565300
C	2.46823000	-1.43948600	4.02433000
C	1.48222900	-0.58605900	4.54630400
F	3.92458700	-2.14867600	2.30306000
F	3.00104900	-2.44114500	4.82691200
F	1.02811300	-0.73901600	5.84831100
F	0.00516400	1.30670800	4.21632900
F	0.90992100	1.63212100	1.67778700
C	1.50832900	0.04288500	-0.76297600
H	0.94705700	0.95755800	-0.52566600
H	1.91813700	0.04174900	-1.78621200
H	0.96762400	-0.87557800	-0.49565300
C	-2.90407500	2.52737800	-0.67949500
C	-3.37129300	3.43348100	-1.66675400
C	-1.76855400	2.89457500	0.08699100
C	-2.72508800	4.66843200	-1.88144600
H	-4.25305800	3.17994500	-2.25780600
C	-1.11958500	4.13001700	-0.12438900
H	-1.40642800	2.23116700	0.87114000
C	-1.59625500	5.02355100	-1.10901100
H	-3.10692100	5.35405100	-2.64127400
H	-0.25341900	4.39403700	0.48556300
H	-1.09958800	5.98321100	-1.26741400
C	-5.71264600	2.56959000	0.43379400
C	-6.94748800	2.85646400	-0.20462700
C	-5.24260100	3.47019900	1.42441500
C	-7.68233800	4.01616300	0.12162500
H	-7.33040900	2.17518900	-0.96798000
C	-5.97937800	4.62539100	1.75855300
H	-4.30722500	3.26280400	1.94539500
C	-7.20013200	4.90658000	1.10584600

H	-8.62611100	4.22156500	-0.38914200
H	-5.60193100	5.30117000	2.52946800
H	-7.76844300	5.80319500	1.36357800
C	-5.85458200	-2.39427600	0.64496000
C	-7.09539200	-2.66144400	0.00912300
C	-5.44947900	-3.23973600	1.70981400
C	-7.89956100	-3.74872600	0.41190200
H	-7.42784700	-2.02311500	-0.81268600
C	-6.25550800	-4.32185800	2.12019200
H	-4.50989900	-3.04637700	2.22807100
C	-7.48212400	-4.58435600	1.47087400
H	-8.84662400	-3.94063800	-0.09801700
H	-5.92657500	-4.95564500	2.94696900
H	-8.10414100	-5.42453300	1.78793700
C	-3.02260500	-2.59344400	-0.41008700
C	-3.46788000	-3.53591000	-1.37135700
C	-1.95959800	-2.96192400	0.45418900
C	-2.87357900	-4.81192800	-1.46277400
H	-4.29029200	-3.27554000	-2.04040600
C	-1.36620000	-4.23916900	0.36934100
H	-1.60922700	-2.25605600	1.21054500
C	-1.82326900	-5.17034500	-0.58945500
H	-3.23487800	-5.52553700	-2.20691100
H	-0.55211700	-4.50404600	1.04681500
H	-1.36477200	-6.15929400	-0.65502100

Frequencies --	3.9649	11.2002	14.5950
Frequencies --	16.8335	23.7698	25.1251
Frequencies --	27.9565	28.7191	31.4428
Frequencies --	37.0563	39.4956	42.6964
Frequencies --	43.9515	45.5296	47.0954
Frequencies --	48.1824	52.9600	58.3728
Frequencies --	62.1564	64.5919	71.0846
Frequencies --	74.6640	81.1961	88.5170
Frequencies --	92.0147	99.9206	107.3771
Frequencies --	112.1263	114.6466	118.3143
Frequencies --	122.8157	124.6721	124.9176
Frequencies --	138.0010	141.5814	147.5968
Frequencies --	151.2891	151.5452	156.1344
Frequencies --	158.5015	161.5337	169.0552
Frequencies --	192.9731	193.6421	202.8718
Frequencies --	211.6751	213.2178	215.0201
Frequencies --	217.1277	223.0027	228.4787
Frequencies --	236.5060	247.6254	252.6427
Frequencies --	257.8176	260.7599	264.1970
Frequencies --	264.5447	264.9768	272.9626
Frequencies --	274.5025	275.3814	280.4375
Frequencies --	285.5582	292.7117	300.3348
Frequencies --	302.1368	311.5310	322.8455
Frequencies --	327.8589	328.5749	335.1618
Frequencies --	337.7316	348.7426	350.2271
Frequencies --	370.1252	374.0529	378.1973
Frequencies --	379.4277	379.9793	401.0312
Frequencies --	401.6466	404.5746	405.6269
Frequencies --	407.1054	408.6417	412.6085
Frequencies --	431.6338	433.2055	433.7036
Frequencies --	445.9816	450.8084	457.9418
Frequencies --	458.2846	475.8704	488.9598
Frequencies --	517.7587	520.7274	529.4103
Frequencies --	541.2786	542.8266	543.9722

Frequencies --	548.2878	549.2273	557.2965
Frequencies --	567.1666	588.5656	596.7448
Frequencies --	602.8159	613.5195	616.2734
Frequencies --	618.0086	620.0704	624.5830
Frequencies --	632.3241	633.5916	634.9932
Frequencies --	637.9920	640.4117	642.0245
Frequencies --	651.8375	657.2738	668.0325
Frequencies --	687.5647	692.1703	696.3611
Frequencies --	700.3956	709.8132	710.7371
Frequencies --	715.0763	718.5107	719.8133
Frequencies --	731.2817	741.3589	743.6448
Frequencies --	748.4424	751.3480	764.6900
Frequencies --	766.0565	770.1180	773.0807
Frequencies --	784.5024	797.2346	802.1982
Frequencies --	806.6227	813.5333	825.2036
Frequencies --	839.3502	842.5357	843.4127
Frequencies --	857.8671	859.4252	859.6497
Frequencies --	861.4384	867.5501	875.6195
Frequencies --	877.7830	879.5323	902.4617
Frequencies --	912.7934	914.0381	915.8037
Frequencies --	916.6892	934.8984	936.8494
Frequencies --	940.6918	948.5635	965.6086
Frequencies --	985.6476	986.9518	992.2755
Frequencies --	995.5235	999.6656	1005.2885
Frequencies --	1006.2938	1011.1237	1012.4669
Frequencies --	1013.3154	1017.5469	1020.2911
Frequencies --	1021.0998	1026.7315	1028.3864
Frequencies --	1031.3074	1033.3025	1039.9809
Frequencies --	1045.6444	1048.8943	1050.2444
Frequencies --	1052.2745	1054.2993	1054.3923
Frequencies --	1055.0720	1080.4111	1085.5215
Frequencies --	1090.2358	1091.0320	1091.6034
Frequencies --	1092.2517	1092.4434	1094.0528
Frequencies --	1123.7362	1129.1094	1129.5967
Frequencies --	1135.3977	1183.5156	1183.6068
Frequencies --	1185.2264	1186.3097	1199.7359
Frequencies --	1204.6395	1205.7835	1207.1225
Frequencies --	1209.4787	1214.3361	1215.8383
Frequencies --	1218.1943	1232.3721	1254.5661
Frequencies --	1282.3424	1286.7779	1304.8029
Frequencies --	1317.1973	1321.2012	1322.9763
Frequencies --	1326.5173	1327.7595	1331.3816
Frequencies --	1332.6460	1335.0385	1340.0330
Frequencies --	1345.1833	1349.0960	1366.1619
Frequencies --	1368.0485	1370.1212	1371.3059
Frequencies --	1378.9012	1391.2375	1396.5787
Frequencies --	1413.3716	1419.6793	1423.4465
Frequencies --	1426.9425	1441.4119	1441.7310
Frequencies --	1443.3123	1443.6875	1446.2114
Frequencies --	1447.7631	1449.8479	1451.1299
Frequencies --	1457.3968	1468.4657	1469.2435
Frequencies --	1471.7299	1475.2954	1496.9358
Frequencies --	1497.4349	1502.4548	1509.1022
Frequencies --	1527.1123	1587.3555	1593.9798
Frequencies --	1594.9106	1595.2350	1596.9525
Frequencies --	1597.6600	1598.1274	1598.9643
Frequencies --	1618.9911	1620.8597	1621.6185
Frequencies --	1622.8635	1623.2690	1623.9489
Frequencies --	1624.5134	2976.0030	3010.1234
Frequencies --	3116.2328	3133.6724	3139.3906
Frequencies --	3150.2063	3152.9564	3153.0949
Frequencies --	3157.9591	3159.4572	3161.0625
Frequencies --	3161.2074	3161.9201	3171.1633

Frequencies --	3173.2019	3173.4487	3174.1294
Frequencies --	3182.5174	3183.1729	3185.8832
Frequencies --	3186.7039	3193.5989	3194.9001
Frequencies --	3197.6098	3198.0551	3198.9715
Frequencies --	3213.4980	3244.3495	3259.2324
Frequencies --	3273.8945	3276.7248	3297.7999

Catalyst 20:**distal conformation**

vacuum	toluene-like solvent	D3 dispersion
-3054.962514	-3054.973941	-0.55747543

Ti	2.01723900	-1.71230800	-0.43123600
C	1.84446700	-2.08102800	-2.48468300
H	1.57876600	-1.10050500	-2.91764300
H	2.77933500	-2.42575000	-2.94861700
H	1.04749400	-2.81068600	-2.69752000
O	3.11152100	-0.30751700	-0.57438600
C	4.06304300	0.65505000	-0.82387400
C	4.32090200	1.71586300	0.08647200
C	4.78461900	0.60678000	-2.04565400
C	5.28041300	2.70216600	-0.22048300
C	5.74223500	1.59033200	-2.35017800
C	5.99250800	2.63890300	-1.43717700
H	5.46359600	3.51556700	0.48170400
H	6.28257500	1.54295200	-3.29729700
C	2.61948300	-2.81663800	1.57973300
C	1.40260300	-3.49202800	1.17377900
C	3.63290800	-3.08367100	0.57968100
C	1.65992000	-4.16980100	-0.07393800
C	3.03642500	-3.92549600	-0.44162600

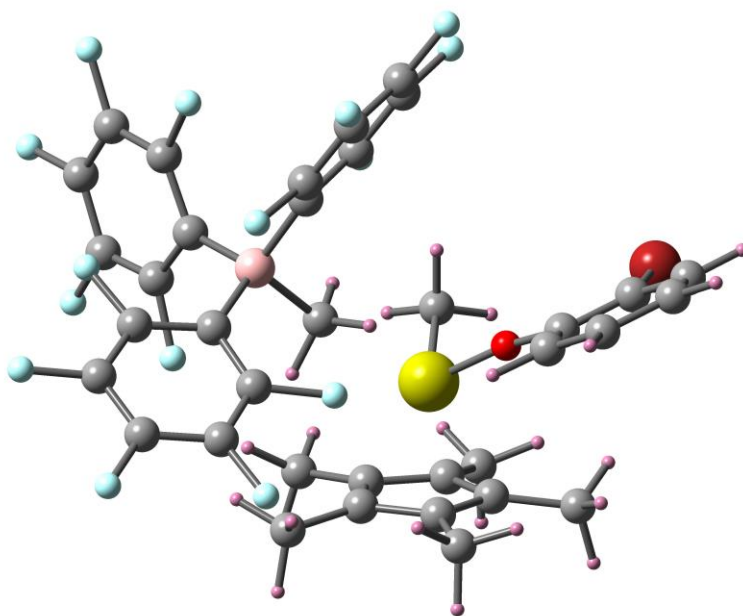
F	0.23179300	5.93700400	-0.94574600
C	-0.21573900	4.63921900	-0.74319500
C	-1.04720200	4.32834500	0.34359200
C	0.15267200	3.60991600	-1.62505300
C	-1.48695900	3.00101200	0.53326900
F	-1.43386500	5.33365800	1.22233300
C	-0.31062700	2.30537800	-1.38641200
F	0.96618500	3.89070000	-2.71884400
C	-1.13609200	1.91657900	-0.30372600
F	-2.33882000	2.81963500	1.62955500
F	0.07494300	1.35114800	-2.35122900
B	-1.57893500	0.32486300	-0.07662700
C	-2.32955300	0.06953300	1.38918800
C	-2.51987200	-0.25851200	-1.32613400
C	-0.10520300	-0.56570600	-0.11738500
C	-3.73197800	-0.03939700	1.55253400
C	-1.62882500	-0.04984000	2.61054900
C	-3.20694000	0.53939600	-2.27206600
C	-2.71547300	-1.64263000	-1.53453000
H	0.59909100	-0.00494700	0.51249500
H	-0.35065800	-1.56026100	0.26865100
H	0.15900200	-0.55161900	-1.18344800
C	-4.37772600	-0.28027200	2.78230900
F	-4.59129100	0.13153100	0.46162000
C	-2.21986100	-0.29159800	3.86373100
F	-0.22582900	0.10742400	2.64474400
C	-3.96830900	0.02745500	-3.34231500
F	-3.19893200	1.93358800	-2.16983100
C	-3.46535600	-2.20855000	-2.58132600
F	-2.16225300	-2.57937700	-0.63095000
C	-3.61514200	-0.41624600	3.95347900
F	-5.76219100	-0.37858200	2.84870400
F	-1.43540800	-0.40879000	5.00916600
C	-4.09579000	-1.36156700	-3.50638400
F	-4.60455100	0.88388500	-4.23240900
F	-3.58665300	-3.59065400	-2.70527900
F	-4.22637100	-0.66111000	5.17450600
F	-4.83685800	-1.88693400	-4.55488600
C	3.78699500	-4.60711000	-1.56091900
H	4.64600300	-4.01837200	-1.90975600
H	4.18188500	-5.57292900	-1.20039400
H	3.14969600	-4.82153700	-2.42760800
C	5.09559000	-2.71308300	0.67631500
H	5.64985700	-3.51298700	1.19702900
H	5.56138900	-2.58313100	-0.30986600
H	5.25328800	-1.78581800	1.24136000
C	0.68770300	-5.07376800	-0.79508200
H	0.95099200	-5.21301300	-1.85103100
H	0.69036200	-6.07361100	-0.32639900
H	-0.34419300	-4.70104400	-0.74988200
C	0.15565000	-3.64000100	2.01639500
H	-0.75325600	-3.76044900	1.41388900
H	0.25055400	-4.54500900	2.64161500
H	0.00604600	-2.79418900	2.69732500
C	2.82599400	-2.10482500	2.89682100
H	3.02763800	-2.84857700	3.68768100
H	3.67935700	-1.41691400	2.87136800

H	1.94487000	-1.53045700	3.21107200
H	6.72898000	3.41002300	-1.66807500
Br	3.33137400	1.85073500	1.76994500
H	4.56849000	-0.19894900	-2.74661500

Frequencies --	6.1878	12.8696	16.9649
Frequencies --	19.5497	21.5033	25.9568
Frequencies --	27.3558	30.7669	33.3773
Frequencies --	37.5647	41.5483	42.3669
Frequencies --	45.0651	70.1489	74.7017
Frequencies --	90.2887	103.5426	104.9499
Frequencies --	106.1017	108.6394	114.0139
Frequencies --	115.4327	118.0425	119.3446
Frequencies --	120.0427	124.8896	130.5063
Frequencies --	133.0219	141.3174	150.5677
Frequencies --	153.6431	155.2651	157.3784
Frequencies --	159.4118	160.1792	162.8996
Frequencies --	168.1485	168.5100	177.4602
Frequencies --	182.7993	200.3840	212.8351
Frequencies --	217.6257	220.0074	221.8033
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Frequencies --	264.8346	264.9878	266.7146
Frequencies --	268.8654	273.6543	278.0367
Frequencies --	281.9212	286.9996	290.9513
Frequencies --	294.6733	295.2459	303.4612
Frequencies --	308.1915	308.3089	313.3317
Frequencies --	321.0646	324.1058	331.3032
Frequencies --	334.3935	338.3429	356.3716
Frequencies --	357.7547	379.3086	379.6389
Frequencies --	380.8679	386.3203	388.1815
Frequencies --	391.4964	395.0414	418.6928
Frequencies --	432.1666	432.8553	433.0448
Frequencies --	446.5466	453.3948	456.5393
Frequencies --	457.7928	473.8574	490.4946
Frequencies --	504.1903	530.2989	535.7658
Frequencies --	538.4446	541.1482	542.4675
Frequencies --	548.0613	557.1015	579.4217
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Frequencies --	631.8432	638.3337	639.4182
Frequencies --	642.4637	660.5965	663.4959
Frequencies --	671.7041	694.1781	703.8613
Frequencies --	708.5364	726.5734	729.8009
Frequencies --	742.2486	757.4250	760.2242
Frequencies --	765.1963	770.2075	803.5382
Frequencies --	805.3340	837.2274	861.5091
Frequencies --	864.5894	867.9846	906.4046
Frequencies --	908.2405	911.3867	932.8834
Frequencies --	956.1250	971.1802	974.2768
Frequencies --	993.4284	1013.9688	1022.7047
Frequencies --	1026.0670	1028.8023	1043.0501
Frequencies --	1044.1070	1047.5638	1048.1860
Frequencies --	1048.7338	1049.1488	1050.8688
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Frequencies --	1318.8792	1321.9053	1327.3206
Frequencies --	1338.8788	1341.2499	1345.7059
Frequencies --	1357.5949	1411.9458	1417.1575

Frequencies --	1417.6995	1418.1205	1420.3871
Frequencies --	1425.7416	1427.6523	1428.6063
Frequencies --	1430.3745	1434.2287	1435.4669
Frequencies --	1437.4043	1447.2494	1448.9263
Frequencies --	1454.8861	1459.9073	1465.5990
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Frequencies --	1493.1450	1495.5848	1499.3392
Frequencies --	1502.0127	1507.2789	1509.3382
Frequencies --	1514.2132	1516.6547	1519.2220
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Frequencies --	3104.7421	3106.6797	3107.4799
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Frequencies --	3135.6249	3142.9083	3144.9839
Frequencies --	3148.2641	3152.9584	3156.4699
Frequencies --	3164.9524	3175.6539	3175.9981
Frequencies --	3190.5561	3206.1560	3213.9486

proximal conformation



vacuum	toluene-like solvent	D3 dispersion
-3054.9633056	-3054.9745635	-0.55652851

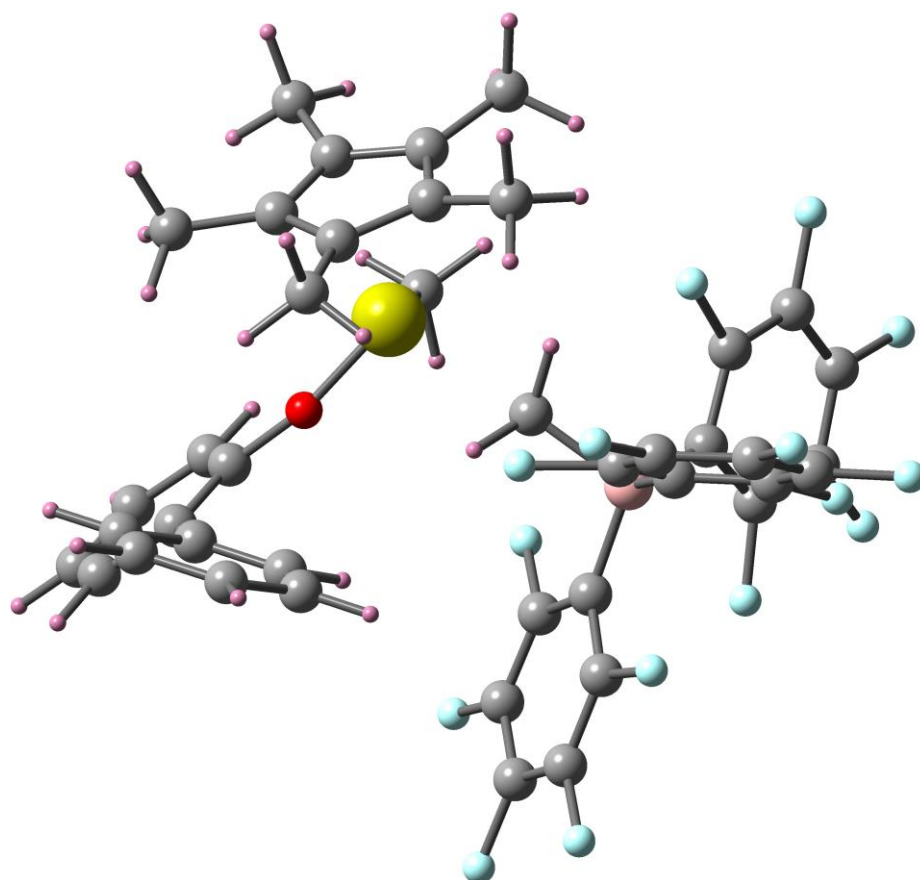
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H	3.29355600	-1.74027200	-2.61803700
H	1.60800400	-2.33899900	-2.80049600
O	2.94343800	-0.06388300	0.14236100
C	3.60664600	1.00455300	0.70636900

C	4.73328100	1.60314100	0.07912000
C	3.12818300	1.55044000	1.92732100
C	5.36634900	2.71836400	0.66536500
C	3.75944000	2.66416900	2.50906400
C	4.88099000	3.24858700	1.88005200
H	6.22573000	3.17295900	0.17233000
H	3.37192900	3.07602000	3.44248100
C	2.52240800	-2.86298500	1.65262200
C	1.32520100	-3.47881900	1.11660000
C	3.57910100	-3.02481300	0.67695300
C	1.63866400	-4.01419300	-0.18883100
C	3.03145400	-3.74595700	-0.46009600
F	0.02558900	5.95368100	-0.85107800
C	-0.40822500	4.64837600	-0.66979700
C	-1.24191500	4.31334500	0.40830900
C	-0.02363600	3.63568700	-1.56427500
C	-1.66884500	2.97900300	0.57629300
F	-1.64335900	5.30194000	1.29979500
C	-0.47374500	2.32229900	-1.34633400
F	0.79067900	3.94149900	-2.64962500
C	-1.30153500	1.91049000	-0.27388400
F	-2.52684300	2.77293700	1.66420100
F	-0.07324400	1.38489400	-2.31941200
B	-1.73233200	0.31144100	-0.07663600
C	-2.45422600	0.02643400	1.39982500
C	-2.68400800	-0.24568100	-1.32660100
C	-0.26063000	-0.57864000	-0.13660800
C	-3.85028200	-0.12070900	1.58657800
C	-1.73087900	-0.08565100	2.60842700
C	-3.38331800	0.57094200	-2.24702900
C	-2.86966300	-1.62562200	-1.56890700
H	0.42603900	0.02129500	0.47459000
H	-0.48260100	-1.56477400	0.27887500
H	0.00905300	-0.60762600	-1.20083900
C	-4.46756300	-0.39042300	2.82520800
F	-4.73225200	0.03660900	0.51276900
C	-2.29200600	-0.35353000	3.86960900
F	-0.32796300	0.10775200	2.62376200
C	-4.14726500	0.08066400	-3.32564100
F	-3.38478600	1.96246300	-2.10914600
C	-3.62183400	-2.17021800	-2.62512500
F	-2.30510700	-2.57854400	-0.69076800
C	-3.68170100	-0.51656200	3.98216500
F	-5.84707800	-0.52668500	2.91455000
F	-1.48364000	-0.45926900	4.99999900
C	-4.26437500	-1.30461000	-3.52460100
F	-4.79521400	0.95473500	-4.18961900
F	-3.73474500	-3.54934900	-2.78296800
F	-4.26448700	-0.78905000	5.21096300
F	-5.00778300	-1.80894300	-4.58157100
C	3.83644600	-4.31428700	-1.60364800
H	4.72552500	-3.71116600	-1.83000400
H	4.18860000	-5.32558600	-1.33517900
H	3.25109500	-4.40955800	-2.52682600
C	5.03702100	-2.67686100	0.87290100
H	5.58602200	-3.56577300	1.22927100
H	5.51951800	-2.34550900	-0.05621800

H	5.17876300	-1.88530100	1.61911000
C	0.70052700	-4.81301900	-1.06352800
H	0.99299900	-4.78501700	-2.12132000
H	0.71180700	-5.87278600	-0.75344200
H	-0.33904500	-4.46863800	-0.99153600
C	0.04218800	-3.70693200	1.88406400
H	-0.83268200	-3.81132500	1.23120200
H	0.13129400	-4.64581900	2.45810500
H	-0.16409500	-2.90896300	2.60797200
C	2.66819100	-2.30276300	3.04943700
H	2.87412900	-3.12453100	3.75731500
H	3.49900100	-1.59058900	3.13063600
H	1.75691300	-1.79914000	3.39917000
H	5.37436300	4.11577200	2.32161200
Br	5.42355400	0.91461800	-1.61894200
H	2.25411900	1.10139300	2.39747300

Frequencies --	2.7252	10.4610	14.7560
Frequencies --	16.2203	21.7315	22.9619
Frequencies --	26.1789	29.3697	31.7139
Frequencies --	37.3283	40.0784	43.6930
Frequencies --	51.6663	59.6754	71.4729
Frequencies --	91.2509	97.3625	103.2921
Frequencies --	105.2838	107.8090	113.0869
Frequencies --	117.3257	117.7108	118.7948
Frequencies --	120.9141	124.4194	132.2284
Frequencies --	138.4585	140.1699	149.8905
Frequencies --	150.6957	153.3231	155.8763
Frequencies --	157.1828	159.7315	160.7931
Frequencies --	161.3917	168.5640	173.4091
Frequencies --	181.4653	202.1010	210.3851
Frequencies --	214.5841	216.7456	219.0612
Frequencies --	225.7442	238.3119	256.0105
Frequencies --	264.8837	265.0117	265.2842
Frequencies --	268.9760	272.3004	279.5905
Frequencies --	281.5576	284.2078	288.4470
Frequencies --	289.9722	291.0620	297.6757
Frequencies --	302.5267	307.6946	311.5700
Frequencies --	319.0490	325.8202	330.1884
Frequencies --	333.4974	336.5332	347.0863
Frequencies --	353.7470	379.2140	379.5497
Frequencies --	380.2649	386.0195	387.5756
Frequencies --	390.1724	391.3683	417.6654
Frequencies --	431.9791	432.8681	433.1553
Frequencies --	448.0518	451.5617	456.2296
Frequencies --	457.5934	472.9440	490.6996
Frequencies --	515.5565	529.7601	535.5210
Frequencies --	540.8541	541.2796	542.3639
Frequencies --	547.9548	553.7199	572.9421
Frequencies --	582.1941	591.8664	596.1738
Frequencies --	599.8627	609.7297	629.8844
Frequencies --	631.5484	638.3330	638.8425
Frequencies --	641.5622	661.2368	663.2588
Frequencies --	669.1955	694.1051	702.1521
Frequencies --	710.8523	726.6775	729.0877
Frequencies --	741.9191	757.5569	759.0964
Frequencies --	768.3590	770.2155	799.9409
Frequencies --	803.3122	838.7794	859.4933
Frequencies --	866.8018	869.8516	906.1780
Frequencies --	907.2437	910.5932	927.2833
Frequencies --	960.2487	967.2148	972.2039

Frequencies --	995.7608	1009.7928	1023.8462
Frequencies --	1024.0139	1028.6388	1042.5819
Frequencies --	1042.9383	1045.9004	1046.1616
Frequencies --	1047.1788	1049.0138	1049.3374
Frequencies --	1051.6736	1053.9017	1075.1695
Frequencies --	1088.7854	1090.0990	1095.5504
Frequencies --	1126.2749	1131.1373	1135.9187
Frequencies --	1171.0226	1175.5354	1185.5587
Frequencies --	1190.4643	1213.9301	1215.3691
Frequencies --	1216.2448	1251.2180	1277.4726
Frequencies --	1318.9486	1321.4703	1326.3574
Frequencies --	1339.0075	1341.6880	1345.3809
Frequencies --	1358.2668	1409.8579	1414.1048
Frequencies --	1417.3459	1417.8908	1420.2540
Frequencies --	1421.6840	1426.7689	1428.0918
Frequencies --	1428.4058	1429.8274	1435.6001
Frequencies --	1436.2096	1439.4665	1447.3895
Frequencies --	1454.2086	1458.3977	1463.9781
Frequencies --	1467.9483	1469.4710	1469.9713
Frequencies --	1471.8600	1478.0898	1480.3785
Frequencies --	1491.9059	1494.3451	1499.2689
Frequencies --	1499.4807	1504.3249	1507.3458
Frequencies --	1511.9572	1517.4850	1518.0515
Frequencies --	1579.4489	1595.6688	1595.9676
Frequencies --	1596.6568	1597.5884	1620.4738
Frequencies --	1620.8734	1622.5467	2991.9111
Frequencies --	3010.7965	3011.6411	3011.8541
Frequencies --	3012.9057	3014.4593	3016.4511
Frequencies --	3104.1002	3104.6060	3106.6634
Frequencies --	3107.6481	3113.3022	3113.6960
Frequencies --	3143.2136	3144.5364	3146.2295
Frequencies --	3148.6070	3150.3828	3152.6350
Frequencies --	3161.6340	3177.1679	3191.5717
Frequencies --	3192.2301	3207.1016	3218.0741

Catalyst 21:**distal conformation**

vacuum	toluene-like solvent	D3 dispersion
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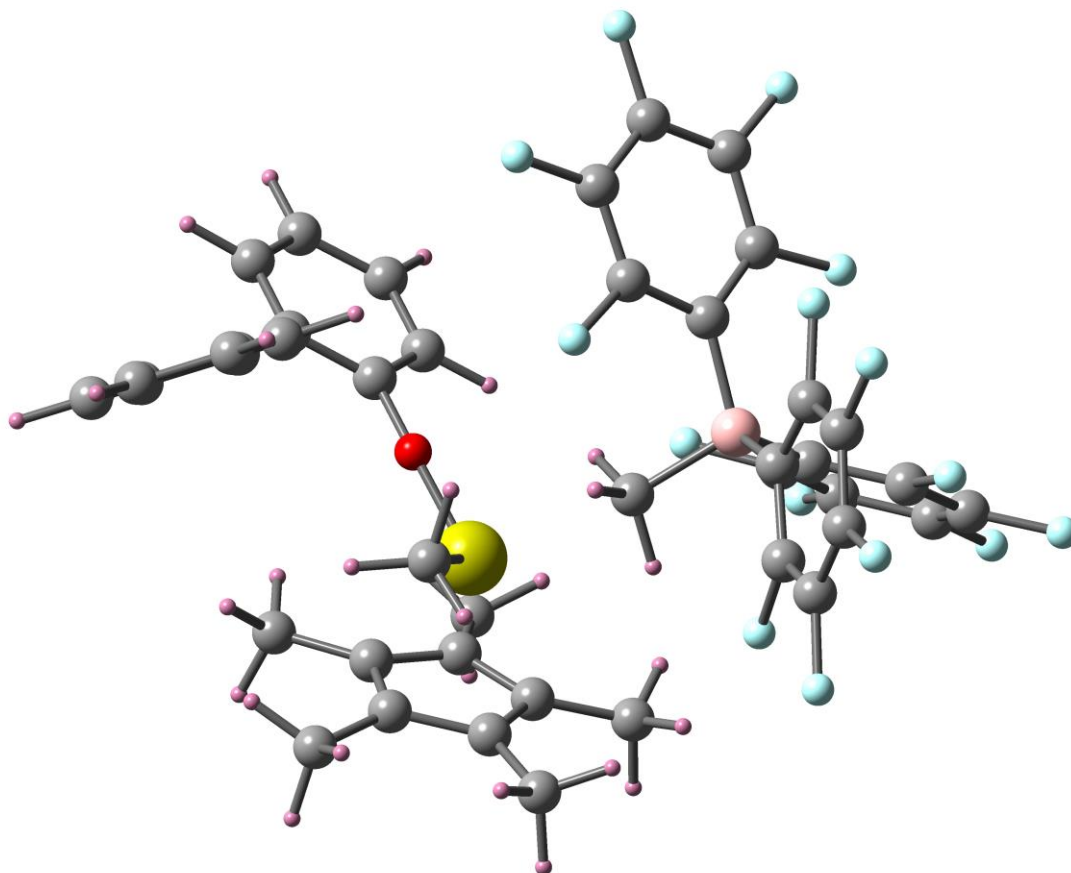
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H	-3.34326900	-1.68694700	2.29246600
H	-1.69485400	-2.31657500	2.64111100
O	-2.77666800	-0.13940400	-0.49241500
C	-3.41927900	0.85102900	-1.22882400
C	-4.61016400	1.46980900	-0.74116400
C	-2.86061900	1.21765000	-2.47994900
C	-5.23302200	2.42508000	-1.58760300
C	-3.49235600	2.18418800	-3.28276500
C	-4.69351000	2.78119600	-2.83996100
H	-6.13998700	2.91696600	-1.23262100
H	-3.04932200	2.46710700	-4.23955000
C	-2.13626900	-3.00928200	-1.84826200

C	-1.01809300	-3.58589300	-1.12894500
C	-3.31033300	-3.12601400	-1.01031000
C	-1.49871300	-4.05951400	0.14819400
C	-2.91379200	-3.78397200	0.22412900
F	-0.04335600	5.98802700	-0.18477300
C	0.41835600	4.68291600	-0.09570200
C	1.51180300	4.25362100	-0.86460200
C	-0.19337300	3.76411100	0.77184000
C	1.95847000	2.91938900	-0.76445200
F	2.14687800	5.15038600	-1.71593100
C	0.29341100	2.44686100	0.83212300
F	-1.27280900	4.15963000	1.55846900
C	1.36682300	1.93719600	0.06452600
F	3.08277100	2.61857500	-1.54260600
F	-0.35489100	1.62205900	1.77583000
B	1.83009600	0.33624800	0.14512600
C	2.77603400	-0.09638300	-1.15841600
C	2.56174800	-0.03876700	1.59505300
C	0.39283400	-0.60193700	0.06832400
C	4.16737700	-0.34979200	-1.10447300
C	2.24525500	-0.24543900	-2.45984000
C	3.06604000	0.90278800	2.52296400
C	2.73187400	-1.37556700	2.02424400
H	-0.20602900	-0.11738200	-0.71537300
H	0.70215200	-1.61910900	-0.17925700
H	-0.04379600	-0.51864900	1.07255000
C	4.94890600	-0.74979600	-2.20822400
F	4.87969800	-0.17859700	0.08708000
C	2.97557300	-0.64003300	-3.59445000
F	0.88271000	0.04167900	-2.70813100
C	3.64256200	0.56650600	3.76541700
F	3.04870400	2.27178600	2.23533000
C	3.30131500	-1.76778300	3.24840500
F	2.35277500	-2.44193500	1.17861000
C	4.34872400	-0.90415900	-3.46818800
F	6.31038600	-0.98638800	-2.06342300
F	2.35140000	-0.77095000	-4.83338400
C	3.75800200	-0.78213800	4.13832000
F	4.10552600	1.55768300	4.62235800
F	3.41920600	-3.11477600	3.58131900
F	5.09574800	-1.30339100	-4.56690000
F	4.31862900	-1.13586400	5.35706000
C	-3.86015400	-4.28791000	1.28735000
H	-4.77137600	-3.67951200	1.35694800
H	-4.17277000	-5.31768500	1.04113800
H	-3.40028800	-4.31795900	2.28308100
C	-4.73224400	-2.79840200	-1.40662100
H	-5.23038800	-3.70678300	-1.78764500
H	-5.32801500	-2.43009100	-0.56041800
H	-4.78051300	-2.04155700	-2.19917800
C	-0.67806700	-4.80527000	1.17485500
H	-1.12887000	-4.76658600	2.17465800
H	-0.60464400	-5.87075100	0.89430200
H	0.34842000	-4.42271900	1.25288500
C	0.35651100	-3.84372200	-1.70437400
H	1.13843700	-3.88467700	-0.93579300
H	0.35486400	-4.82277200	-2.21476100

H	0.64935800	-3.09466800	-2.45016200
C	-2.09826900	-2.53072700	-3.28216600
H	-2.17414900	-3.39683600	-3.96254500
H	-2.93129700	-1.85838200	-3.52086800
H	-1.16296000	-2.01011700	-3.52983200
H	-1.93524300	0.74809000	-2.81029000
H	-5.19401000	3.53208400	-3.45384800
C	-5.20515100	1.19212500	0.60720300
C	-4.48255600	1.47248900	1.79655700
C	-6.54254300	0.72894700	0.72240400
C	-5.08135300	1.29596300	3.06136000
H	-3.46445800	1.85792300	1.73354700
C	-7.13912100	0.54107100	1.98773700
H	-7.11583000	0.51174800	-0.18177800
C	-6.40992600	0.82645800	3.16335000
H	-4.51346700	1.53469000	3.96356900
H	-8.16892100	0.18196200	2.05373800
H	-6.87231200	0.69378300	4.14407500

Frequencies --	4.9018	9.0469	14.6843
Frequencies --	15.3866	22.1479	26.6203
Frequencies --	28.4783	30.0735	31.5098
Frequencies --	37.5028	42.3093	42.5847
Frequencies --	43.5189	62.5016	66.6819
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Frequencies --	149.8248	153.5118	157.4945
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Frequencies --	201.3063	204.8600	215.6975
Frequencies --	216.1279	220.1496	234.4653
Frequencies --	252.7662	261.8503	263.6080
Frequencies --	264.7872	264.9323	265.6716
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Frequencies --	589.8941	596.5423	600.8137
Frequencies --	614.4908	614.8851	621.9606
Frequencies --	630.7023	637.8098	638.6818
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Frequencies --	713.4052	725.5597	729.4046
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Frequencies --	770.2826	780.8825	802.9504
Frequencies --	806.8027	842.2494	854.3314
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Frequencies --	1048.3149	1048.9263	1050.4351
Frequencies --	1051.8519	1063.0374	1071.5448
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Frequencies --	1185.9759	1187.0042	1190.0917
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Frequencies --	1425.7514	1427.3606	1429.1437
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Frequencies --	3016.4352	3103.7927	3105.6003
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Frequencies --	3181.0926	3182.6681	3192.2971
Frequencies --	3199.0465	3208.9658	3223.8367

proximal conformation

vacuum	toluene-like solvent	D3 dispersion
-3273.3540006	-3273.3659841	-0.62568555

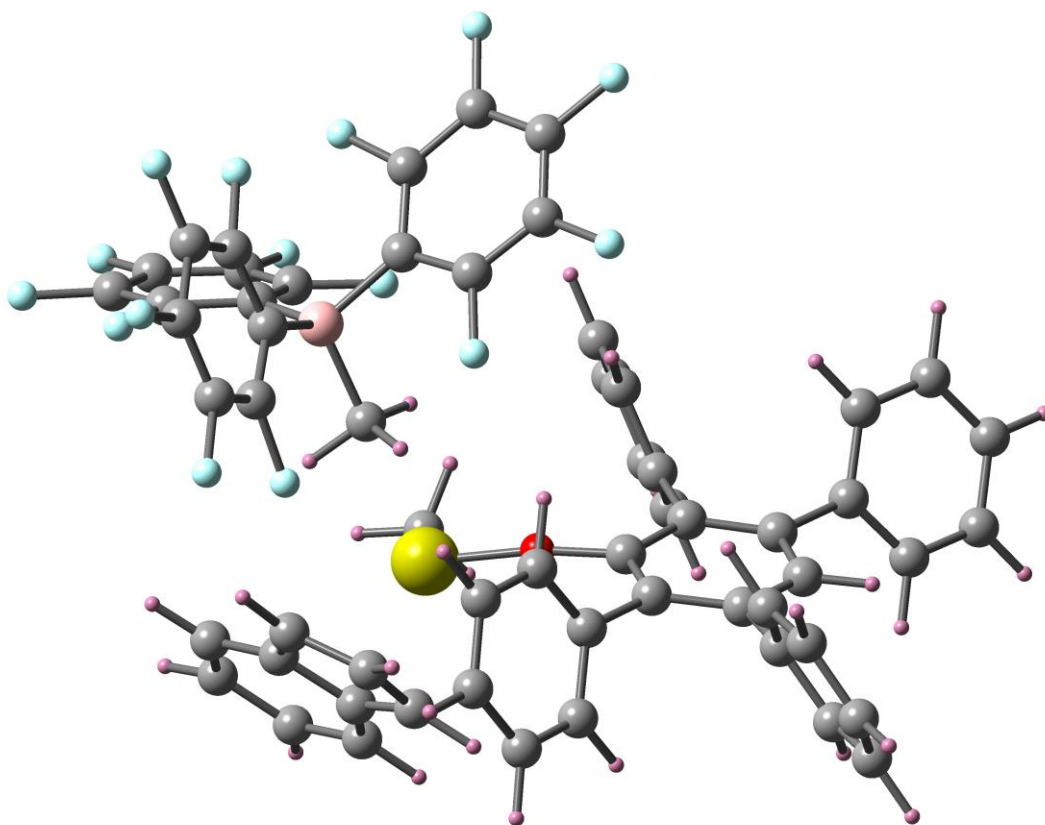
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H	-3.34326900	-1.68694700	2.29246600
H	-1.69485400	-2.31657500	2.64111100
O	-2.77666800	-0.13940400	-0.49241500
C	-3.41927900	0.85102900	-1.22882400
C	-4.61016400	1.46980900	-0.74116400
C	-2.86061900	1.21765000	-2.47994900
C	-5.23302200	2.42508000	-1.58760300
C	-3.49235600	2.18418800	-3.28276500
C	-4.69351000	2.78119600	-2.83996100
H	-6.13998700	2.91696600	-1.23262100
H	-3.04932200	2.46710700	-4.23955000
C	-2.13626900	-3.00928200	-1.84826200
C	-1.01809300	-3.58589300	-1.12894500
C	-3.31033300	-3.12601400	-1.01031000
C	-1.49871300	-4.05951400	0.14819400
C	-2.91379200	-3.78397200	0.22412900

F	-0.04335600	5.98802700	-0.18477300
C	0.41835600	4.68291600	-0.09570200
C	1.51180300	4.25362100	-0.86460200
C	-0.19337300	3.76411100	0.77184000
C	1.95847000	2.91938900	-0.76445200
F	2.14687800	5.15038600	-1.71593100
C	0.29341100	2.44686100	0.83212300
F	-1.27280900	4.15963000	1.55846900
C	1.36682300	1.93719600	0.06452600
F	3.08277100	2.61857500	-1.54260600
F	-0.35489100	1.62205900	1.77583000
B	1.83009600	0.33624800	0.14512600
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C	0.39283400	-0.60193700	0.06832400
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C	2.24525500	-0.24543900	-2.45984000
C	3.06604000	0.90278800	2.52296400
C	2.73187400	-1.37556700	2.02424400
H	-0.20602900	-0.11738200	-0.71537300
H	0.70215200	-1.61910900	-0.17925700
H	-0.04379600	-0.51864900	1.07255000
C	4.94890600	-0.74979600	-2.20822400
F	4.87969800	-0.17859700	0.08708000
C	2.97557300	-0.64003300	-3.59445000
F	0.88271000	0.04167900	-2.70813100
C	3.64256200	0.56650600	3.76541700
F	3.04870400	2.27178600	2.23533000
C	3.30131500	-1.76778300	3.24840500
F	2.35277500	-2.44193500	1.17861000
C	4.34872400	-0.90415900	-3.46818800
F	6.31038600	-0.98638800	-2.06342300
F	2.35140000	-0.77095000	-4.83338400
C	3.75800200	-0.78213800	4.13832000
F	4.10552600	1.55768300	4.62235800
F	3.41920600	-3.11477600	3.58131900
F	5.09574800	-1.30339100	-4.56690000
F	4.31862900	-1.13586400	5.35706000
C	-3.86015400	-4.28791000	1.28735000
H	-4.77137600	-3.67951200	1.35694800
H	-4.17277000	-5.31768500	1.04113800
H	-3.40028800	-4.31795900	2.28308100
C	-4.73224400	-2.79840200	-1.40662100
H	-5.23038800	-3.70678300	-1.78764500
H	-5.32801500	-2.43009100	-0.56041800
H	-4.78051300	-2.04155700	-2.19917800
C	-0.67806700	-4.80527000	1.17485500
H	-1.12887000	-4.76658600	2.17465800
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C	0.35651100	-3.84372200	-1.70437400
H	1.13843700	-3.88467700	-0.93579300
H	0.35486400	-4.82277200	-2.21476100
H	0.64935800	-3.09466800	-2.45016200
C	-2.09826900	-2.53072700	-3.28216600
H	-2.17414900	-3.39683600	-3.96254500
H	-2.93129700	-1.85838200	-3.52086800

H	-1.16296000	-2.01011700	-3.52983200
H	-1.93524300	0.74809000	-2.81029000
H	-5.19401000	3.53208400	-3.45384800
C	-5.20515100	1.19212500	0.60720300
C	-4.48255600	1.47248900	1.79655700
C	-6.54254300	0.72894700	0.72240400
C	-5.08135300	1.29596300	3.06136000
H	-3.46445800	1.85792300	1.73354700
C	-7.13912100	0.54107100	1.98773700
H	-7.11583000	0.51174800	-0.18177800
C	-6.40992600	0.82645800	3.16335000
H	-4.51346700	1.53469000	3.96356900
H	-8.16892100	0.18196200	2.05373800
H	-6.87231200	0.69378300	4.14407500

Frequencies --	7.7461	11.7983	12.3823
Frequencies --	16.3378	20.5082	25.4906
Frequencies --	28.1619	29.4661	30.3087
Frequencies --	35.3867	39.1274	40.5669
Frequencies --	44.5527	54.4601	61.4821
Frequencies --	70.4921	86.9654	90.0311
Frequencies --	90.8664	103.2498	104.8692
Frequencies --	107.2058	117.4478	118.1089
Frequencies --	118.9516	122.8630	123.5223
Frequencies --	127.6795	135.1574	135.5927
Frequencies --	140.1948	141.8873	152.0766
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Frequencies --	160.5087	161.0658	165.9811
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Frequencies --	208.0775	210.8014	216.3716
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Frequencies --	319.2067	330.6567	333.5892
Frequencies --	336.5655	344.2633	348.6399
Frequencies --	360.0390	378.8346	379.0793
Frequencies --	379.4732	387.1417	390.5483
Frequencies --	392.5743	394.9139	406.9081
Frequencies --	418.2878	432.5900	433.0075
Frequencies --	433.1168	451.5079	456.1789
Frequencies --	457.5462	472.6059	473.5531
Frequencies --	499.5599	518.6670	531.8952
Frequencies --	536.7941	541.3931	542.1247
Frequencies --	547.9813	548.8647	556.7487
Frequencies --	562.3012	581.4004	583.3728
Frequencies --	592.5233	595.6668	604.9636
Frequencies --	613.7595	616.2907	620.5866
Frequencies --	630.3330	638.3208	638.9453
Frequencies --	641.7370	649.8568	660.8467
Frequencies --	662.9110	694.6223	698.0665
Frequencies --	712.4768	727.9276	728.2283
Frequencies --	739.5130	741.8194	743.8226
Frequencies --	757.4168	758.1344	767.4683
Frequencies --	770.4420	780.2040	802.9444
Frequencies --	805.6049	842.7166	856.1540
Frequencies --	866.0797	869.1475	878.2054
Frequencies --	906.8473	907.5761	909.7199

Frequencies --	922.3779	937.7556	962.2826
Frequencies --	970.9836	974.2373	990.3272
Frequencies --	994.9739	999.3008	1008.1981
Frequencies --	1008.8786	1023.7405	1024.3681
Frequencies --	1035.6445	1042.1445	1044.0780
Frequencies --	1046.0465	1046.8640	1048.0487
Frequencies --	1049.2711	1049.4602	1050.5949
Frequencies --	1051.5173	1062.4340	1072.9660
Frequencies --	1089.9635	1090.8276	1091.8839
Frequencies --	1098.2165	1126.6476	1128.2965
Frequencies --	1137.4574	1173.1300	1175.7132
Frequencies --	1184.5242	1188.1855	1195.3163
Frequencies --	1208.0890	1213.8466	1214.6958
Frequencies --	1215.4577	1220.7726	1267.1004
Frequencies --	1301.5984	1320.1791	1320.4492
Frequencies --	1326.0436	1334.5060	1339.3224
Frequencies --	1342.9055	1343.5158	1356.7290
Frequencies --	1370.3104	1413.6681	1414.9683
Frequencies --	1417.6849	1418.6937	1419.1650
Frequencies --	1424.2154	1427.5532	1428.2653
Frequencies --	1429.8867	1432.3801	1434.7122
Frequencies --	1436.4728	1443.0720	1448.4562
Frequencies --	1451.0058	1455.4970	1460.5622
Frequencies --	1467.8524	1469.5790	1469.7252
Frequencies --	1471.6751	1479.4441	1481.1640
Frequencies --	1482.1017	1492.9062	1495.2863
Frequencies --	1500.5395	1501.7048	1506.8373
Frequencies --	1507.8090	1508.7261	1513.4555
Frequencies --	1517.4625	1519.3641	1578.6288
Frequencies --	1595.7754	1595.9303	1597.2031
Frequencies --	1597.3900	1610.6515	1620.4181
Frequencies --	1620.5025	1622.2938	1624.0326
Frequencies --	2998.0767	3008.4622	3011.4521
Frequencies --	3011.6823	3013.1698	3014.4886
Frequencies --	3015.5467	3102.6168	3105.2233
Frequencies --	3105.9988	3107.6469	3112.3357
Frequencies --	3118.0624	3141.5204	3144.7004
Frequencies --	3145.1539	3147.0771	3150.4638
Frequencies --	3152.9649	3154.4211	3159.9800
Frequencies --	3163.3370	3169.2661	3175.3468
Frequencies --	3181.2692	3189.1358	3197.6124
Frequencies --	3203.0972	3203.3195	3216.8707

Catalyst 22:

vacuum	toluene-like solvent	D3 dispersion
-3923.278477	-3923.2957256	-0.83374868

Ti	0.33506400	-0.21389100	2.16690200
C	0.08034700	-2.23742600	2.49899600
H	-0.03959200	-2.69132000	1.50499900
H	0.99336300	-2.64086200	2.96129800
H	-0.78804600	-2.45989900	3.13349900
O	1.77946900	-0.18510100	1.13529300
C	3.01078500	-0.09358100	0.48017100
C	3.66792500	1.17569800	0.40090100
C	3.58408500	-1.30365800	-0.02681200
C	4.98477100	1.20753700	-0.15034400
C	4.90449000	-1.24184700	-0.56375600
C	5.57730000	0.00089200	-0.58619000
H	6.57226600	0.04278100	-1.02730000
F	-6.24213400	-4.10242100	1.73407700
C	-5.45449800	-3.10612900	1.17439700
C	-5.85141800	-1.76115200	1.23155300
C	-4.23160800	-3.42213900	0.55808400

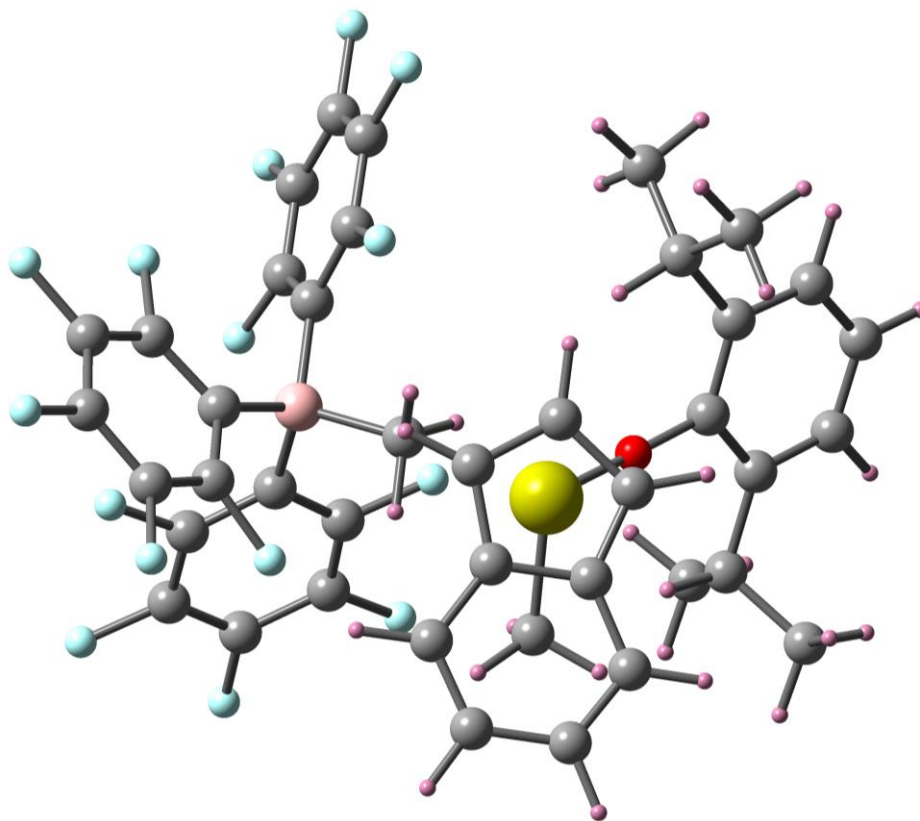
C	-5.03191600	-0.76383800	0.66030700
F	-7.04319300	-1.42115200	1.86294300
C	-3.45626700	-2.38917800	0.00528600
F	-3.80068900	-4.74405600	0.50931700
C	-3.81145700	-1.01873600	-0.00613600
F	-5.50540600	0.54633700	0.82118900
F	-2.23488700	-2.79322100	-0.56543700
B	-2.77754600	0.13835600	-0.61301100
C	-3.47070400	1.64994100	-0.74008900
C	-3.10556800	2.81431000	-0.03415500
C	-4.50479800	1.88246200	-1.68129600
C	-3.67191000	4.08921000	-0.23547700
F	-2.11260100	2.77208200	0.96682600
C	-5.11272400	3.12833000	-1.91799100
F	-5.00606800	0.81117100	-2.42732100
C	-4.68782800	4.25248200	-1.18884200
F	-3.23070100	5.18415600	0.50439700
F	-6.12833300	3.25894100	-2.85725300
F	-5.26305400	5.49633000	-1.40502000
C	-2.19102900	-0.19024600	-2.14728000
C	-1.08486300	0.52356300	-2.66382300
C	-2.73380300	-1.10896600	-3.07915400
C	-0.52439600	0.34191000	-3.94164900
C	-2.21133600	-1.33211400	-4.37048000
C	-1.09136900	-0.60623300	-4.80799000
F	-3.86674300	-1.86214900	-2.76907000
F	-2.79786300	-2.26314200	-5.21946500
F	-0.56015500	-0.81498100	-6.07277600
F	0.57722400	1.08962400	-4.35021100
F	-0.47295900	1.52892800	-1.88660300
C	-1.46599600	0.06230100	0.48908400
H	-0.79768500	0.91208000	0.29691400
H	-1.94680700	0.10762500	1.47941200
H	-1.00335200	-0.90741800	0.26526700
C	3.02250600	2.44657500	0.88357200
C	3.55367200	3.14718500	1.99734100
C	1.92964500	3.02016800	0.18394600
C	3.01475300	4.38755700	2.39781200
H	4.40368800	2.72969300	2.54011300
C	1.38923500	4.26248900	0.58118400
H	1.52064500	2.51352700	-0.68964000
C	1.93146100	4.95282100	1.68796600
H	3.44487800	4.91480000	3.25233300
H	0.55424900	4.69080900	0.02316200
H	1.51823200	5.91770400	1.98946300
C	5.78105600	2.47289700	-0.33541600
C	7.04378000	2.61793600	0.29624700
C	5.34044900	3.50603500	-1.20239600
C	7.83536600	3.76674900	0.08362600
H	7.40444000	1.83272400	0.96468500
C	6.13326600	4.65130500	-1.42321500
H	4.38463200	3.40920300	-1.71843600
C	7.38248200	4.78944900	-0.77840700
H	8.80053600	3.86070100	0.58708300
H	5.77763900	5.43052700	-2.10135600
H	7.99494600	5.67782000	-0.94884600
C	5.62444600	-2.42989100	-1.14611500

C	6.86503400	-2.84656900	-0.59643200
C	5.13559200	-3.10827800	-2.29222500
C	7.58759400	-3.91836600	-1.16281400
H	7.26140000	-2.33687500	0.28476400
C	5.85952500	-4.17439900	-2.86513400
H	4.19545300	-2.79513000	-2.74702800
C	7.08689400	-4.58740700	-2.30115200
H	8.53620400	-4.22768400	-0.71747500
H	5.46661300	-4.67789300	-3.75144000
H	7.64576000	-5.41498200	-2.74404700
C	2.83397600	-2.60755500	0.00293200
C	3.25732300	-3.67159300	0.83899800
C	1.73220200	-2.82667100	-0.86304400
C	2.60246800	-4.92068200	0.80730700
H	4.10906600	-3.52597500	1.50617700
C	1.07845200	-4.07621800	-0.90188700
H	1.40083000	-2.02546200	-1.52693400
C	1.51286100	-5.12892900	-0.06663600
H	2.94703800	-5.72947100	1.45583400
H	0.23546300	-4.22617600	-1.57903200
H	1.00757600	-6.09660100	-0.09690800
H	-3.06923200	-0.36142800	4.94027600
C	-2.02336600	-0.61542900	5.12245100
C	-0.97604800	0.14644200	4.52501800
C	-1.67883800	-1.66826400	5.97600200
C	0.41761700	-0.19698900	4.77391600
C	-0.99114900	1.31186200	3.66464700
C	-0.30527100	-1.99326700	6.23927600
H	-2.46310900	-2.25068300	6.46399600
C	0.73926900	-1.27904400	5.64412600
C	1.24243900	0.74641100	4.03058000
C	0.35672700	1.72313300	3.44345500
H	-1.87285200	1.83671900	3.31286400
H	-0.07934400	-2.81164600	6.92620500
H	1.77973800	-1.53313000	5.85480100
H	2.32280000	0.82994900	4.09375800
H	0.66141000	2.60543000	2.89500700

Frequencies --	1.6199	6.7225	11.1486
Frequencies --	12.7554	19.6192	21.6580
Frequencies --	26.5565	29.1485	30.1009
Frequencies --	31.3228	36.6591	37.5180
Frequencies --	38.6823	41.9742	44.8875
Frequencies --	45.8758	46.8521	48.6705
Frequencies --	58.7755	59.7658	64.3159
Frequencies --	69.7606	74.7660	77.6777
Frequencies --	80.7613	91.6251	99.2226
Frequencies --	101.3816	111.1614	113.5263
Frequencies --	115.0060	120.7189	124.3467
Frequencies --	125.1027	136.8783	139.5667
Frequencies --	141.2479	145.2524	147.6654
Frequencies --	155.4055	158.4608	160.8573
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Frequencies --	214.1101	218.2837	222.8644
Frequencies --	228.0453	233.4539	243.6164
Frequencies --	245.4698	249.6428	255.6958
Frequencies --	263.9836	264.2836	264.3885
Frequencies --	268.4626	270.9073	273.8259

Frequencies --	274.7805	280.7716	287.5099
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Frequencies --	327.3160	334.6565	336.0782
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Frequencies --	547.9196	549.1870	566.8721
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Frequencies --	713.2768	717.4538	717.6554
Frequencies --	730.9004	737.8944	741.4339
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Frequencies --	769.8896	770.7686	773.3852
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Frequencies --	857.7734	858.8370	859.3939
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Frequencies --	871.3116	876.8241	880.8386
Frequencies --	884.8194	895.9265	901.8793
Frequencies --	913.0350	914.7822	916.3011
Frequencies --	935.0369	936.3764	939.7525
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Frequencies --	995.1929	995.8416	1005.2621
Frequencies --	1005.8540	1007.3230	1008.9569
Frequencies --	1010.3149	1012.3282	1013.9489
Frequencies --	1016.0070	1019.3524	1019.8809
Frequencies --	1026.9876	1028.3193	1038.0434
Frequencies --	1044.7824	1048.2848	1050.2219
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Frequencies --	1054.8116	1059.8044	1078.3827
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Frequencies --	1126.2343	1128.8840	1139.2473
Frequencies --	1150.3936	1182.1771	1183.6412
Frequencies --	1183.7463	1186.0207	1186.3725
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Frequencies --	1207.5182	1209.3748	1210.8409
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Frequencies --	1232.6806	1242.5776	1255.3656
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Frequencies --	1325.4785	1328.8945	1331.8952
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Frequencies --	1345.2797	1349.2636	1359.9080
Frequencies --	1366.7389	1367.7234	1369.7522
Frequencies --	1370.7664	1373.8191	1378.7038

Frequencies --	1412.7206	1419.0040	1420.0661
Frequencies --	1421.1856	1423.1830	1428.7908
Frequencies --	1432.8247	1441.4378	1443.1050
Frequencies --	1445.7331	1447.0800	1456.9399
Frequencies --	1457.4732	1467.6749	1467.9154
Frequencies --	1468.9129	1471.2383	1478.6782
Frequencies --	1496.4372	1496.8789	1498.2225
Frequencies --	1502.1524	1508.9103	1526.6331
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Frequencies --	3018.8113	3123.2502	3143.6568
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Frequencies --	3165.2234	3170.1899	3172.7751
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Frequencies --	3198.9248	3199.4232	3210.6797
Frequencies --	3251.0878	3262.1440	3299.0019

Catalyst 23:

vacuum	toluene-like solvent	D3 dispersion
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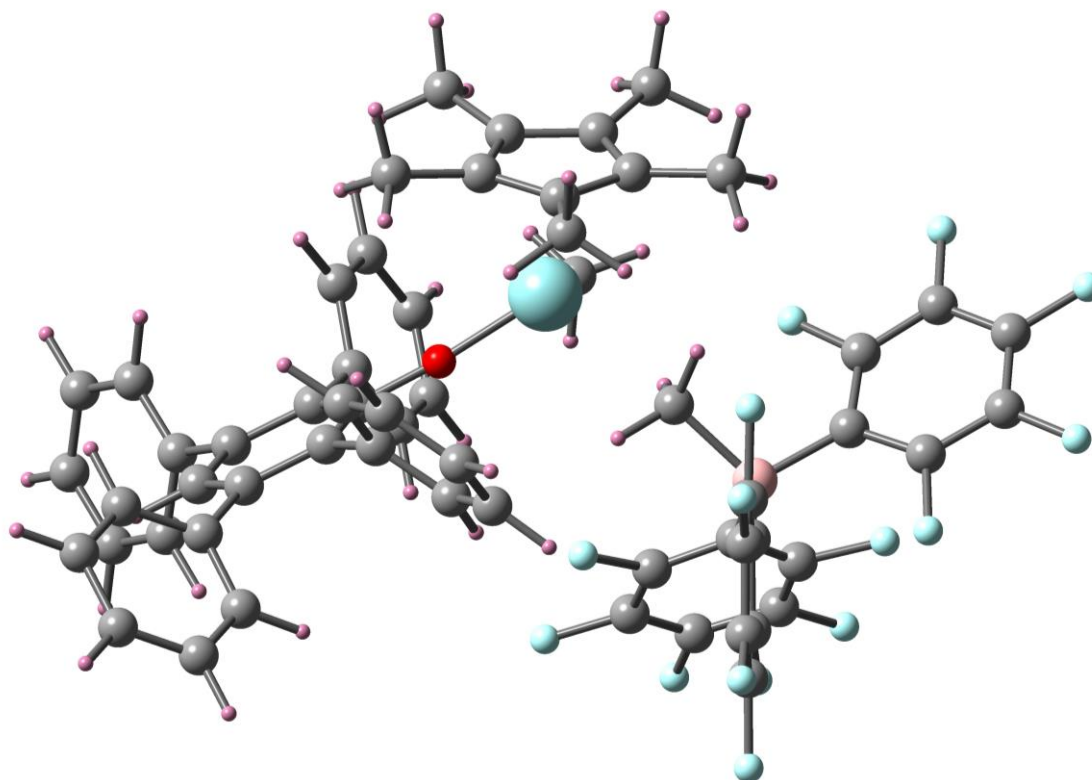
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H	3.03742500	2.70915200	1.74050900
H	1.32021900	3.18962500	1.53567500
O	3.17251200	0.10386300	-0.12254000
C	4.15811700	-0.89399900	-0.07293900
C	4.38543700	-1.71613200	-1.22301400
C	4.89877300	-1.05276600	1.14241300
C	5.41787100	-2.67968100	-1.13665300
C	5.91114100	-2.03973100	1.16139600
C	6.17939100	-2.83922300	0.03538100
H	5.62128500	-3.31912200	-1.99578400
H	6.49288300	-2.18459900	2.07175000
H	6.96960600	-3.59156000	0.07453200
F	-1.57130600	-5.86407800	-2.13549400
C	-1.60961000	-4.58561200	-1.59855700
C	-2.11085800	-4.36396800	-0.30628600
C	-1.15334900	-3.48467100	-2.34122600

C	-2.14037800	-3.05489100	0.21792900
F	-2.58412400	-5.43616200	0.43988400
C	-1.19298000	-2.20315200	-1.76542000
F	-0.67016200	-3.67173900	-3.63364500
C	-1.67329100	-1.90861600	-0.46792900
F	-2.71110300	-2.94708100	1.49080100
F	-0.75080200	-1.15970200	-2.60855300
B	-1.68868000	-0.35691800	0.13592000
C	-1.92539300	-0.31781600	1.78671900
C	-0.93155000	-0.72711500	2.70740100
C	-3.11067300	0.12218900	2.42257300
C	-1.05461600	-0.67622100	4.10727600
F	0.28334200	-1.27551100	2.24247000
C	-3.28762800	0.19567700	3.81964500
F	-4.23118800	0.49314500	1.67015000
C	-2.24712000	-0.19976200	4.67510500
F	-0.01168200	-1.09443300	4.92954700
F	-4.48532200	0.64944200	4.35855900
F	-2.39585000	-0.13001500	6.05244100
C	3.55954800	-1.60818800	-2.51287000
H	2.75135600	-0.88502600	-2.34220100
C	4.62263400	-0.22193000	2.40322100
H	3.83511700	0.49839200	2.16722600
C	-2.78532900	0.60817900	-0.67139900
C	-2.73908300	2.01954600	-0.59795400
C	-3.84304500	0.14117600	-1.48789600
C	-3.59260300	2.89788800	-1.28815700
C	-4.73040700	0.97529800	-2.19990200
C	-4.60178400	2.37060700	-2.10943800
F	-4.10114500	-1.22768800	-1.61303600
F	-5.73671100	0.42921400	-2.98656000
F	-5.45667200	3.21029400	-2.80764700
F	-3.44363100	4.27858200	-1.16259400
F	-1.80506000	2.65280700	0.25138600
C	-0.12064400	0.30049100	-0.15162800
H	-0.12247700	1.22811900	0.44181300
H	0.57621800	-0.46129400	0.21132900
H	-0.07260100	0.46820900	-1.23465400
C	2.87425600	-2.95700600	-2.87730300
H	2.19938000	-2.82109100	-3.73563500
H	3.60906100	-3.72936900	-3.14888700
H	2.27953500	-3.34063800	-2.03491700
C	4.41651800	-1.08262900	-3.70298900
H	5.22432800	-1.78597800	-3.95540200
H	3.79036100	-0.96031200	-4.60160100
H	4.88245600	-0.11204000	-3.47121300
C	4.08405500	-1.11336300	3.56210400
H	4.82469500	-1.86341800	3.87922300
H	3.84121100	-0.48990400	4.43731000
H	3.16804900	-1.64433300	3.26244500
C	5.86964600	0.59637600	2.84886800
H	6.23413700	1.24420000	2.03519000
H	5.61250300	1.23711500	3.70758000
H	6.70220000	-0.05374300	3.15789600
C	3.54233400	4.73518700	-0.43185800
C	2.84405800	3.75012100	-1.19182700
C	2.81492200	5.79732000	0.11215200

H	4.62406800	4.67256400	-0.29984600
C	1.40336800	3.86273700	-1.38245400
C	3.29449700	2.56952300	-1.91477000
C	1.39252300	5.89694900	-0.06113200
H	3.33344600	6.57634300	0.67512200
C	0.67979400	4.94076000	-0.78976700
C	0.99091700	2.77034300	-2.23832900
C	2.15671100	2.04257200	-2.62746900
H	4.32818800	2.26812500	-2.05359000
H	0.86456900	6.74444200	0.38079200
H	-0.39926900	5.02526800	-0.92023800
H	-0.01830400	2.59073100	-2.59573200
H	2.17515500	1.21772400	-3.33241700

Frequencies --	-2.6514	8.9363	12.8143
Frequencies --	16.1733	20.1556	25.1046
Frequencies --	28.8115	30.9435	32.1696
Frequencies --	34.1003	38.6117	39.8297
Frequencies --	46.6471	48.8089	56.2246
Frequencies --	63.1332	67.6498	79.2563
Frequencies --	93.3835	101.8142	105.7701
Frequencies --	107.2581	115.8803	118.2940
Frequencies --	120.4155	123.2970	125.4290
Frequencies --	134.9586	140.7349	148.5051
Frequencies --	152.5622	153.6351	157.9627
Frequencies --	158.2543	161.1381	162.7811
Frequencies --	187.1517	210.0239	212.3936
Frequencies --	216.0356	218.5791	219.7129
Frequencies --	232.8547	237.3687	238.9459
Frequencies --	246.5412	249.3721	258.8898
Frequencies --	262.6826	264.7979	265.3521
Frequencies --	265.4626	271.4201	273.6723
Frequencies --	275.7975	278.8393	283.2488
Frequencies --	290.5662	292.4482	295.4314
Frequencies --	308.1531	309.4571	312.2188
Frequencies --	317.0348	318.4403	330.9882
Frequencies --	332.9434	338.4495	341.4127
Frequencies --	351.1280	375.7217	378.7920
Frequencies --	379.2118	381.0551	387.6398
Frequencies --	390.7624	393.6630	423.6460
Frequencies --	427.5915	431.7333	432.3098
Frequencies --	433.0062	434.4463	442.3934
Frequencies --	454.7722	456.5225	457.2799
Frequencies --	474.5070	519.6930	535.8162
Frequencies --	538.2237	541.1545	541.7470
Frequencies --	544.1553	545.5096	547.8316
Frequencies --	564.1814	584.6427	593.0483
Frequencies --	596.2094	599.0093	599.2910
Frequencies --	609.2990	629.9303	630.4308
Frequencies --	639.1458	640.2519	643.4179
Frequencies --	659.5814	662.9290	673.3246
Frequencies --	692.9191	726.9963	728.2749
Frequencies --	728.8158	736.9385	741.0023
Frequencies --	742.2381	758.6797	760.3055
Frequencies --	763.5269	770.5184	772.1127
Frequencies --	796.1250	805.1408	817.6444
Frequencies --	819.9929	836.5190	856.4933
Frequencies --	863.5265	870.4098	877.1313
Frequencies --	878.5658	883.5056	886.7994
Frequencies --	906.6735	908.6776	910.8004
Frequencies --	924.6332	930.5550	933.0677

Frequencies --	937.8003	939.7243	961.5118
Frequencies --	963.2814	980.2909	993.1709
Frequencies --	1009.6386	1010.5656	1012.9830
Frequencies --	1024.0301	1025.9319	1046.6906
Frequencies --	1048.8339	1050.7764	1055.6386
Frequencies --	1058.9173	1068.3478	1072.9525
Frequencies --	1073.3434	1096.6032	1113.6576
Frequencies --	1116.1352	1117.3802	1120.1887
Frequencies --	1140.4151	1166.8218	1178.7415
Frequencies --	1183.5445	1185.0105	1187.8317
Frequencies --	1204.2002	1208.1419	1214.4465
Frequencies --	1215.1933	1216.3614	1244.1758
Frequencies --	1252.5392	1269.6572	1275.3867
Frequencies --	1310.0291	1319.7449	1320.8927
Frequencies --	1325.0028	1325.8989	1328.7500
Frequencies --	1336.0199	1338.5697	1342.1126
Frequencies --	1343.3415	1362.2967	1372.8990
Frequencies --	1384.2809	1399.7201	1400.3203
Frequencies --	1415.8943	1416.9783	1417.7793
Frequencies --	1418.8686	1418.9066	1421.8032
Frequencies --	1423.0536	1430.2961	1436.5575
Frequencies --	1439.1927	1460.6074	1467.2909
Frequencies --	1468.8974	1469.7417	1470.0356
Frequencies --	1471.9619	1473.9501	1486.3990
Frequencies --	1487.4917	1488.6297	1492.1917
Frequencies --	1498.8712	1499.6758	1503.6418
Frequencies --	1506.3155	1508.9424	1561.4057
Frequencies --	1594.9463	1595.3712	1596.7505
Frequencies --	1597.1646	1604.4875	1620.2245
Frequencies --	1620.9535	1622.6607	1627.6925
Frequencies --	2993.4505	3001.6408	3006.9502
Frequencies --	3007.6230	3013.1897	3019.3098
Frequencies --	3077.4470	3105.9064	3108.9474
Frequencies --	3112.2040	3113.8365	3116.4179
Frequencies --	3124.5015	3124.8159	3128.4318
Frequencies --	3129.9197	3136.3947	3151.6157
Frequencies --	3161.2757	3166.8491	3167.1825
Frequencies --	3178.1658	3178.2605	3188.8120
Frequencies --	3192.9525	3201.3255	3207.2748
Frequencies --	3243.5401	3249.4949	3271.4472

Catalyst 24:

vacuum	toluene-like solvent	bromobenzene-like solvent	1,2-dichlorobenzene-like solvent	D3 dispersion
-3954.663659	-3954.675539*	-3954.6874613	-3954.6918592	-0.8671433

* estimated LANL2DZ energy using the solvation energy calculated with 6-311++G** basis sets (because the PCM calculation did not converge with LANL2DZ basis sets)

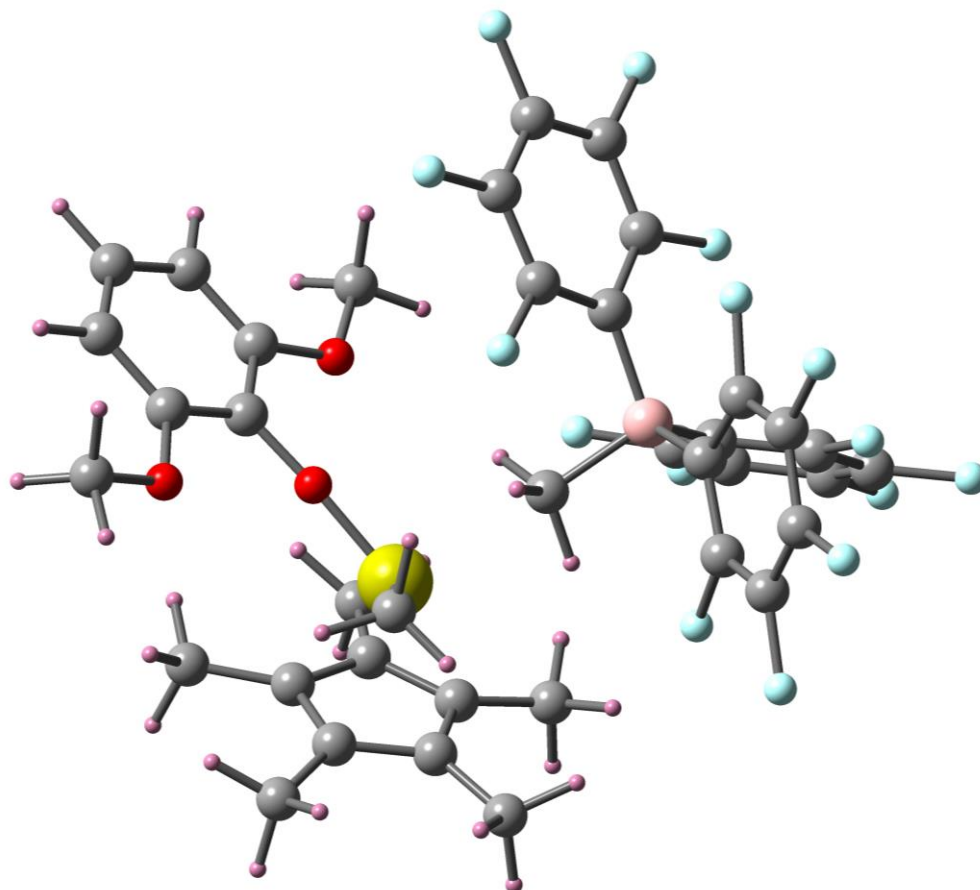
C	-0.14710600	-3.05753100	-1.13779600
H	-0.28049300	-3.00003600	-0.04209300
H	-0.93635700	-3.71535700	-1.52835400
H	0.83147100	-3.51139500	-1.35516100
O	-1.94130300	-0.40473600	-0.93578200
C	-3.16003100	0.00765300	-0.38685300
C	-3.48336400	1.40208800	-0.36397800
C	-4.03822900	-0.98901800	0.14466000
C	-4.74363100	1.79467800	0.18268300
C	-5.29468000	-0.57120300	0.67513000
C	-5.62132400	0.80186700	0.67077500
H	-6.57596800	1.11135700	1.09414500
C	0.17103100	0.15203900	-4.08825000
C	1.15167100	-0.91546800	-4.01779700
C	-1.14335800	-0.45383800	-4.17893500
C	0.44817400	-2.17613300	-4.06442200
C	-0.96914600	-1.89337000	-4.14973800
F	7.99398100	-2.23903700	-1.54085400
C	6.84069700	-1.70248800	-0.98708700
C	6.87926100	-0.48955800	-0.28062600

C	5.60985200	-2.36489100	-1.11441200
C	5.69259100	0.03967600	0.26592100
F	8.09017000	0.17328200	-0.12042100
C	4.45750900	-1.79046400	-0.54788000
F	5.53738100	-3.57582000	-1.80008700
C	4.41595500	-0.56127300	0.14724800
F	5.86092300	1.22083600	0.99683500
F	3.28311600	-2.55894500	-0.69576300
B	3.00129400	0.08615900	0.75677500
C	3.15460300	1.73378900	0.94750800
C	3.28313100	2.59431600	-0.16682000
C	3.20211700	2.41983400	2.18351700
C	3.42902300	3.99068000	-0.09665100
F	3.30000500	2.05748400	-1.47156800
C	3.33962200	3.81756300	2.31170300
F	3.14789100	1.72110500	3.39419600
C	3.45369800	4.61463800	1.16127100
F	3.53702800	4.75715800	-1.25471600
F	3.37349900	4.41462600	3.56635100
F	3.58492500	5.99264900	1.26347100
C	2.52600400	-0.68707700	2.16052700
C	1.20581900	-0.59017500	2.66041300
C	3.34828900	-1.52306400	2.95255600
C	0.71376000	-1.26876200	3.78885600
C	2.90881900	-2.22453800	4.09507500
C	1.57503200	-2.10577900	4.51621300
F	4.70437800	-1.68907300	2.65108600
F	3.78512700	-3.03225100	4.80989800
F	1.11687300	-2.79560700	5.62970600
F	-0.61489600	-1.12484600	4.18463700
F	0.27292100	0.26138200	2.03105700
C	1.74787600	-0.17573500	-0.38662000
H	0.96224000	0.55663000	-0.15220800
H	2.17736600	-0.02731900	-1.38403900
H	1.44375800	-1.21783300	-0.19852700
C	-2.54048600	2.45682500	-0.87861800
C	-2.88718200	3.25336300	-2.00062300
C	-1.34431100	2.76646400	-0.18167600
C	-2.07401200	4.33137400	-2.40897600
H	-3.81390900	3.04622700	-2.53855700
C	-0.53316300	3.84944600	-0.58290200
H	-1.07520400	2.19291600	0.70634800
C	-0.89340600	4.63770400	-1.69734100
H	-2.37206400	4.94069000	-3.26558000
H	0.36323800	4.09257400	-0.01188500
H	-0.26894500	5.48186900	-1.99782800
C	-5.19659600	3.22691100	0.30753300
C	-6.38633400	3.65271400	-0.33917900
C	-4.51189200	4.15703400	1.13203400
C	-6.86744200	4.97045400	-0.18457200
H	-6.93397900	2.95123000	-0.97268600
C	-4.99485800	5.47218100	1.29513700
H	-3.60736400	3.85028200	1.65833200
C	-6.17221700	5.88719000	0.63409200
H	-7.78149900	5.27743400	-0.69863100
H	-4.45484100	6.16876700	1.94079600
H	-6.54423100	6.90667300	0.75969200

C	-6.29496600	-1.51520100	1.29501600
C	-7.07215100	-2.40634500	0.51237100
C	-6.53300500	-1.46652700	2.69322400
C	-8.05156000	-3.22885300	1.10841200
H	-6.92214500	-2.44839600	-0.56772200
C	-7.50600800	-2.29362300	3.29360300
H	-5.94788100	-0.78490900	3.31438400
C	-8.27038800	-3.17913900	2.50270900
H	-8.64281500	-3.90413400	0.48516400
H	-7.66541100	-2.24534800	4.37343300
H	-9.02630700	-3.81815200	2.96510400
C	-3.64153000	-2.43989500	0.25194800
C	-3.95697300	-3.38052700	-0.75836500
C	-3.02502400	-2.90912200	1.44078400
C	-3.68637400	-4.75469500	-0.58253800
H	-4.44086600	-3.04136300	-1.67717200
C	-2.75105200	-4.28153300	1.62017200
H	-2.77788000	-2.20266300	2.23621700
C	-3.08604600	-5.21108400	0.61105500
H	-3.95667400	-5.46623000	-1.36690400
H	-2.28798000	-4.62298300	2.54892600
H	-2.88552500	-6.27517100	0.75508700
C	1.09229900	-3.53642600	-4.20439600
H	1.28099000	-3.74848100	-5.27151400
H	2.05841700	-3.59810100	-3.68608300
H	0.45454300	-4.34218100	-3.82019600
C	2.65486000	-0.74893900	-4.11473800
H	3.20068000	-1.54168900	-3.58712900
H	2.96072700	-0.79895900	-5.17421900
H	3.00111400	0.21759800	-3.72769200
C	0.48315500	1.62795100	-4.22503700
H	1.41483000	1.91221700	-3.71849100
H	0.60729100	1.87902400	-5.29324200
H	-0.31669600	2.26497100	-3.83171000
C	-2.44190300	0.26550000	-4.48253600
H	-3.30622700	-0.18141500	-3.97125000
H	-2.40068500	1.32377400	-4.20517600
H	-2.64302600	0.21551400	-5.56700000
C	-2.06335200	-2.91336100	-4.38251000
H	-3.04203900	-2.55881500	-4.03348800
H	-2.15705500	-3.11514200	-5.46415000
H	-1.85575900	-3.87167800	-3.88967600
Zr	-0.31208100	-0.96252900	-1.85882400
Frequencies --	6.0550	9.0843	12.3342
Frequencies --	15.0120	17.1668	21.7968
Frequencies --	23.9552	25.0681	27.2945
Frequencies --	27.6315	30.3400	32.4174
Frequencies --	38.3976	40.4702	42.9423
Frequencies --	45.7983	46.4200	48.6294
Frequencies --	53.8575	54.7626	63.4076
Frequencies --	65.0195	74.3805	78.1988
Frequencies --	80.2236	85.0431	85.2473
Frequencies --	103.0778	105.0419	106.4830
Frequencies --	116.8348	117.7248	118.0650
Frequencies --	118.6344	123.7461	125.4969
Frequencies --	127.3265	129.6259	130.6123
Frequencies --	138.5315	139.8743	144.8962

Frequencies --	150.4483	150.9497	152.5946
Frequencies --	157.4374	158.2719	160.6130
Frequencies --	161.3523	162.8413	176.1445
Frequencies --	180.8001	189.0681	193.4809
Frequencies --	209.5809	210.8323	213.6552
Frequencies --	214.3694	219.0431	220.5930
Frequencies --	230.2540	234.2568	248.1835
Frequencies --	255.3031	256.3852	264.3590
Frequencies --	264.8621	265.0784	267.9741
Frequencies --	270.0408	272.5515	285.6035
Frequencies --	287.1336	288.8014	289.6167
Frequencies --	290.3868	296.4464	301.3556
Frequencies --	310.9399	315.7587	316.1962
Frequencies --	317.1903	330.0398	332.0145
Frequencies --	333.2027	335.2864	344.2157
Frequencies --	350.7469	378.8767	380.2335
Frequencies --	382.1424	386.4911	387.1686
Frequencies --	391.2255	397.1081	402.8369
Frequencies --	403.0445	406.7636	408.5697
Frequencies --	411.0783	414.9480	432.2013
Frequencies --	432.5984	433.0785	433.9196
Frequencies --	450.6013	456.6612	457.8628
Frequencies --	472.3366	490.4286	497.2053
Frequencies --	512.4444	528.5256	538.5005
Frequencies --	540.1618	541.9869	542.6516
Frequencies --	543.7397	548.4911	548.7196
Frequencies --	555.2681	565.6897	582.4471
Frequencies --	592.2703	592.7277	595.0702
Frequencies --	604.1634	614.5644	617.3847
Frequencies --	617.8891	620.8471	625.0354
Frequencies --	629.9946	635.2818	636.1862
Frequencies --	639.6958	640.4931	642.8800
Frequencies --	654.9171	660.6714	661.2678
Frequencies --	665.5525	688.3124	696.5378
Frequencies --	699.8469	709.6186	711.2710
Frequencies --	712.3546	717.2307	722.3554
Frequencies --	726.6730	728.0479	743.1520
Frequencies --	744.5642	759.4302	760.9737
Frequencies --	770.6070	773.1025	775.8758
Frequencies --	778.0712	795.9215	801.3959
Frequencies --	802.3319	807.6591	847.6064
Frequencies --	854.9137	857.6921	859.1082
Frequencies --	861.9712	868.8618	870.8252
Frequencies --	874.6731	907.9623	908.8884
Frequencies --	909.6536	910.8948	930.2826
Frequencies --	937.6264	940.8081	948.1078
Frequencies --	956.0587	969.4722	974.2506
Frequencies --	983.9208	987.8552	992.1563
Frequencies --	996.6968	998.6360	1004.4184
Frequencies --	1005.6838	1007.6514	1011.0482
Frequencies --	1012.2600	1015.2631	1021.1659
Frequencies --	1024.2146	1025.5416	1026.7761
Frequencies --	1040.5717	1043.0939	1044.7322
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Frequencies --	1049.6672	1050.0978	1050.7592
Frequencies --	1052.0304	1052.3097	1055.7890
Frequencies --	1056.7855	1074.9487	1087.0323
Frequencies --	1088.4270	1088.5407	1089.5542
Frequencies --	1090.7906	1091.1440	1104.6385
Frequencies --	1126.1351	1127.4517	1130.6980
Frequencies --	1160.6322	1171.5855	1175.3321
Frequencies --	1182.5741	1182.7628	1182.9835
Frequencies --	1184.3284	1202.9159	1204.7576

Frequencies --	1205.1974	1206.5319	1206.8220
Frequencies --	1213.5682	1215.0651	1215.8800
Frequencies --	1230.9262	1267.5582	1279.6579
Frequencies --	1305.6464	1319.5059	1323.5836
Frequencies --	1324.6529	1327.9295	1327.9503
Frequencies --	1329.1967	1330.4864	1333.8915
Frequencies --	1339.4258	1341.6493	1344.5676
Frequencies --	1366.1120	1367.8315	1369.2429
Frequencies --	1370.5273	1381.5944	1414.3990
Frequencies --	1417.2527	1418.7896	1419.4337
Frequencies --	1420.2226	1425.4393	1427.4599
Frequencies --	1428.5464	1428.9542	1435.7043
Frequencies --	1438.8381	1440.5257	1441.4472
Frequencies --	1443.3481	1443.6295	1447.1726
Frequencies --	1448.8318	1454.9599	1455.2101
Frequencies --	1459.1308	1468.2966	1469.4786
Frequencies --	1471.5078	1482.0001	1485.2493
Frequencies --	1486.9456	1493.8650	1495.6015
Frequencies --	1496.2190	1496.9191	1501.3701
Frequencies --	1502.2644	1503.1547	1507.9754
Frequencies --	1508.8402	1509.3086	1512.2854
Frequencies --	1515.2135	1519.6723	1529.2312
Frequencies --	1591.9732	1594.0885	1595.7333
Frequencies --	1595.8899	1596.9028	1597.0877
Frequencies --	1597.5971	1601.1412	1619.9289
Frequencies --	1620.3330	1622.0485	1623.4613
Frequencies --	1623.6855	1624.2957	1624.7796
Frequencies --	2984.9988	2996.6259	3010.8668
Frequencies --	3011.0835	3011.9239	3012.7233
Frequencies --	3016.5417	3100.4103	3104.7324
Frequencies --	3107.2002	3109.4462	3110.8721
Frequencies --	3112.4419	3120.6403	3141.3746
Frequencies --	3147.0345	3148.4750	3151.9135
Frequencies --	3152.5421	3153.0063	3155.7299
Frequencies --	3156.4622	3158.0404	3159.3562
Frequencies --	3159.7870	3160.5768	3162.3881
Frequencies --	3166.4345	3169.1711	3172.2983
Frequencies --	3172.6577	3172.6907	3176.9922
Frequencies --	3181.4109	3184.2269	3185.2540
Frequencies --	3186.8365	3191.6190	3192.4022
Frequencies --	3193.3664	3197.3256	3209.9971

Catalyst 30:

vacuum	toluene-like solvent	D3 dispersion
-3271.3511915	-3271.3620576	-0.58924176

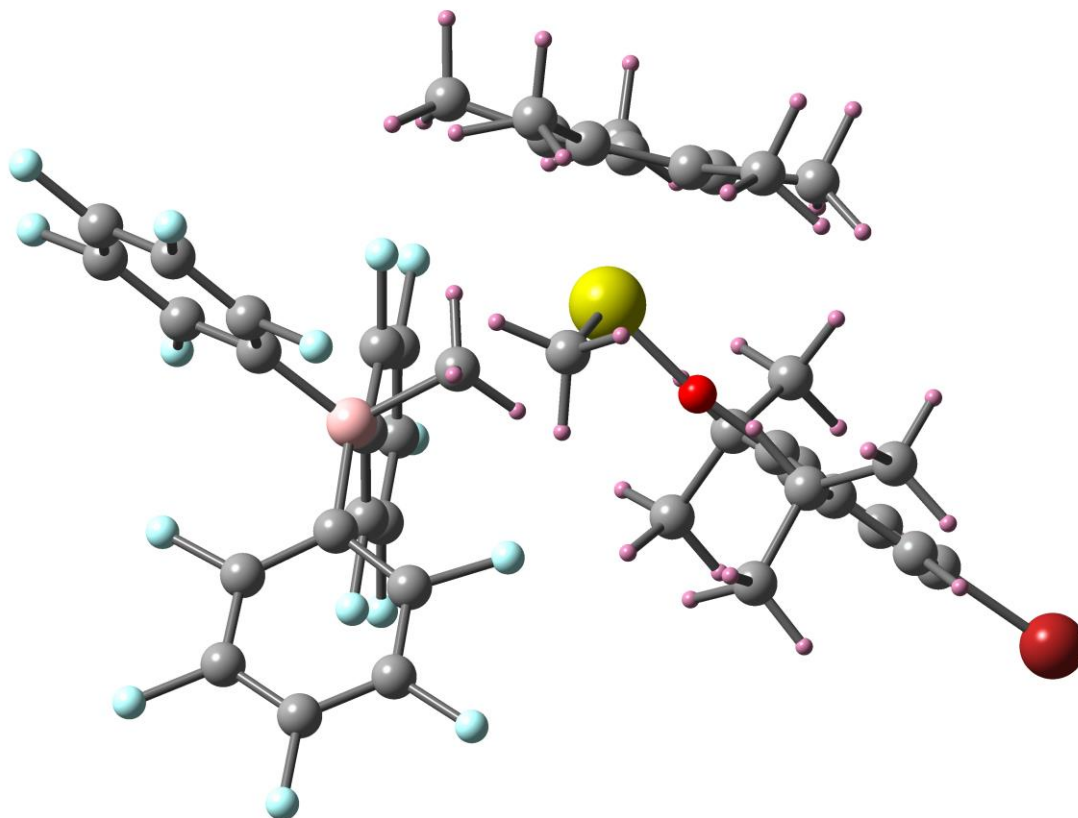
Ti	-2.11248200	-1.56249600	0.11484300
C	-2.17204400	-1.96903000	2.16298200
H	-1.84723900	-1.02069800	2.62724600
H	-3.20009000	-2.17025900	2.49481300
H	-1.50856000	-2.79091600	2.47152400
O	-3.11057300	-0.09599400	0.11569200
C	-3.94095700	0.98619700	-0.01194800
C	-3.69844800	1.94989200	-1.03810600
C	-5.02031900	1.17600900	0.90196200
C	-4.52553500	3.09250600	-1.14037700
C	-5.84005100	2.32353300	0.78861300
C	-5.58275800	3.26627900	-0.22594900
H	-4.34920200	3.84175200	-1.90886900
H	-6.66423000	2.49113400	1.47837800
H	-6.21486600	4.15277600	-0.30349400
C	-2.59104000	-2.57711900	-1.97071200
C	-1.43309500	-3.31069600	-1.49827800
C	-3.68569700	-2.84164800	-1.06160300

C	-1.80882400	-4.02233900	-0.30011200
C	-3.19843300	-3.73853100	-0.02835300
F	0.08699900	6.03104900	0.55625900
C	0.47487100	4.70021000	0.46804600
C	1.44542900	4.29646300	-0.46146600
C	-0.09269200	3.73132500	1.31179900
C	1.81994800	2.93828800	-0.53856700
F	2.03276300	5.24212300	-1.29650700
C	0.31324700	2.39138700	1.18836400
F	-1.04250000	4.10680500	2.25744900
C	1.26585400	1.90953700	0.25794900
F	2.82595800	2.66493200	-1.47448400
F	-0.27381800	1.50694100	2.11355100
B	1.63067600	0.28437800	0.14323100
C	2.53843700	-0.06436000	-1.21288400
C	2.37436100	-0.29323000	1.52254700
C	0.12715600	-0.53142100	0.02446300
C	3.92399100	-0.35513600	-1.20194400
C	1.98897700	-0.09077900	-2.51479400
C	2.96530800	0.50437000	2.53068800
C	2.47221500	-1.67747400	1.79408100
H	-0.46764300	0.01451300	-0.72193100
H	0.36280900	-1.55926500	-0.26875200
H	-0.28528600	-0.45272600	1.03931700
C	4.68143100	-0.68343600	-2.34544500
F	4.65926900	-0.29480400	-0.01300100
C	2.69538500	-0.40923900	-3.68791500
F	0.63674500	0.26084700	-2.72097100
C	3.54805800	-0.00373200	3.70981600
F	3.03947900	1.89488100	2.39139200
C	3.04373300	-2.23941700	2.94945300
F	2.01250000	-2.61829400	0.84506500
C	4.06199000	-0.71958100	-3.60456200
F	6.03874400	-0.96337400	-2.23977300
F	2.05354100	-0.41701700	-4.92544200
C	3.58300300	-1.39016600	3.92884000
F	4.09853800	0.85401400	4.65508300
F	3.08300900	-3.62040300	3.12698100
F	4.78466200	-1.04494500	-4.74368800
F	4.14767900	-1.91201600	5.08410600
C	-4.05526600	-4.41911400	1.01247800
H	-4.92244900	-3.80983700	1.30009500
H	-4.44402700	-5.36911800	0.60562700
H	-3.49661800	-4.66120900	1.92530400
C	-5.12348600	-2.41198900	-1.24381500
H	-5.68938400	-3.20687100	-1.76002300
H	-5.62455100	-2.21843500	-0.28579800
H	-5.20971800	-1.50204100	-1.85100000
C	-0.92441400	-4.97900500	0.46568100
H	-1.28497900	-5.15014200	1.48785600
H	-0.90536100	-5.96027600	-0.04039700
H	0.11509500	-4.63041600	0.53033500
C	-0.12580400	-3.47296100	-2.24111600
H	0.72597600	-3.63970900	-1.56908500
H	-0.19305800	-4.35582400	-2.90066400
H	0.10516400	-2.61234400	-2.87919900
C	-2.67301600	-1.79264300	-3.26049600

H	-2.96777400	-2.46364200	-4.08646000
H	-3.41426400	-0.98549200	-3.20907400
H	-1.71211300	-1.33908200	-3.53547900
O	-2.61628400	1.65888700	-1.87031800
O	-5.17887000	0.16728900	1.85595600
C	-2.22570700	2.63265100	-2.90154900
H	-1.97684200	3.60777600	-2.45296700
H	-1.33381100	2.19942600	-3.36746700
H	-3.02290300	2.75615500	-3.65295000
C	-6.17613300	0.35831800	2.91703700
H	-5.97407600	1.27591800	3.49275800
H	-7.19929600	0.38770500	2.50649400
H	-6.06379200	-0.51745100	3.56750300

Frequencies --	7.6005	14.6215	16.1900
Frequencies --	19.4163	23.1142	24.9575
Frequencies --	29.1133	30.9520	32.0345
Frequencies --	40.1076	41.1537	44.7085
Frequencies --	51.0765	63.4378	66.7788
Frequencies --	73.4269	86.0244	94.3290
Frequencies --	103.1143	104.5818	105.5985
Frequencies --	106.5945	109.1042	113.6853
Frequencies --	115.6929	118.2091	119.1917
Frequencies --	120.9103	122.2042	129.6208
Frequencies --	138.5684	151.7508	152.7543
Frequencies --	154.2036	157.3677	160.3864
Frequencies --	161.5865	163.4038	168.3005
Frequencies --	170.4927	177.0265	184.3287
Frequencies --	195.4786	198.1118	203.4081
Frequencies --	211.1534	217.6959	219.2597
Frequencies --	231.2576	239.9431	251.9113
Frequencies --	259.1224	264.5699	264.7365
Frequencies --	265.2013	266.9182	270.9068
Frequencies --	274.1145	278.5268	279.0295
Frequencies --	285.7755	287.7673	292.4093
Frequencies --	294.1782	297.5733	306.2712
Frequencies --	307.3519	314.3998	319.8772
Frequencies --	327.5565	331.0651	333.8518
Frequencies --	340.0299	347.7632	348.0565
Frequencies --	360.3590	378.6237	379.3772
Frequencies --	379.4328	379.8818	386.7294
Frequencies --	390.8630	392.6228	396.9082
Frequencies --	417.4669	432.2293	432.7169
Frequencies --	433.5164	452.5197	456.5142
Frequencies --	457.5099	472.9010	509.5707
Frequencies --	519.9055	532.3236	537.1060
Frequencies --	541.4472	542.0608	542.6993
Frequencies --	548.0614	556.0287	580.3671
Frequencies --	581.6977	585.1301	592.9588
Frequencies --	595.8194	596.8212	605.8119
Frequencies --	610.7745	618.4569	630.8617
Frequencies --	638.6080	639.6825	642.3163
Frequencies --	659.6851	661.5138	688.8645
Frequencies --	698.8069	725.2425	727.4220
Frequencies --	728.6009	729.1839	743.1024
Frequencies --	756.8788	758.3574	760.4901
Frequencies --	770.9051	802.6838	804.9084
Frequencies --	842.6501	848.1699	852.0643
Frequencies --	862.2083	866.6055	907.4192
Frequencies --	908.9519	911.2260	926.3127
Frequencies --	953.2945	969.6686	975.3625

Frequencies --	986.0500	1016.9288	1023.2087
Frequencies --	1024.5022	1043.7519	1044.4929
Frequencies --	1048.1888	1048.9444	1049.7171
Frequencies --	1050.7097	1051.0385	1052.2537
Frequencies --	1083.0418	1084.5608	1090.5727
Frequencies --	1091.8383	1097.3645	1099.5133
Frequencies --	1126.7477	1128.6391	1129.3896
Frequencies --	1158.9757	1168.3458	1173.7156
Frequencies --	1176.3310	1178.4239	1190.8351
Frequencies --	1208.8943	1213.5804	1214.2258
Frequencies --	1214.4657	1236.8150	1256.2892
Frequencies --	1295.9300	1319.3774	1320.8495
Frequencies --	1326.1186	1338.9395	1342.2526
Frequencies --	1344.3429	1375.1790	1410.8072
Frequencies --	1415.9437	1417.0970	1418.1456
Frequencies --	1419.4634	1423.3319	1426.7292
Frequencies --	1427.5094	1429.8379	1430.6689
Frequencies --	1436.5177	1442.8713	1446.6325
Frequencies --	1448.4106	1454.8544	1455.9964
Frequencies --	1461.1609	1468.2587	1469.3452
Frequencies --	1471.2382	1471.7463	1478.3199
Frequencies --	1479.3991	1479.8196	1481.3356
Frequencies --	1485.0180	1490.4855	1491.6320
Frequencies --	1493.7346	1494.3635	1495.9901
Frequencies --	1500.1246	1501.1062	1505.5640
Frequencies --	1508.1975	1513.4586	1517.8111
Frequencies --	1518.8814	1591.6760	1596.1111
Frequencies --	1597.6113	1597.7770	1606.2165
Frequencies --	1619.7362	1620.4707	1622.0618
Frequencies --	2992.3396	3000.7453	3004.6823
Frequencies --	3005.5356	3010.0266	3010.8505
Frequencies --	3011.4817	3013.2224	3015.9851
Frequencies --	3102.7329	3102.9104	3103.8630
Frequencies --	3105.8109	3106.2167	3109.4534
Frequencies --	3111.7177	3112.1676	3136.0371
Frequencies --	3142.6087	3145.3791	3146.7612
Frequencies --	3149.7047	3152.8263	3159.4031
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Frequencies --	3178.8133	3217.8002	3225.5078

Catalyst 31:

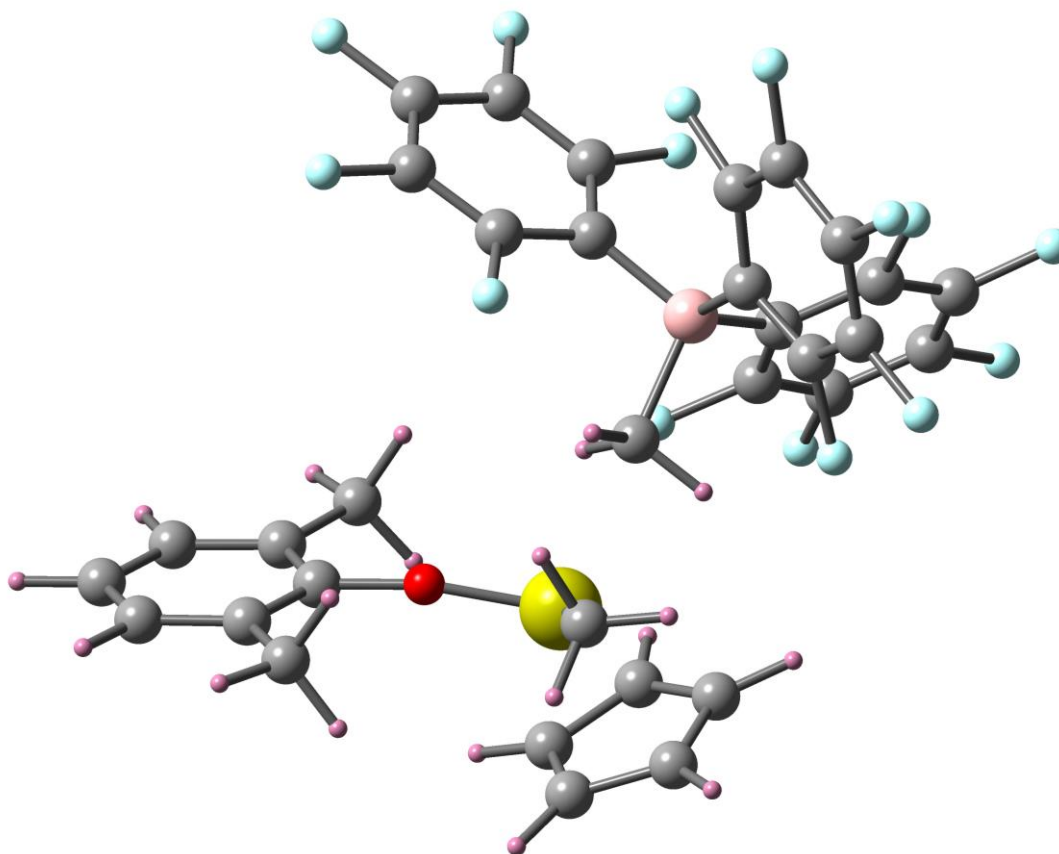
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C	0.78456700	2.66272200	1.95134500
H	0.89765000	1.71299700	2.50078600
H	1.52147200	3.38644900	2.32497400
H	-0.22569900	3.06576900	2.11740400
O	2.44119400	1.00601700	0.10387800
C	3.62891500	0.26931000	0.08483000
C	3.84195700	-0.69757100	-0.94901700
C	4.58955500	0.48307800	1.12595400
C	5.06437000	-1.40883100	-0.95003700
C	5.79501400	-0.25378500	1.07710300
C	6.02746000	-1.17458500	0.04335600
H	5.25302000	-2.15028700	-1.72320200
H	6.54266600	-0.11012200	1.85366900
C	0.82219000	3.10854900	-2.21660500
C	-0.19882800	3.75640100	-1.41287900
C	2.11343700	3.46761600	-1.67329800
C	0.46005900	4.51142100	-0.37599400
C	1.88687900	4.31992400	-0.52399100

F	-1.86176500	-4.14056800	-4.63762700
C	-1.96501400	-3.32482700	-3.51993000
C	-1.89775000	-3.86526800	-2.22684300
C	-2.12651100	-1.93626300	-3.65989900
C	-1.99543900	-3.01541600	-1.10350900
F	-1.72658600	-5.23479400	-2.06346500
C	-2.22125000	-1.13913000	-2.50748300
F	-2.19069100	-1.36777100	-4.92940800
C	-2.16738900	-1.61340100	-1.17484700
F	-1.90315200	-3.67088200	0.12956500
F	-2.41036500	0.23818300	-2.75166000
B	-2.23348300	-0.56070700	0.11843200
C	-2.11545200	-1.32853300	1.59778000
C	-0.93341400	-1.48158700	2.35544300
C	-3.24661800	-1.89829000	2.23364300
C	-0.85919400	-2.09107300	3.62311800
F	0.31022200	-1.04306300	1.85141800
C	-3.23061900	-2.52147800	3.49567400
F	-4.48359700	-1.91075500	1.57945700
C	-2.02289200	-2.61267000	4.20773800
F	0.35744600	-2.18261700	4.29487500
F	-4.39258500	-3.05411300	4.04052200
F	-1.97938600	-3.21649400	5.45575000
C	2.77772200	-1.05591700	-1.99742100
H	1.98256100	-0.29950400	-1.94913500
C	4.32390800	1.41157100	2.31983000
H	3.47420600	2.05208300	2.06133300
C	-3.62923000	0.36311400	0.13571700
C	-3.74748500	1.50183500	0.96530300
C	-4.80704100	0.10492200	-0.60652800
C	-4.87516600	2.34039800	1.03856100
C	-5.96283600	0.91143700	-0.57462700
C	-5.99952800	2.04677000	0.25126300
F	-4.90742600	-1.02835200	-1.41764100
F	-7.07328600	0.58843700	-1.34505700
F	-7.12437500	2.85787800	0.29416400
F	-4.88125500	3.45448100	1.87541800
F	-2.68494100	1.86542300	1.82163700
C	-0.90892000	0.50151500	-0.12027700
H	-0.85068000	1.07750600	0.81503100
H	-0.03457100	-0.13810000	-0.29118900
H	-1.17247800	1.11439700	-0.98754300
C	2.12829300	-2.43063200	-1.65306900
H	1.33317800	-2.66844100	-2.37583500
H	2.87107800	-3.24148500	-1.69329400
H	1.69119400	-2.42705000	-0.64378500
C	3.32198100	-1.05566500	-3.45450000
H	4.04523700	-1.86671700	-3.62507300
H	2.49270000	-1.20722800	-4.16349500
H	3.82056600	-0.10674100	-3.70509400
C	3.90415300	0.57386500	3.56696200
H	4.72299100	-0.08234700	3.90019100
H	3.64253500	1.24115700	4.40374400
H	3.03213700	-0.06049600	3.34981400
C	5.51735100	2.34933300	2.65526500
H	5.84208400	2.92546600	1.77423800
H	5.21849900	3.06277000	3.43976200

H	6.38970800	1.79745200	3.03595100
C	-0.21520200	5.46887600	0.57534900
H	-0.28583400	6.46606300	0.10666200
H	-1.23729200	5.15691100	0.82698900
H	0.33850300	5.59093200	1.51454400
C	-1.67775100	3.80816800	-1.72665300
H	-2.29702300	3.88081200	-0.82334400
H	-1.88911800	4.70531800	-2.33453700
H	-2.02143700	2.94198400	-2.30392800
C	0.57821700	2.34198800	-3.49730100
H	0.49817300	3.05171500	-4.33933500
H	1.39875300	1.65437300	-3.73721400
H	-0.35371500	1.76339800	-3.47935300
C	3.46074500	3.17614100	-2.29171400
H	3.44512600	2.28431200	-2.92864900
H	3.76512100	4.02592100	-2.92719200
H	4.24832700	3.03379200	-1.54003200
C	2.96651600	5.02956300	0.25938800
H	3.86980400	4.41628600	0.37796700
H	3.26800900	5.94825400	-0.27368400
H	2.62879800	5.33269200	1.25847300
Br	7.72376800	-2.16990000	-0.00141400

Frequencies --	7.6242	10.6024	15.7302
Frequencies --	18.8895	21.8114	25.8004
Frequencies --	26.6394	27.6765	33.5308
Frequencies --	34.7967	39.3279	45.5982
Frequencies --	46.3072	50.4294	58.1773
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Frequencies --	92.9547	96.4284	101.6298
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Frequencies --	154.4548	155.4673	157.0665
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Frequencies --	168.8930	177.5268	182.9491
Frequencies --	194.0123	214.3202	216.3051
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Frequencies --	224.2588	232.5871	245.4662
Frequencies --	251.0817	256.5047	258.4571
Frequencies --	262.8590	264.2188	264.3429
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Frequencies --	275.1778	279.7585	287.5883
Frequencies --	289.3539	291.4812	295.7969
Frequencies --	299.4148	299.5046	303.7688
Frequencies --	305.6283	307.3879	314.9975
Frequencies --	319.9828	323.8601	327.7002
Frequencies --	328.6110	333.9955	337.2406
Frequencies --	353.6888	366.0803	377.6939
Frequencies --	378.1324	379.7593	381.4260
Frequencies --	387.4927	397.1751	401.2102
Frequencies --	421.4557	427.1708	432.2651
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Frequencies --	444.5186	456.4187	457.3912
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Frequencies --	587.0881	591.4416	596.8327
Frequencies --	598.7112	608.6735	609.7425
Frequencies --	618.4749	625.4513	629.9423
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Frequencies --	653.1281	666.6118	696.0200
Frequencies --	698.7638	721.2119	729.6064
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Frequencies --	878.6511	896.2439	903.1462
Frequencies --	903.7790	910.8510	911.0090
Frequencies --	925.7668	931.0956	934.3883
Frequencies --	945.8851	963.7996	964.6421
Frequencies --	968.4085	972.6283	1008.0532
Frequencies --	1019.3917	1024.9904	1040.3675
Frequencies --	1042.1937	1044.6127	1045.8401
Frequencies --	1047.7423	1049.6065	1049.9614
Frequencies --	1052.6109	1066.4359	1070.9905
Frequencies --	1086.8414	1088.1586	1088.7126
Frequencies --	1090.0608	1110.5501	1116.3554
Frequencies --	1124.1853	1126.1428	1139.9686
Frequencies --	1169.3496	1173.0814	1175.9464
Frequencies --	1186.2149	1189.4489	1197.0386
Frequencies --	1213.5423	1214.4163	1215.6464
Frequencies --	1257.1824	1262.5784	1302.2943
Frequencies --	1316.8768	1317.4355	1321.6252
Frequencies --	1325.6254	1326.7943	1337.4622
Frequencies --	1338.9825	1341.1486	1346.2823
Frequencies --	1376.1390	1402.3741	1404.1391
Frequencies --	1412.8180	1414.1847	1415.5599
Frequencies --	1417.8920	1419.9219	1420.3373
Frequencies --	1421.9372	1424.8508	1427.1880
Frequencies --	1427.9436	1428.4184	1431.0857
Frequencies --	1435.2747	1437.1836	1442.2761
Frequencies --	1448.8583	1450.4592	1457.7406
Frequencies --	1461.0683	1468.7039	1469.4023
Frequencies --	1471.6557	1477.3164	1478.0439
Frequencies --	1483.2405	1486.4359	1487.8490
Frequencies --	1488.9424	1492.1481	1494.2580
Frequencies --	1496.3623	1500.7839	1502.2524
Frequencies --	1503.7752	1504.7057	1507.7199
Frequencies --	1508.7125	1509.5749	1511.6556
Frequencies --	1512.3044	1516.3940	1520.1636
Frequencies --	1575.7247	1586.5700	1595.4057
Frequencies --	1596.5948	1597.2862	1619.4146
Frequencies --	1620.4080	1622.1117	3002.1569
Frequencies --	3005.5589	3008.8413	3011.9740
Frequencies --	3013.0782	3013.5207	3013.9342
Frequencies --	3014.2662	3015.2944	3016.8939
Frequencies --	3019.6861	3070.7362	3103.5285
Frequencies --	3105.8372	3106.2512	3108.5545
Frequencies --	3109.9691	3110.2177	3113.0529
Frequencies --	3113.4418	3114.1270	3120.6257
Frequencies --	3123.3770	3125.2039	3128.6843
Frequencies --	3132.2267	3138.8784	3142.6352
Frequencies --	3144.8727	3146.9452	3151.5551
Frequencies --	3155.2628	3160.0841	3162.4227
Frequencies --	3181.8566	3216.7533	3219.0152

Catalyst 33:

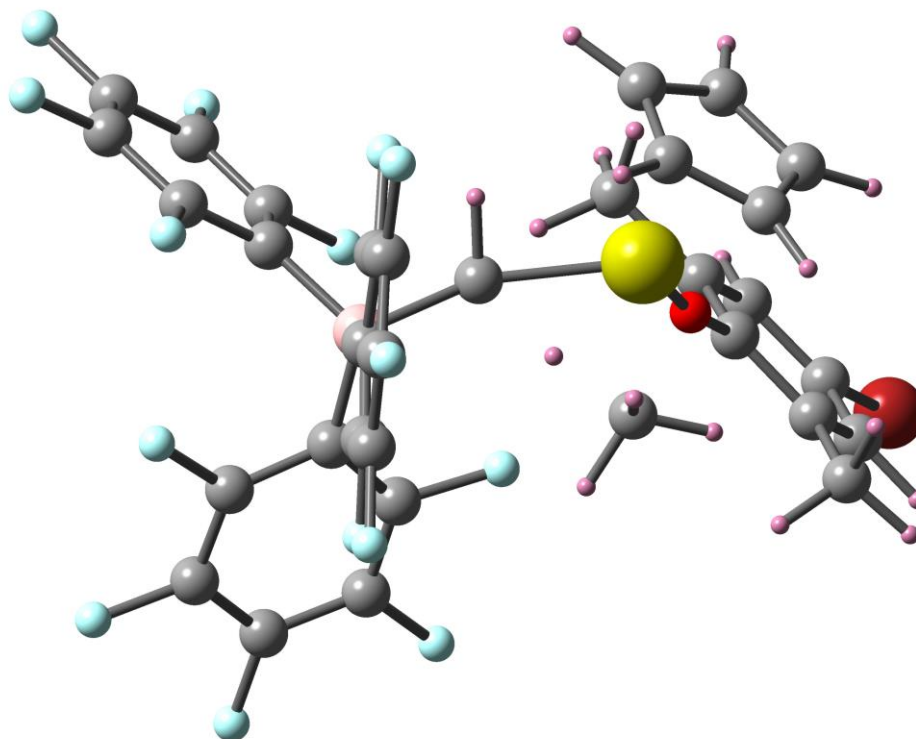
vacuum	toluene-like solvent	D3 dispersion	
-2924.520432	-2924.5333682	-0.48901926	
Ti	-2.21192500	-1.98396900	0.50932600
C	-2.05923800	-2.30730500	2.56254800
H	-2.05933300	-1.29043800	2.99508200
H	-2.89462000	-2.88032500	2.99065100
H	-1.11009100	-2.81501200	2.79953300
O	-3.50431400	-0.77578600	0.43543900
C	-4.64821200	-0.02560300	0.15340600
C	-4.75058000	0.63857900	-1.10534900
C	-5.65738800	0.06539700	1.15748200
C	-5.92083700	1.39490800	-1.34736100
C	-6.80570500	0.83409100	0.85917400
C	-6.94233400	1.49138700	-0.38061000
H	-6.02434500	1.91775800	-2.29972200
H	-7.59256500	0.92225700	1.61040200
H	-7.83532600	2.08358000	-0.58870100
H	-1.47287700	-2.87890800	-2.36768600
C	-1.89578200	-3.32426900	-1.47236200
C	-1.15677700	-3.99517600	-0.43378600
C	-3.28622500	-3.35685500	-1.12043700
H	-0.08204400	-4.15116600	-0.41169400
C	-2.08885200	-4.43069100	0.56185000
H	-4.10593300	-2.94327500	-1.69940300

C	-3.40511900	-4.02424800	0.14608400
H	-1.84580100	-4.96814400	1.47215400
H	-4.33011000	-4.20893500	0.68539400
F	-0.72212700	5.72147900	-1.27086000
C	-0.25452800	4.44988900	-0.97414300
C	0.73752700	3.84838800	-1.76441800
C	-0.76077400	3.74098400	0.12794200
C	1.19573200	2.55253100	-1.44718500
F	1.26449600	4.53932700	-2.84860400
C	-0.27192800	2.45024900	0.39591700
F	-1.72999900	4.32028200	0.93999500
C	0.70902000	1.77521000	-0.37004800
F	2.21784700	2.07402400	-2.27475700
F	-0.80295200	1.84102200	1.55180000
B	1.20291200	0.22877200	0.00097400
C	2.07580700	-0.47871700	-1.22920200
C	2.01636700	0.15796000	1.45348300
C	-0.23907400	-0.69619600	0.21356600
C	3.47138000	-0.71405600	-1.19678900
C	1.47837700	-0.91098800	-2.43546400
C	2.59468500	1.26922300	2.11176600
C	2.20472000	-1.05449400	2.15704100
H	-0.86192300	-0.45396100	-0.66127200
H	0.12179400	-1.73187500	0.23653800
H	-0.65801300	-0.33517900	1.16137500
C	4.19745100	-1.34791400	-2.22662300
F	4.24428600	-0.28432800	-0.11335200
C	2.15136000	-1.54742200	-3.49308600
F	0.10415900	-0.67333600	-2.66962700
C	3.25256800	1.20304000	3.35701900
F	2.57801000	2.53757900	1.52239800
C	2.85336700	-1.17889600	3.39834700
F	1.76315800	-2.27416800	1.59539800
C	3.53258000	-1.77733300	-3.38637400
F	5.56690700	-1.54577400	-2.10776200
F	1.46503300	-1.94429800	-4.63753900
C	3.37904200	-0.03148700	4.01396200
F	3.78599900	2.34688700	3.93693900
F	2.98156400	-2.41985900	4.01461700
F	4.22499700	-2.40712700	-4.40918400
F	4.01897000	-0.11880200	5.24093300
C	-3.64923000	0.57164200	-2.14901900
H	-2.69909000	0.96769300	-1.76057800
H	-3.45994400	-0.45713400	-2.49128200
H	-3.91561800	1.16674900	-3.03244200
C	-5.51068200	-0.61826600	2.50497700
H	-5.42561000	-1.71183700	2.40311700
H	-4.61038900	-0.27093500	3.03408800
H	-6.37929000	-0.40870200	3.14349400
Frequencies --	6.6977	12.3442	14.8152
Frequencies --	16.1650	25.9849	26.6810
Frequencies --	30.5211	31.7814	34.7348
Frequencies --	40.1510	42.8331	45.3662
Frequencies --	62.2725	80.7552	81.4538
Frequencies --	102.3667	104.1667	107.6339
Frequencies --	110.9245	116.0653	117.6017
Frequencies --	119.7213	121.0528	124.9982

Frequencies --	140.1605	147.1657	151.8568
Frequencies --	153.0864	157.4373	160.0912
Frequencies --	161.3564	162.5124	205.8557
Frequencies --	211.4631	214.9982	218.0142
Frequencies --	219.5464	221.6477	225.7878
Frequencies --	227.3798	242.3307	261.0903
Frequencies --	264.5522	264.9391	265.5237
Frequencies --	266.2126	272.4552	273.1727
Frequencies --	280.8820	289.3961	293.0657
Frequencies --	308.0665	316.8691	319.4252
Frequencies --	326.0788	333.3381	335.9039
Frequencies --	340.4386	346.7289	351.7142
Frequencies --	358.8812	379.5159	380.2878
Frequencies --	380.4367	388.3834	391.4806
Frequencies --	400.8664	431.5891	432.1253
Frequencies --	432.3857	456.8411	457.5317
Frequencies --	458.8167	478.5105	491.8759
Frequencies --	513.2982	518.1751	541.1824
Frequencies --	541.5750	547.4687	549.1374
Frequencies --	552.4464	560.9906	565.2856
Frequencies --	571.4768	594.8113	597.4539
Frequencies --	600.6089	632.4909	639.3658
Frequencies --	640.0889	642.7215	661.3189
Frequencies --	663.5043	680.1155	694.2292
Frequencies --	728.4782	729.5694	737.1526
Frequencies --	742.9069	746.0720	759.3803
Frequencies --	761.3579	771.1447	786.7401
Frequencies --	797.7493	805.7864	816.6901
Frequencies --	835.4568	840.6512	841.1934
Frequencies --	865.0886	870.4858	871.4144
Frequencies --	897.2296	906.7475	909.4072
Frequencies --	910.2861	912.1634	922.1810
Frequencies --	934.0402	990.8920	1003.3979
Frequencies --	1018.1401	1021.5130	1026.0361
Frequencies --	1027.4785	1036.5282	1047.8656
Frequencies --	1049.9054	1050.1480	1052.3689
Frequencies --	1054.5172	1059.6463	1076.6850
Frequencies --	1086.8492	1090.1091	1096.1520
Frequencies --	1108.2663	1110.7919	1127.3454
Frequencies --	1187.6168	1194.5974	1198.5032
Frequencies --	1215.9811	1217.1243	1217.4531
Frequencies --	1279.2459	1280.6812	1286.0926
Frequencies --	1320.2384	1321.1720	1326.1709
Frequencies --	1338.6505	1342.0378	1343.1689
Frequencies --	1361.6622	1390.1117	1397.6349
Frequencies --	1417.1069	1418.0135	1418.7998
Frequencies --	1420.9025	1422.0853	1424.8755
Frequencies --	1426.7199	1439.6436	1442.5502
Frequencies --	1447.9951	1450.6274	1455.0145
Frequencies --	1469.5301	1470.2582	1472.0971
Frequencies --	1473.3936	1489.3796	1491.4245
Frequencies --	1502.8200	1503.0765	1595.0274
Frequencies --	1596.3041	1596.8098	1604.0043
Frequencies --	1606.5961	1620.0216	1620.8587
Frequencies --	1622.4339	2983.3243	2988.8552
Frequencies --	3018.2384	3025.4969	3102.9366
Frequencies --	3107.3723	3110.5290	3132.1775
Frequencies --	3134.0882	3135.8885	3137.8322
Frequencies --	3160.5006	3167.4838	3178.4758
Frequencies --	3198.1609	3240.5670	3243.9377
Frequencies --	3257.0596	3265.3473	3279.6281

4. Transition States for Transfer of H from Counterion to Cation ([return to table of contents](#))

Catalyst 1:



vacuum	toluene-like solvent	D3 dispersion
-2937.0328612	-2937.0465161	-0.50581106

Imaginary frequency corresponding to vibration along the reaction coordinate: -1067 cm^{-1} .

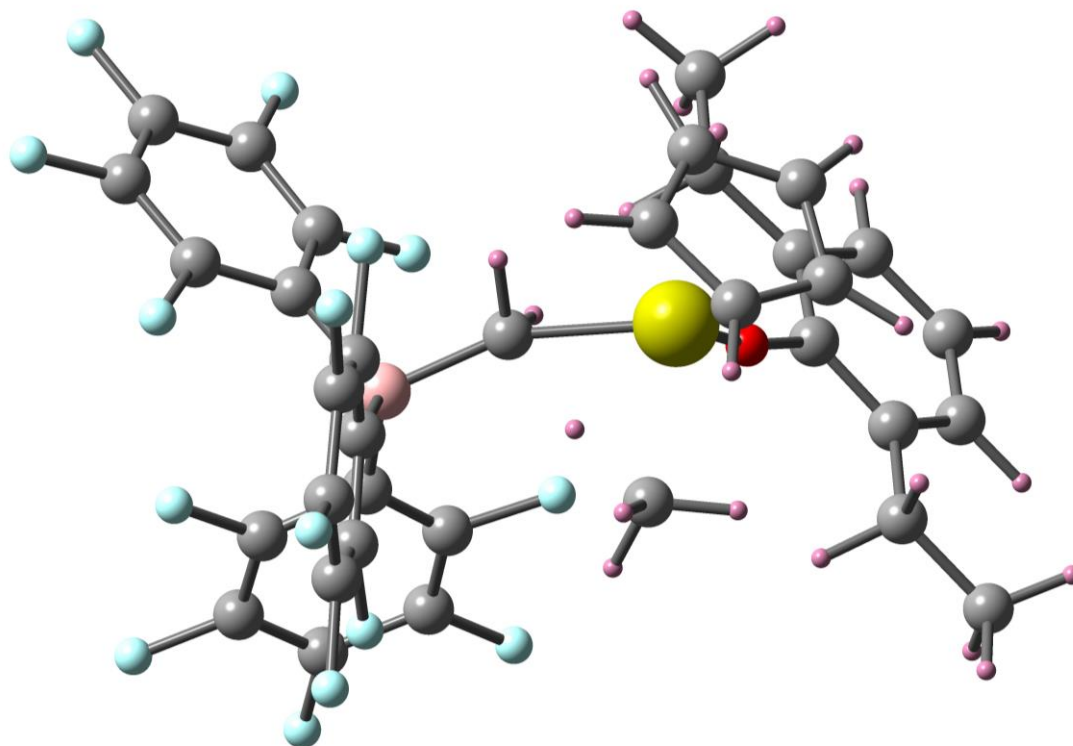
Ti	-1.03590100	2.15729500	0.50226500
C	-0.24244300	2.43494900	-1.66184800
H	-0.04616400	1.65971200	-2.41614700
H	-1.22947400	2.85607800	-1.89932800
H	0.51801300	3.21823400	-1.73802500
O	-2.60346600	1.38088700	0.20802300
C	-3.89641600	0.86743800	0.17731100
C	-4.31340100	-0.02120100	1.21149300
C	-4.75211800	1.24050600	-0.89973500
C	-5.63432200	-0.52198200	1.15765500
C	-6.06381600	0.71520300	-0.91737700
C	-6.49306500	-0.15109800	0.10589400
H	-5.97730200	-1.20356500	1.93499900
H	-6.73568300	0.98172700	-1.73231100
H	-2.11481600	3.03232200	3.23543300
C	-1.50800700	3.45164800	2.43750800
C	-0.06577800	3.44029100	2.37149900
C	-1.99722700	4.19338500	1.30789400
H	0.60276200	2.97674300	3.09139500

C	0.32844400	4.12705600	1.18519000
H	-3.04060500	4.39513000	1.08286000
C	-0.86576300	4.58293000	0.51702700
H	1.34827200	4.27383800	0.84492000
H	-0.89873500	5.16340300	-0.40000600
F	0.38787600	-4.60102400	-3.89799800
C	0.68221800	-3.57053400	-3.01789100
C	1.97953200	-3.41918700	-2.49793900
C	-0.30711300	-2.65352000	-2.63277500
C	2.24696200	-2.36458000	-1.60724400
F	2.98104400	-4.30492300	-2.87455000
C	0.01899200	-1.61543400	-1.73665900
F	-1.59835200	-2.77181000	-3.13852000
C	1.29439000	-1.41020300	-1.17155300
F	3.56982400	-2.26400000	-1.16478000
F	-1.05111400	-0.74728100	-1.43692800
B	1.72210200	-0.25554100	-0.04538300
C	2.28397000	-1.14103600	1.27234900
C	2.82196500	0.86315900	-0.61217800
C	0.43029500	0.67093300	0.52303900
C	3.62772800	-1.24788300	1.70727200
C	1.39422400	-1.92698800	2.04265000
C	3.21459300	1.03227600	-1.95965200
C	3.39972100	1.82543100	0.25029700
H	-0.41836900	-0.00078000	0.74798700
H	0.82302400	1.16769100	1.43106000
H	0.17564500	1.57656900	-0.70067200
C	4.04599500	-2.01875600	2.81184800
F	4.65708500	-0.58972100	1.03137100
C	1.75789300	-2.71385000	3.15095300
F	0.02633200	-1.98451400	1.69933600
C	4.13067300	2.00835300	-2.40775600
F	2.67173900	0.23181700	-2.97384100
C	4.30916700	2.82212900	-0.14036500
F	3.06277800	1.82401700	1.61896500
C	3.10412100	-2.75561400	3.54790800
F	5.38590800	-2.06149900	3.17626600
F	0.80235700	-3.44529800	3.84996800
C	4.69256400	2.90951900	-1.49007300
F	4.46589400	2.09794200	-3.75327100
F	4.82350700	3.72289400	0.78757400
F	3.49564400	-3.51624300	4.63949700
F	5.58689700	3.88310000	-1.90852200
C	-3.38526200	-0.44801300	2.33466900
H	-2.52820900	-1.02126700	1.95211100
H	-2.98626100	0.41636300	2.88880100
H	-3.91278900	-1.08587300	3.05575900
C	-4.27825300	2.15073200	-2.01823000
H	-3.91456500	3.11608200	-1.63206800
H	-3.45445300	1.68448900	-2.58092900
H	-5.09096700	2.35988200	-2.72632400
Br	-8.32233700	-0.86269000	0.06100600

Frequencies --	-1067.2478	8.9848	10.9244
Frequencies --	19.9051	26.2355	27.4697
Frequencies --	29.0179	32.5599	36.9614
Frequencies --	38.9138	40.3233	43.7078

Frequencies --	48.5773	61.0562	73.6806
Frequencies --	76.6272	101.8292	107.3321
Frequencies --	111.3786	120.3382	122.1725
Frequencies --	126.5722	135.2095	137.3865
Frequencies --	140.5030	141.7091	145.1679
Frequencies --	147.3017	149.8217	152.8092
Frequencies --	156.3253	160.9581	161.5340
Frequencies --	169.7308	181.8900	202.7123
Frequencies --	204.0165	215.5043	216.4179
Frequencies --	221.6765	222.0527	223.7619
Frequencies --	230.0017	240.8516	247.5903
Frequencies --	260.8624	264.2016	264.5178
Frequencies --	264.9074	267.2849	275.2742
Frequencies --	275.8259	282.1726	302.9202
Frequencies --	303.5553	313.3784	320.8530
Frequencies --	326.1317	329.6123	336.5572
Frequencies --	348.0525	356.2185	363.6822
Frequencies --	375.8690	377.8200	379.0712
Frequencies --	381.5949	393.4769	401.8793
Frequencies --	425.4891	431.5679	432.2706
Frequencies --	433.2980	450.9742	456.8930
Frequencies --	463.8386	481.8062	502.1078
Frequencies --	508.2669	537.1944	537.9915
Frequencies --	544.3827	553.9122	563.9766
Frequencies --	566.6637	567.4596	568.0869
Frequencies --	572.0749	576.6482	596.1000
Frequencies --	607.1856	634.7641	636.2049
Frequencies --	638.1680	643.7749	655.3708
Frequencies --	675.0374	707.9814	719.1574
Frequencies --	725.4998	727.7389	736.0941
Frequencies --	748.8833	750.0491	763.1412
Frequencies --	772.9326	780.7664	801.5196
Frequencies --	804.4966	814.0225	838.3752
Frequencies --	841.0968	849.7799	868.5820
Frequencies --	871.3375	881.5171	884.8594
Frequencies --	888.4783	889.3790	898.3146
Frequencies --	902.9804	912.3303	919.5235
Frequencies --	934.5692	949.4552	1002.5882
Frequencies --	1010.0913	1018.0666	1021.7081
Frequencies --	1028.2512	1033.6026	1039.8187
Frequencies --	1050.0916	1050.5910	1053.3079
Frequencies --	1054.8780	1056.5831	1060.3079
Frequencies --	1085.9473	1088.9567	1090.7252
Frequencies --	1123.7696	1126.7364	1208.5521
Frequencies --	1211.8841	1214.6561	1216.8637
Frequencies --	1265.4565	1266.7342	1280.6462
Frequencies --	1287.4997	1288.4409	1318.1711
Frequencies --	1319.7528	1325.3724	1338.8388
Frequencies --	1342.1214	1344.5794	1349.6201
Frequencies --	1355.4795	1389.2627	1392.6391
Frequencies --	1412.2319	1414.6873	1420.0778
Frequencies --	1421.4377	1423.0236	1425.7666
Frequencies --	1429.6053	1436.9329	1452.2413
Frequencies --	1465.9035	1468.0850	1469.2268
Frequencies --	1471.7552	1486.3250	1491.2317
Frequencies --	1491.5875	1503.2479	1505.2611
Frequencies --	1588.2991	1591.3335	1593.8093
Frequencies --	1595.7749	1597.6468	1618.1781
Frequencies --	1619.9464	1622.6628	1830.1501
Frequencies --	2973.5849	3014.7731	3022.2786
Frequencies --	3038.4902	3078.4060	3100.5694
Frequencies --	3110.3979	3135.9947	3138.7465
Frequencies --	3140.9502	3189.2172	3202.5228

Frequencies --	3204.4169	3235.6615	3242.6822
Frequencies --	3254.8340	3259.7821	3279.1552

Catalyst 2:

vacuum	toluene-like solvent	D3 dispersion
-3003.0479695	-3003.0611067	-0.53199011

Imaginary frequency corresponding to vibration along the reaction coordinate: -1067 cm^{-1} .

Ti	1.90130800	1.60618000	-0.85487700
C	1.19502000	2.46007500	1.18495100
H	1.00079700	1.85499600	2.08132100
H	2.21971400	2.84826300	1.28007600
H	0.49747600	3.30300700	1.15313500
O	3.28559600	0.61466100	-0.36929600
C	4.48471400	-0.09307300	-0.24529200
C	4.73063400	-1.17721200	-1.14236000
C	5.39262400	0.29517000	0.78532000
C	5.95870600	-1.86167700	-0.99564000
C	6.60043100	-0.43180600	0.88286400
C	6.88500800	-1.49267900	0.00003700
H	6.19099800	-2.69433200	-1.65711200
H	7.32151300	-0.17484300	1.65661600
H	7.82488400	-2.03999100	0.09524200
H	1.46116600	1.67103900	-3.91477100
C	1.75201100	2.36546100	-3.13004400
C	0.86370600	3.22178700	-2.39297700
C	3.09641300	2.60950900	-2.67522500
H	-0.21152100	3.28282100	-2.51809500
C	1.65776600	3.97818900	-1.46951900
H	3.99608400	2.12408600	-3.04209200

C	3.03563300	3.60374500	-1.64391400
H	1.28620200	4.72528300	-0.77524800
H	3.88328800	4.00952500	-1.09828100
F	-0.69500700	-3.65076100	4.84383600
C	-0.80543500	-2.80584000	3.74932700
C	-2.06083100	-2.52537200	3.18253600
C	0.33327500	-2.20961400	3.18757800
C	-2.13983300	-1.66538100	2.07295400
F	-3.20597200	-3.09333200	3.72701900
C	0.19355900	-1.35428400	2.07576500
F	1.58914800	-2.46329700	3.73210300
C	-1.03135200	-1.03525000	1.45432700
F	-3.42830300	-1.41617200	1.58938100
F	1.40402000	-0.80382400	1.60949000
B	-1.25490200	-0.10148600	0.08809800
C	-1.96505200	-1.15845600	-1.01622100
C	-2.14500100	1.28218500	0.36157100
C	0.16980900	0.45238800	-0.62751300
C	-3.31398200	-1.14953300	-1.44897900
C	-1.21940100	-2.22657300	-1.57031600
C	-2.45688600	1.83017300	1.62690900
C	-2.59007900	2.09310100	-0.70955900
H	0.87582000	-0.39522000	-0.70059000
H	-0.14083800	0.81771100	-1.62536800
H	0.60687500	1.52754100	0.39999400
C	-3.86118000	-2.07342500	-2.36377500
F	-4.21957500	-0.20417700	-0.96360400
C	-1.71519400	-3.17417200	-2.48459000
F	0.12536200	-2.42297400	-1.18844500
C	-3.18784100	3.02180500	1.82220700
F	-2.01217800	1.21760800	2.80668500
C	-3.31459700	3.28917200	-0.57511200
F	-2.30243000	1.71227500	-2.03554300
C	-3.05553400	-3.09349800	-2.89465200
F	-5.19530100	-1.98734500	-2.74230500
F	-0.89494400	-4.18405500	-2.97982000
C	-3.63108500	3.75739600	0.71195900
F	-3.45634200	3.48413500	3.10524700
F	-3.71163300	4.01342000	-1.69502100
F	-3.57404600	-4.00902300	-3.79863100
F	-4.34371000	4.93530700	0.88004800
C	3.68418000	-1.57661600	-2.18449000
H	2.76147800	-1.86534200	-1.65570600
C	5.03229900	1.43196600	1.74289300
H	4.06865700	1.18356300	2.21850700
C	4.06293400	-2.72076700	-3.14968000
H	3.22950000	-2.90428300	-3.84522300
H	4.95498000	-2.48087700	-3.74973900
H	4.25144300	-3.66245600	-2.61211800
C	6.05782700	1.75918800	2.85008400
H	7.02981100	2.06995100	2.43594700
H	5.68068100	2.58790900	3.46963400
H	6.22620200	0.89956500	3.51655500
H	4.85224300	2.34806800	1.15253800
H	3.42212300	-0.68834300	-2.78655600

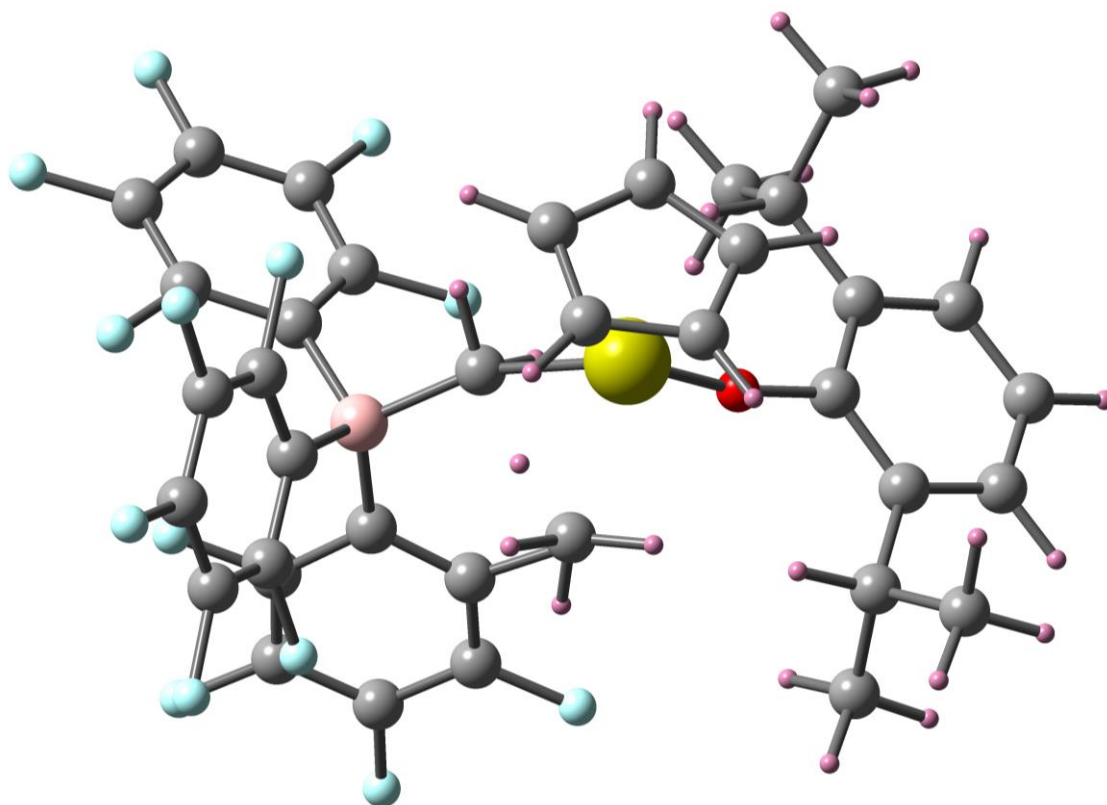
Frequencies -- -1067.1387

12.8762

14.8625

Frequencies --	20.9310	23.9972	28.2653
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Frequencies --	39.1938	41.2013	41.8663
Frequencies --	49.9843	52.7636	60.4120
Frequencies --	72.4587	75.6369	93.4391
Frequencies --	102.5390	110.2819	112.1171
Frequencies --	121.9567	123.5950	125.4437
Frequencies --	135.4012	139.8313	141.4278
Frequencies --	146.0206	151.3573	156.2121
Frequencies --	160.2477	161.1659	170.0614
Frequencies --	174.7740	187.1034	190.0030
Frequencies --	206.0454	211.4260	215.5987
Frequencies --	217.4909	221.7347	223.3264
Frequencies --	239.4046	256.7436	263.4496
Frequencies --	264.5151	264.8244	265.2408
Frequencies --	274.3687	275.2572	278.1229
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Frequencies --	301.9866	305.0448	310.7307
Frequencies --	324.1948	325.2819	327.2499
Frequencies --	332.6109	337.4314	354.6351
Frequencies --	361.4123	367.8902	375.9514
Frequencies --	377.6131	378.9247	381.2131
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Frequencies --	432.1538	432.9742	450.4741
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Frequencies --	505.1268	528.0812	536.9183
Frequencies --	538.5177	543.3976	545.5458
Frequencies --	555.7918	565.8878	568.2348
Frequencies --	571.6879	577.8180	597.7706
Frequencies --	603.8687	611.4428	634.9988
Frequencies --	636.2870	638.1658	643.0945
Frequencies --	656.1976	674.2309	708.3789
Frequencies --	710.8453	718.8731	724.7848
Frequencies --	730.5546	736.2398	748.4208
Frequencies --	749.4905	762.5904	772.7553
Frequencies --	773.7417	778.6444	793.0165
Frequencies --	797.1319	813.2896	830.5594
Frequencies --	837.5739	840.2763	848.8383
Frequencies --	852.4495	863.9009	872.8790
Frequencies --	880.5180	889.2062	892.1267
Frequencies --	902.5806	912.3829	920.9198
Frequencies --	924.6995	938.2452	995.0298
Frequencies --	995.6571	1007.1901	1019.4201
Frequencies --	1025.4322	1028.3826	1029.2273
Frequencies --	1032.3513	1040.8016	1050.4890
Frequencies --	1052.9900	1056.4997	1058.2677
Frequencies --	1087.9779	1091.3649	1093.5427
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Frequencies --	1120.3344	1126.4430	1186.8602
Frequencies --	1203.7575	1211.1888	1214.2389
Frequencies --	1216.2969	1256.4240	1260.2115
Frequencies --	1279.0331	1283.1936	1284.5462
Frequencies --	1289.0907	1293.1435	1318.0989
Frequencies --	1319.4753	1324.8385	1326.8957
Frequencies --	1338.3600	1342.3594	1343.0355
Frequencies --	1344.4918	1350.0133	1380.2959
Frequencies --	1391.6414	1392.2302	1411.8612
Frequencies --	1413.5164	1417.1311	1420.2892
Frequencies --	1422.6448	1432.7577	1441.6578
Frequencies --	1447.6770	1464.5972	1468.0606
Frequencies --	1468.4627	1469.0890	1471.5451
Frequencies --	1480.3599	1493.2543	1499.4997
Frequencies --	1500.8766	1505.8775	1506.1944

Frequencies --	1509.2468	1593.9846	1596.0038
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Frequencies --	1617.9082	1619.7860	1622.5290
Frequencies --	1833.0125	2971.7243	3003.8050
Frequencies --	3007.4633	3014.9049	3015.8219
Frequencies --	3034.7576	3058.3421	3068.5911
Frequencies --	3076.8286	3115.5448	3118.3121
Frequencies --	3122.7448	3122.9098	3136.8838
Frequencies --	3172.5082	3184.9569	3207.5024
Frequencies --	3215.9002	3232.3420	3237.8217
Frequencies --	3254.9692	3262.0647	3282.4968

Catalyst 3:

vacuum	toluene-like solvent	D3 dispersion
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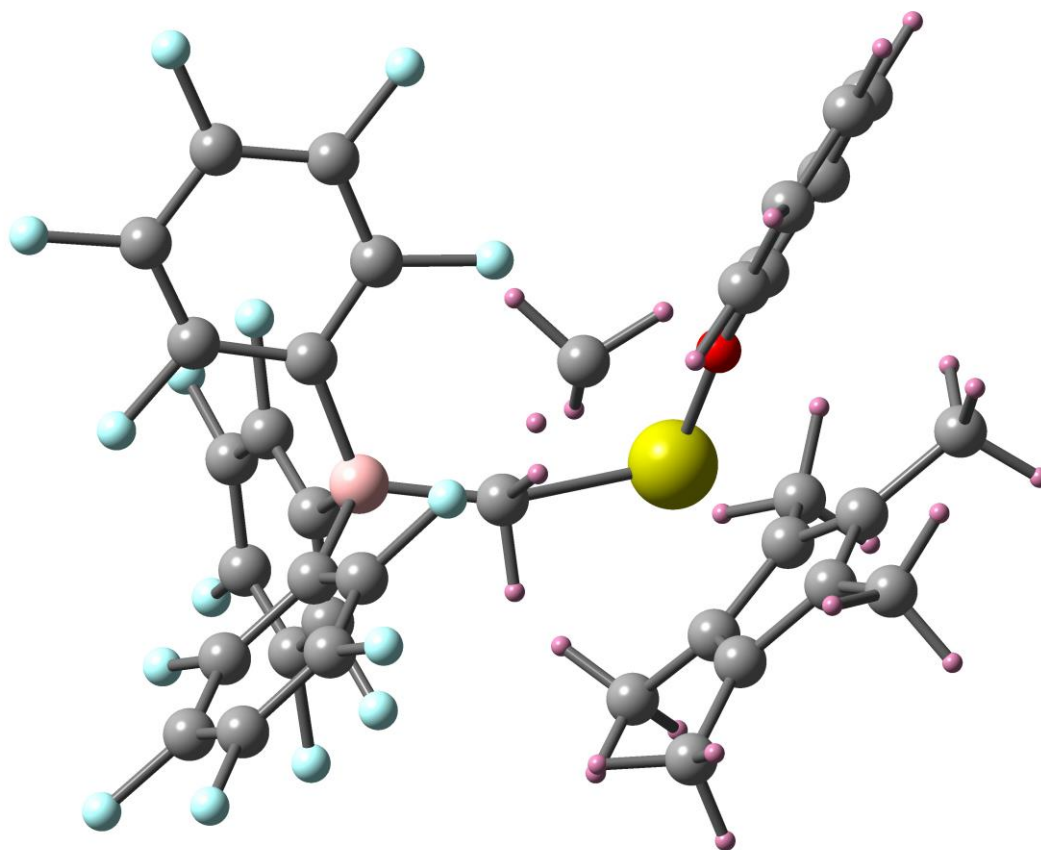
Imaginary frequency corresponding to vibration along the reaction coordinate: -1051 cm^{-1} .

Ti	1.75506200	1.55364600	-0.87870000
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H	0.92488000	1.88637000	2.03953300
H	1.99298000	2.98375700	1.15297900
H	0.24031400	3.26286100	1.11024900
O	3.13984600	0.58184600	-0.35729400
C	4.34321200	-0.12063700	-0.20480800
C	4.68744400	-1.11830300	-1.17099200
C	5.16622700	0.17968000	0.92465600
C	5.91914400	-1.79084200	-0.99011500
C	6.38145400	-0.53326700	1.04670000
C	6.76182400	-1.50162000	0.09915800
H	6.21695700	-2.55681900	-1.70666700
H	7.03278800	-0.33266600	1.89773500
H	7.70545900	-2.03818900	0.21531700
H	2.08050700	1.43332800	-3.91209500
C	2.00650100	2.19698700	-3.14212600
C	0.79517600	2.86183500	-2.72552400
C	3.10904300	2.78171800	-2.42560100
H	-0.20283300	2.66852500	-3.10359800
C	1.14675200	3.81476700	-1.72268200
H	4.15401500	2.50252400	-2.52207700

C	2.57474200	3.76157900	-1.52817500
H	0.45853900	4.47217400	-1.19997200
H	3.14839000	4.37645800	-0.83982600
F	-1.01249000	-3.36693300	5.06175600
C	-1.08690900	-2.59038200	3.91492300
C	-2.32552100	-2.32721900	3.30432200
C	0.07192400	-2.04650700	3.34180700
C	-2.36797500	-1.53498100	2.14337900
F	-3.49053500	-2.84362900	3.85769400
C	-0.03100300	-1.26000500	2.17664200
F	1.31358300	-2.28257900	3.92746900
C	-1.23743800	-0.95909400	1.51164900
F	-3.64207000	-1.29646400	1.61865000
F	1.19984400	-0.76208400	1.70373800
B	-1.41875100	-0.10168600	0.09006100
C	-2.12119100	-1.20726600	-0.96881400
C	-2.29842300	1.30587400	0.26203100
C	0.03270400	0.39212500	-0.61497200
C	-3.46037000	-1.20470200	-1.43075200
C	-1.37821100	-2.31284800	-1.44758900
C	-2.63760300	1.92887900	1.48481700
C	-2.70337600	2.05924200	-0.86564700
H	0.73814100	-0.45859900	-0.60957200
H	-0.23990300	0.69429700	-1.64604300
H	0.44476600	1.53251900	0.36313200
C	-3.99940900	-2.16786600	-2.30909800
F	-4.36395700	-0.22443200	-1.01505800
C	-1.86614600	-3.29990800	-2.32353600
F	-0.04624600	-2.50376600	-1.02436900
C	-3.35379100	3.14065200	1.59128400
F	-2.23668400	1.37760500	2.70943300
C	-3.41190800	3.27149400	-0.82010400
F	-2.39327900	1.59444900	-2.15929700
C	-3.19567000	-3.22369600	-2.76833200
F	-5.32357300	-2.08503100	-2.72222400
F	-1.04849300	-4.34394300	-2.74742400
C	-3.75415900	3.81815900	0.42892600
F	-3.64936500	3.67992200	2.83791100
F	-3.76967400	3.93426700	-1.99008200
F	-3.70618300	-4.17798500	-3.63617600
F	-4.45038900	5.01507400	0.50975300
C	3.78262800	-1.49147000	-2.35588600
H	2.87677200	-0.87048400	-2.31048200
C	4.76491600	1.20439800	1.99563100
H	3.80453400	1.64225300	1.70050200
C	3.30683200	-2.97160300	-2.26818300
H	4.14941300	-3.67399200	-2.35492900
H	2.79460800	-3.16931200	-1.31570700
H	2.59889200	-3.19243400	-3.08236300
C	4.46655100	-1.20310500	-3.72490800
H	4.78371000	-0.15100200	-3.80569000
H	5.35817600	-1.83057900	-3.87264800
H	3.77008300	-1.41907600	-4.55115200
C	4.53573400	0.52112900	3.37647600
H	3.77015700	-0.26566600	3.30648000
H	5.45884000	0.06348500	3.76348300
H	4.19600800	1.26500900	4.11521800

C	5.78804400	2.37257700	2.10132200
H	6.77633100	2.02425500	2.43725100
H	5.92410900	2.87617400	1.13042100
H	5.43509500	3.12018600	2.82998100
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Frequencies --	153.5679	156.1135	159.7829
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Frequencies --	180.7288	210.6890	215.2340
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Frequencies --	222.9067	224.6405	231.6969
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Frequencies --	377.6327	378.1831	381.2114
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Frequencies --	429.4163	430.7754	432.1288
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Frequencies --	1253.2969	1276.7633	1281.9486
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Frequencies --	1325.9421	1328.3047	1338.4123
Frequencies --	1340.1008	1344.4452	1349.6112
Frequencies --	1379.8828	1390.3472	1392.7030
Frequencies --	1401.4135	1401.6220	1411.6837
Frequencies --	1419.9126	1420.7301	1421.9641
Frequencies --	1422.8919	1435.1009	1438.5663
Frequencies --	1452.6632	1458.8752	1467.9216
Frequencies --	1468.7322	1471.4551	1473.6284
Frequencies --	1485.0312	1487.5831	1488.8013
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Frequencies --	1505.2147	1509.1440	1519.4683
Frequencies --	1593.7565	1595.9891	1596.2910
Frequencies --	1597.5069	1603.7423	1617.9302
Frequencies --	1619.5273	1622.5986	1831.3783
Frequencies --	2968.9350	3004.9105	3007.0766
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Frequencies --	3200.2809	3235.5015	3240.2485
Frequencies --	3254.6662	3261.5947	3279.1358

Catalyst 4:

vacuum	toluene-like solvent	D3 dispersion
-3042.3570666	-3042.3694231	-0.55148438

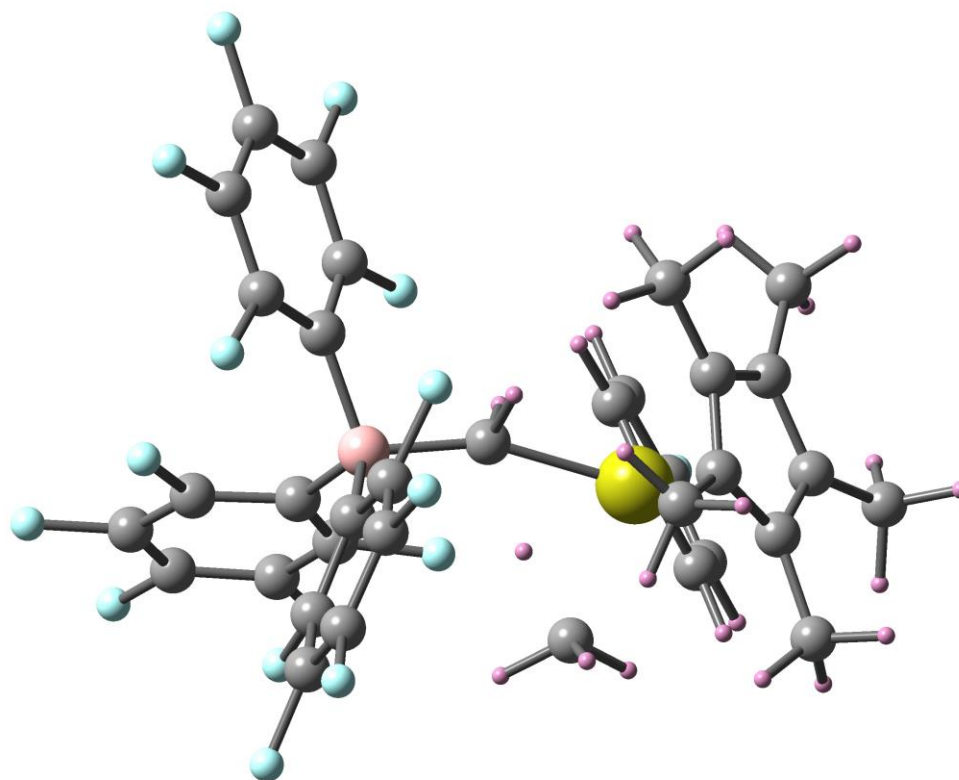
Imaginary frequency corresponding to vibration along the reaction coordinate: -984 cm^{-1} .

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H	2.66219700	-1.14995700	-2.44295200
H	1.28416400	-2.29571000	-2.37316400
O	3.33479200	0.49101100	-0.19480500
C	4.14347600	1.61666100	-0.19505800
C	3.97302900	2.59777900	0.81196700
C	5.10912400	1.78770700	-1.21590200
C	4.78474400	3.74924600	0.79703100
C	5.91193200	2.94637600	-1.22019700
C	5.75658900	3.92694400	-0.21421800
H	4.64962800	4.51033300	1.56831400
H	6.65104300	3.08474600	-2.01220100
H	6.37799300	4.82415300	-0.22401200
C	2.49356000	-2.63297500	1.82582800
C	2.19882100	-3.40158300	0.64740600
C	3.78843200	-1.99150300	1.63663600
C	3.30544100	-3.24027100	-0.27889700

C	4.30111200	-2.39899800	0.34878500
F	-1.73838200	5.43277500	-2.75924600
C	-1.58946900	4.19433000	-2.15111000
C	-2.70739500	3.49092900	-1.67109700
C	-0.32043700	3.61332900	-2.01039400
C	-2.52438200	2.23866200	-1.05737000
F	-3.97857400	4.03495200	-1.81503400
C	-0.19837000	2.35462400	-1.38852000
F	0.80450500	4.27899700	-2.49013000
C	-1.27166500	1.60327200	-0.86967600
F	-3.69557900	1.59124500	-0.64813900
F	1.11196800	1.85154400	-1.33433400
B	-1.17438500	0.14664600	-0.05826900
C	-1.91827300	0.46338900	1.42531300
C	-1.87077700	-1.10911200	-0.91288000
C	0.38231400	-0.40219900	0.32172300
C	-3.19194000	0.01139000	1.85094100
C	-1.29477700	1.30769000	2.37601300
C	-2.19850700	-1.08192300	-2.28879800
C	-2.11289100	-2.37227900	-0.32187600
H	0.92748000	0.43297300	0.81697300
H	0.20936600	-1.23406900	1.02358400
H	0.93576300	-0.86289800	-1.08301700
C	-3.77005900	0.31862000	3.10034300
F	-3.99174800	-0.77413700	1.01885700
C	-1.82681300	1.64715200	3.63388400
F	-0.05010900	1.90857300	2.08515500
C	-2.76453100	-2.16313900	-2.99810200
F	-1.94405700	0.05491600	-3.06953000
C	-2.66958400	-3.48253800	-0.97907500
F	-1.78518800	-2.58309100	1.03025100
C	-3.08073400	1.13862800	4.00782400
F	-5.02292700	-0.17785900	3.44101300
F	-1.12535400	2.47819400	4.50387000
C	-3.01253900	-3.37624900	-2.33752800
F	-3.06186000	-2.04312200	-4.35097700
F	-2.87369300	-4.68244300	-0.30335600
F	-3.63005700	1.44896500	5.24377500
F	-3.55984500	-4.45566200	-3.01601100
C	3.48873900	-4.02025500	-1.56088200
H	4.10191100	-4.91720300	-1.36726100
H	2.53331500	-4.36566900	-1.97537800
H	4.00433600	-3.44443300	-2.34228700
C	1.01746000	-4.32355800	0.44517700
H	0.36525200	-4.00638700	-0.38012500
H	1.36422500	-5.34338200	0.21472800
H	0.39322200	-4.37927300	1.34380900
C	1.67741300	-2.59998300	3.10027200
H	0.60693700	-2.43174600	2.92254600
H	1.76975000	-3.56583600	3.62499000
H	2.02480100	-1.82119300	3.79146000
C	4.53479100	-1.19286100	2.68326800
H	3.87884100	-0.50821000	3.23977900
H	4.99094200	-1.87426800	3.42223500
H	5.34433600	-0.59419700	2.24733000
C	5.67809500	-2.10063800	-0.19939000
H	6.04136300	-1.10526800	0.08619000

H	6.40091700	-2.83615900	0.19504300
H	5.71449200	-2.17154600	-1.29516300
H	3.20682000	2.46569500	1.57630100
H	5.21190900	1.03387800	-1.99689000
Frequencies --	-983.7699	11.5697	14.4898
Frequencies --	18.4619	25.7170	27.2205
Frequencies --	29.0634	30.9317	32.5705
Frequencies --	38.3377	42.0190	48.6101
Frequencies --	51.0677	63.8599	70.3619
Frequencies --	76.9623	94.6402	96.5946
Frequencies --	103.0776	109.8570	113.2895
Frequencies --	115.9298	119.7445	121.1482
Frequencies --	125.0196	128.1082	131.1877
Frequencies --	139.1655	142.5963	143.4527
Frequencies --	144.6747	150.1173	155.3103
Frequencies --	156.3548	160.8065	161.8838
Frequencies --	162.1753	166.5124	176.4498
Frequencies --	191.0406	202.3978	212.5908
Frequencies --	215.6117	220.9985	224.3707
Frequencies --	226.9934	251.4050	264.3586
Frequencies --	264.5672	265.2536	274.8565
Frequencies --	276.3646	277.4327	283.0893
Frequencies --	287.7715	294.9386	297.7034
Frequencies --	303.2419	304.5514	305.4953
Frequencies --	308.6175	321.6859	326.8117
Frequencies --	328.0322	334.8478	350.5895
Frequencies --	361.9166	372.3417	377.3080
Frequencies --	378.4525	379.9074	381.6666
Frequencies --	395.3245	395.4456	405.9373
Frequencies --	408.3287	431.3220	432.2168
Frequencies --	434.2384	439.8077	450.3817
Frequencies --	456.8430	464.1501	480.2614
Frequencies --	509.1985	532.3355	535.7862
Frequencies --	537.0345	539.1779	544.7484
Frequencies --	554.2932	559.8311	576.3345
Frequencies --	581.3213	593.3901	600.6373
Frequencies --	602.8878	614.7108	615.7035
Frequencies --	634.8113	636.6192	638.6201
Frequencies --	643.2689	655.1567	664.2546
Frequencies --	672.1969	687.2634	696.0628
Frequencies --	718.5104	722.5033	733.3135
Frequencies --	746.1755	748.4372	758.9773
Frequencies --	762.4843	770.6167	803.7424
Frequencies --	806.0155	831.1851	842.7513
Frequencies --	871.1020	882.7344	887.4107
Frequencies --	903.7638	912.8196	914.0819
Frequencies --	919.9031	928.0386	970.4690
Frequencies --	972.5833	974.5253	998.1603
Frequencies --	1008.3802	1011.2031	1018.7669
Frequencies --	1028.2655	1030.7014	1039.3720
Frequencies --	1042.0149	1043.5309	1045.7105
Frequencies --	1046.4569	1050.4833	1053.6585
Frequencies --	1055.8271	1057.5184	1088.1379
Frequencies --	1089.3897	1090.5815	1095.9817
Frequencies --	1125.1209	1171.0385	1175.2080
Frequencies --	1183.0026	1189.8929	1209.3484
Frequencies --	1213.3294	1216.0966	1243.1617
Frequencies --	1263.8838	1301.6534	1315.7526
Frequencies --	1319.5038	1324.5038	1326.0606
Frequencies --	1336.4034	1342.9169	1349.8048
Frequencies --	1351.7474	1376.5392	1410.1315
Frequencies --	1410.7176	1416.0100	1419.2634

Frequencies --	1422.2172	1424.5952	1425.5633
Frequencies --	1430.3479	1432.0235	1436.6108
Frequencies --	1450.3955	1453.1834	1455.6304
Frequencies --	1462.7786	1466.4275	1467.0324
Frequencies --	1469.0499	1471.2511	1483.4008
Frequencies --	1483.7599	1490.1032	1491.9057
Frequencies --	1494.2883	1501.2396	1502.7447
Frequencies --	1505.9807	1506.9610	1511.9588
Frequencies --	1516.6353	1522.6376	1593.6799
Frequencies --	1595.9209	1598.4946	1598.8541
Frequencies --	1608.5896	1616.8413	1619.2777
Frequencies --	1622.3780	1815.3006	2927.6620
Frequencies --	3009.7024	3011.6957	3013.9182
Frequencies --	3018.8256	3027.3822	3030.4964
Frequencies --	3096.8411	3099.3581	3099.5769
Frequencies --	3101.8863	3108.6244	3109.0875
Frequencies --	3127.7477	3139.4161	3142.4600
Frequencies --	3144.0137	3147.4121	3161.7704
Frequencies --	3166.7336	3174.7339	3187.3309
Frequencies --	3191.0938	3199.1584	3207.7447

Catalyst 5:

vacuum	toluene-like solvent	D3 dispersion
-3141.5835662	-3141.5876831	-0.55143640

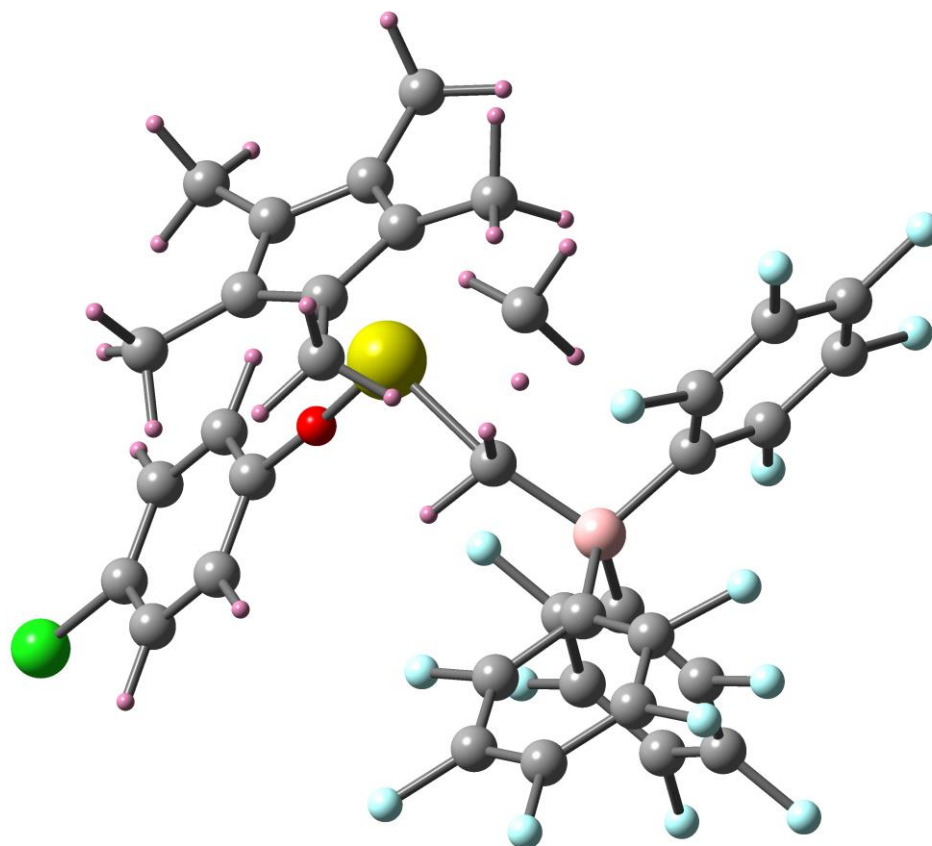
Imaginary frequency corresponding to vibration along the reaction coordinate: -1062 cm^{-1} .

Ti	1.97361800	-1.56415900	-0.01980800
C	1.14828300	-1.66874300	-2.18604500
H	0.68134800	-0.88974600	-2.80564200
H	2.20122800	-1.71521700	-2.50296900
H	0.65845600	-2.62714900	-2.38126700
O	3.23288500	-0.31961200	-0.22097600
C	4.21492000	0.65388300	-0.18292000
C	4.18943900	1.63537400	0.83978100
C	5.21844000	0.67761100	-1.18241500
C	5.17740400	2.63739700	0.87013900
C	6.20660300	1.68050000	-1.15761700
C	6.16760200	2.63729500	-0.12822100
H	5.17683200	3.40814600	1.64028500
H	6.98533700	1.72728100	-1.91828600
C	1.55823200	-3.30471100	1.66896900
C	1.34433800	-3.95846200	0.40865400
C	2.93961500	-2.83790700	1.70625200
C	2.59091700	-3.90605200	-0.34049400
C	3.58553400	-3.25781200	0.48357100
F	-0.69577300	5.60476700	-2.78558900
C	-0.80846400	4.36495700	-2.17318400
C	-2.04147800	3.92811200	-1.65917200

C	0.30333500	3.51664800	-2.06193100
C	-2.12489400	2.66735400	-1.04133100
F	-3.16332700	4.74032500	-1.77432500
C	0.15899500	2.26320000	-1.43441600
F	1.53503700	3.91408300	-2.57515600
C	-1.03988400	1.76988900	-0.88260400
F	-3.39862700	2.29586600	-0.59709500
F	1.32677400	1.48109100	-1.40938300
B	-1.24724300	0.32927900	-0.06606200
C	-1.87264100	0.79593100	1.43137100
C	-2.21110800	-0.75112400	-0.89693000
C	0.16202600	-0.53858900	0.28666500
C	-3.20279600	0.62178000	1.88696000
C	-1.06271000	1.48635900	2.36520700
C	-2.57098700	-0.65417900	-2.26132500
C	-2.68236900	-1.94087200	-0.29372500
H	0.88505000	0.16339300	0.75784900
H	-0.16585800	-1.31356500	0.99884200
H	0.58268700	-1.10621400	-1.09665700
C	-3.67307300	1.04013000	3.14916400
F	-4.16905900	0.02638400	1.07408800
C	-1.48067800	1.92646200	3.63479100
F	0.27487700	1.81024400	2.04272400
C	-3.36350100	-1.59941200	-2.94774200
F	-2.11981100	0.41145600	-3.05267800
C	-3.46915700	-2.91649500	-0.92729100
F	-2.35766800	-2.21374800	1.04987700
C	-2.80482700	1.69300200	4.03871600
F	-4.99392100	0.81855700	3.52024200
F	-0.59877800	2.58662600	4.48658500
C	-3.82649600	-2.74074200	-2.27480400
F	-3.67467400	-1.41900900	-4.29047800
F	-3.88218000	-4.05552100	-0.24148300
F	-3.24696200	2.10776600	5.28665100
F	-4.59799400	-3.68854900	-2.93137900
C	2.86424800	-4.62148400	-1.64437000
H	3.26617100	-5.62891200	-1.43932600
H	1.95765100	-4.75556800	-2.24781800
H	3.60639600	-4.10030300	-2.26573700
C	0.10527600	-4.71041700	-0.01939800
H	-0.14559200	-4.55232000	-1.07791200
H	0.27055000	-5.79435900	0.10765300
H	-0.77315800	-4.44417100	0.57760400
C	0.59425800	-3.22979700	2.83207600
H	-0.45026100	-3.34911400	2.52381000
H	0.82028000	-4.03817500	3.54867000
H	0.67341100	-2.28285300	3.38550100
C	3.61710500	-2.20569300	2.90270900
H	2.94191900	-1.54878500	3.46941200
H	3.95958300	-2.99018300	3.59990400
H	4.49788500	-1.61509200	2.61881700
C	5.05777700	-3.13811200	0.16425500
H	5.52425600	-2.27248700	0.65079900
H	5.58764700	-4.03862700	0.52110700
H	5.24860200	-3.05994200	-0.91493000
H	3.39704200	1.62424600	1.58770900
H	5.21303400	-0.07118000	-1.97402600

F	7.15512400	3.63535300	-0.09922200
Frequencies --	-1062.2773	-2.8552	14.8392
Frequencies --	20.6407	22.7626	27.9776
Frequencies --	29.0303	31.5768	35.7732
Frequencies --	38.1734	40.2395	46.7229
Frequencies --	49.6103	57.5199	68.9312
Frequencies --	94.2320	97.9622	102.5197
Frequencies --	109.7922	110.8104	113.4371
Frequencies --	114.7219	116.8288	119.3214
Frequencies --	122.6071	126.5137	130.6337
Frequencies --	135.8934	138.3081	143.1707
Frequencies --	144.3638	149.8678	154.7678
Frequencies --	156.3055	160.5255	161.8994
Frequencies --	164.3627	166.8889	172.4646
Frequencies --	188.5667	202.6037	211.9188
Frequencies --	217.8461	221.2229	224.1927
Frequencies --	238.0300	241.8948	263.7740
Frequencies --	264.3488	264.7137	265.9050
Frequencies --	274.2587	275.6208	278.5487
Frequencies --	284.3762	287.9483	293.0034
Frequencies --	295.5581	302.2377	302.8797
Frequencies --	304.1349	306.7248	325.2541
Frequencies --	326.4664	332.8593	344.3829
Frequencies --	356.6517	361.2883	368.4348
Frequencies --	373.3484	377.5597	378.6737
Frequencies --	381.2763	392.5261	394.0203
Frequencies --	404.6517	409.0387	417.6878
Frequencies --	431.3855	432.2118	433.7444
Frequencies --	449.3251	454.9556	456.4861
Frequencies --	464.0373	481.0656	512.3245
Frequencies --	531.7984	535.0666	537.0444
Frequencies --	537.4784	544.7841	554.2441
Frequencies --	555.2881	568.8539	576.5770
Frequencies --	582.7011	595.2547	601.3223
Frequencies --	607.1379	612.8956	631.7848
Frequencies --	634.9221	636.3487	638.4426
Frequencies --	643.7312	655.3596	672.0059
Frequencies --	701.6719	704.6164	718.8547
Frequencies --	723.6810	734.2071	746.7126
Frequencies --	749.0084	762.2414	771.2080
Frequencies --	791.8203	800.6364	801.9567
Frequencies --	806.2673	831.0818	842.4982
Frequencies --	871.0427	877.9397	886.2346
Frequencies --	903.7194	912.7278	918.9501
Frequencies --	923.7315	945.9300	959.4469
Frequencies --	967.6367	969.6277	1012.8382
Frequencies --	1013.9005	1018.7215	1029.2626
Frequencies --	1039.2024	1041.0427	1044.1093
Frequencies --	1045.3612	1046.7576	1048.2730
Frequencies --	1050.7445	1054.5541	1057.4133
Frequencies --	1086.0770	1088.3751	1097.5120
Frequencies --	1113.4874	1124.2458	1169.1086
Frequencies --	1171.1367	1174.1920	1203.5494
Frequencies --	1209.7857	1213.4802	1216.4399
Frequencies --	1256.3258	1268.1421	1297.9672
Frequencies --	1305.3025	1316.2311	1319.6781
Frequencies --	1326.7347	1337.5477	1343.8556
Frequencies --	1348.2685	1351.2637	1360.3512
Frequencies --	1407.6322	1411.6368	1413.4463
Frequencies --	1419.7171	1421.6424	1422.7746
Frequencies --	1423.5083	1426.5826	1427.2934
Frequencies --	1428.6822	1435.0709	1450.6578

Frequencies --	1452.1606	1464.1917	1467.4962
Frequencies --	1469.1400	1471.6316	1472.1030
Frequencies --	1481.6406	1485.2551	1490.6973
Frequencies --	1494.1867	1495.3379	1498.7593
Frequencies --	1499.1391	1505.3644	1507.7363
Frequencies --	1510.2254	1513.7489	1525.6931
Frequencies --	1593.8814	1595.9743	1598.7194
Frequencies --	1599.6977	1616.1198	1617.5803
Frequencies --	1620.5367	1622.8091	1830.5178
Frequencies --	2936.7918	3008.9551	3010.5056
Frequencies --	3012.0283	3014.0037	3015.1768
Frequencies --	3032.3695	3088.2584	3096.3158
Frequencies --	3096.8100	3098.4350	3100.1340
Frequencies --	3101.7309	3128.7718	3136.7511
Frequencies --	3142.1922	3147.4558	3156.9259
Frequencies --	3168.2547	3193.4623	3197.3828
Frequencies --	3200.1458	3216.4767	3220.1526

Catalyst 6:

vacuum	toluene-like solvent	D3 dispersion
-3056.7114277	-3056.7241282	-0.55922899

Imaginary frequency corresponding to vibration along the reaction coordinate: -900 cm^{-1} .

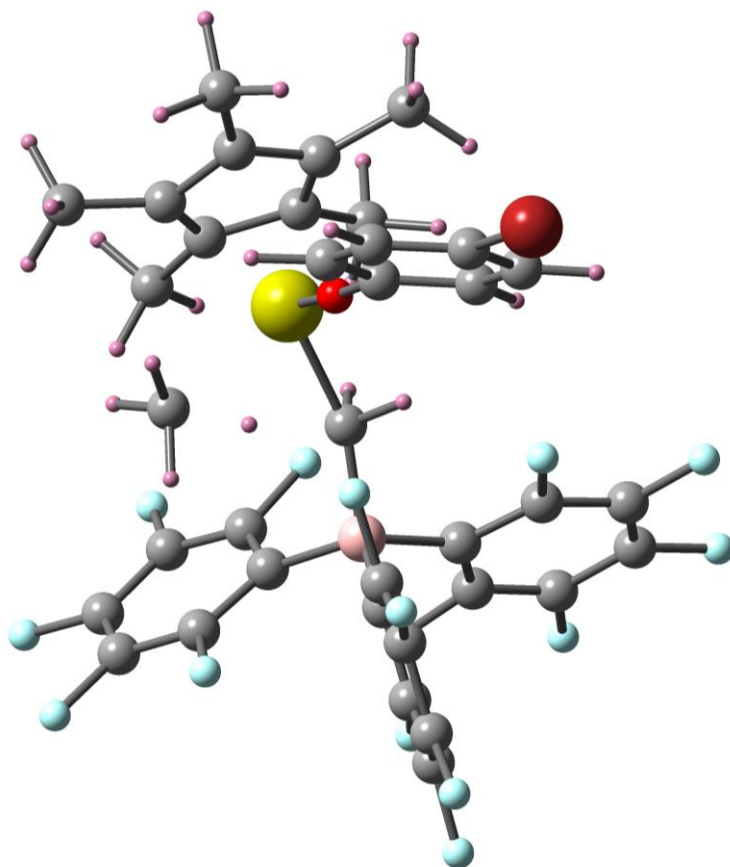
Ti	-1.57445600	1.87057500	0.02018800
C	-0.77644700	1.83934100	-2.16431700
H	-0.51887000	0.97317700	-2.79007200
H	-1.81112000	2.10849200	-2.42637800
H	-0.11040700	2.67345500	-2.40447800
O	-2.98350000	0.79442600	-0.15819300
C	-4.12361800	0.01286400	-0.14727900
C	-4.25262300	-1.02316200	0.81049500
C	-5.13892800	0.23477900	-1.10893400
C	-5.40676100	-1.82929400	0.81258500
C	-6.29122300	-0.57497800	-1.10686400
C	-6.41777500	-1.59662300	-0.14316900
H	-5.50891700	-2.63360800	1.54055300
H	-7.07395700	-0.41444100	-1.84781100
C	-1.14538100	3.43966700	1.83875800
C	-0.55856000	4.05043300	0.67640100
C	-2.57874300	3.31202600	1.60959300
C	-1.62107600	4.29853200	-0.28110700
C	-2.87111700	3.87395900	0.31141400

F	0.05394100	-5.55995500	-2.80444800
C	0.34246800	-4.35137900	-2.18738300
C	1.64072100	-4.07160800	-1.72739700
C	-0.65343900	-3.37856800	-2.01571000
C	1.90146200	-2.83900000	-1.10227400
F	2.65122200	-5.00995800	-1.90100900
C	-0.33230700	-2.16024100	-1.38434000
F	-1.94625300	-3.61972200	-2.47299700
C	0.94021400	-1.82031300	-0.88470700
F	3.22833400	-2.62980900	-0.71061100
F	-1.39711100	-1.24777500	-1.29617200
B	1.35765500	-0.43049700	-0.05801400
C	1.93121400	-1.01045500	1.42180300
C	2.45597500	0.50759400	-0.89575000
C	0.09668900	0.63272800	0.32704500
C	3.27976700	-1.04883800	1.85551800
C	1.04185400	-1.59279800	2.35752800
C	2.74694000	0.39128000	-2.27522300
C	3.13835400	1.58734900	-0.28558300
H	-0.69950300	0.04730900	0.84136600
H	0.55884600	1.36052600	1.01404200
H	-0.27863400	1.24372500	-1.09769900
C	3.70175700	-1.56262100	3.09966400
F	4.31243900	-0.58536200	1.03852600
C	1.40904400	-2.11917500	3.60983900
F	-0.33363100	-1.70860900	2.05379200
C	3.66484900	1.20693100	-2.97111100
F	2.09241900	-0.55850000	-3.07285200
C	4.05875900	2.43242000	-0.92877300
F	2.90634100	1.88036000	1.07129800
C	2.75947100	-2.09682000	3.99288000
F	5.04676100	-1.55169700	3.44919800
F	0.45153900	-2.65915600	4.46455300
C	4.33785000	2.23420500	-2.29166300
F	3.89478700	1.01333900	-4.32846100
F	4.68423400	3.46430900	-0.23509300
F	3.15406200	-2.60215200	5.22326600
F	5.23863400	3.05382300	-2.95597600
C	-1.47266200	5.09119500	-1.55964000
H	-1.69720700	6.15398300	-1.36499800
H	-0.45100100	5.04691900	-1.95770500
H	-2.15696600	4.75823000	-2.35245100
C	0.88070700	4.48700400	0.51815000
H	1.40802000	3.93790600	-0.27297200
H	0.92968300	5.55737000	0.26373900
H	1.44899900	4.33797300	1.44311600
C	-0.43074700	3.11266000	3.13238900
H	0.49951700	2.54903400	2.97974900
H	-0.16065400	4.04669700	3.65301500
H	-1.06243200	2.53138200	3.81629900
C	-3.59289000	2.83800400	2.62768800
H	-3.25005700	1.95561100	3.18686800
H	-3.78456100	3.63476400	3.36705300
H	-4.55462700	2.58333800	2.16503400
C	-4.24582900	4.09158100	-0.27931100
H	-4.95348800	3.29844600	-0.00716100
H	-4.66403400	5.04205800	0.09560800

H	-4.22165800	4.16350100	-1.37541600
H	-3.45443400	-1.20946100	1.52858400
H	-5.02205800	1.01754100	-1.85796300
C1	-7.91411500	-2.63669300	-0.13546200

Frequencies --	-899.8536	9.9785	13.7233
Frequencies --	16.3306	21.4222	27.5231
Frequencies --	28.3740	32.0373	33.5915
Frequencies --	36.7971	40.4971	47.8332
Frequencies --	50.5615	54.9780	62.0971
Frequencies --	68.1757	85.3580	97.7785
Frequencies --	99.6372	102.2363	111.2963
Frequencies --	114.9014	117.8057	120.4170
Frequencies --	125.1494	125.8379	128.4585
Frequencies --	136.0273	138.7736	140.7698
Frequencies --	143.4972	145.9272	155.3998
Frequencies --	156.2675	160.1819	162.0421
Frequencies --	164.7264	168.8198	173.7235
Frequencies --	188.2611	201.5930	205.2561
Frequencies --	215.1928	216.9175	221.8075
Frequencies --	223.8589	229.9366	250.8057
Frequencies --	264.4089	264.6022	264.8620
Frequencies --	269.5499	273.4758	274.9252
Frequencies --	275.7863	278.6348	281.6699
Frequencies --	287.7719	292.1295	301.7752
Frequencies --	302.3838	303.5465	307.4714
Frequencies --	323.0050	326.1390	330.2917
Frequencies --	335.2836	344.2710	360.5617
Frequencies --	371.6345	377.2366	378.1414
Frequencies --	379.5397	381.1800	391.9951
Frequencies --	396.2957	405.3800	408.7593
Frequencies --	430.9788	431.8277	434.3976
Frequencies --	445.5029	447.0217	456.9700
Frequencies --	462.1656	465.2677	482.9588
Frequencies --	490.9093	532.2927	535.8197
Frequencies --	536.6734	540.0956	544.5123
Frequencies --	555.1845	561.0480	579.5558
Frequencies --	581.3442	594.4119	598.5850
Frequencies --	601.3273	621.2444	628.1210
Frequencies --	634.9226	636.1484	638.5909
Frequencies --	642.4565	642.8320	656.1924
Frequencies --	670.1762	693.9309	702.3936
Frequencies --	718.4352	722.7998	733.3378
Frequencies --	746.2975	748.7239	762.1586
Frequencies --	770.7631	777.2829	784.8495
Frequencies --	804.1035	805.5763	840.8753
Frequencies --	871.5654	882.9134	902.6377
Frequencies --	910.5328	912.6814	922.9065
Frequencies --	923.5186	929.9089	943.9255
Frequencies --	968.8402	972.3973	1006.3614
Frequencies --	1013.3335	1018.7404	1028.2356
Frequencies --	1039.3075	1039.5640	1043.9325
Frequencies --	1046.5996	1047.6716	1050.1466
Frequencies --	1052.7542	1055.2743	1057.6631
Frequencies --	1076.3208	1087.6482	1089.6183
Frequencies --	1093.4919	1117.4160	1125.0130
Frequencies --	1170.7895	1175.1707	1190.6843
Frequencies --	1209.5144	1213.6498	1216.5891
Frequencies --	1250.9849	1268.4048	1300.1986
Frequencies --	1308.3646	1315.1426	1319.4780
Frequencies --	1325.5917	1336.4305	1342.6002
Frequencies --	1346.7933	1352.0738	1354.5505

Frequencies --	1410.0277	1410.7875	1415.7290
Frequencies --	1415.8475	1418.9123	1422.1455
Frequencies --	1424.3944	1426.5645	1429.3676
Frequencies --	1431.9646	1435.7252	1450.1356
Frequencies --	1452.7026	1463.1675	1467.2161
Frequencies --	1468.0065	1469.7390	1471.8673
Frequencies --	1484.8133	1485.3920	1490.2837
Frequencies --	1491.8932	1494.3529	1500.1992
Frequencies --	1502.9857	1506.8082	1507.2059
Frequencies --	1511.6757	1515.4088	1521.5623
Frequencies --	1582.3045	1593.4194	1595.4170
Frequencies --	1598.5705	1604.5466	1617.0470
Frequencies --	1619.2362	1622.9451	1815.9251
Frequencies --	2923.0647	3010.5860	3012.2141
Frequencies --	3013.3216	3019.7392	3030.8609
Frequencies --	3031.1868	3090.8153	3099.5007
Frequencies --	3099.7963	3101.9350	3109.2587
Frequencies --	3115.8453	3129.2307	3139.0069
Frequencies --	3141.5690	3144.6789	3147.4090
Frequencies --	3160.0743	3188.5085	3195.0570
Frequencies --	3197.7917	3213.5011	3217.6161

Catalyst 7:

vacuum	toluene-like solvent	D3 dispersion
-3054.9169674	-3054.9294366	-0.56005954

Imaginary frequency corresponding to vibration along the reaction coordinate: -1068 cm^{-1} .

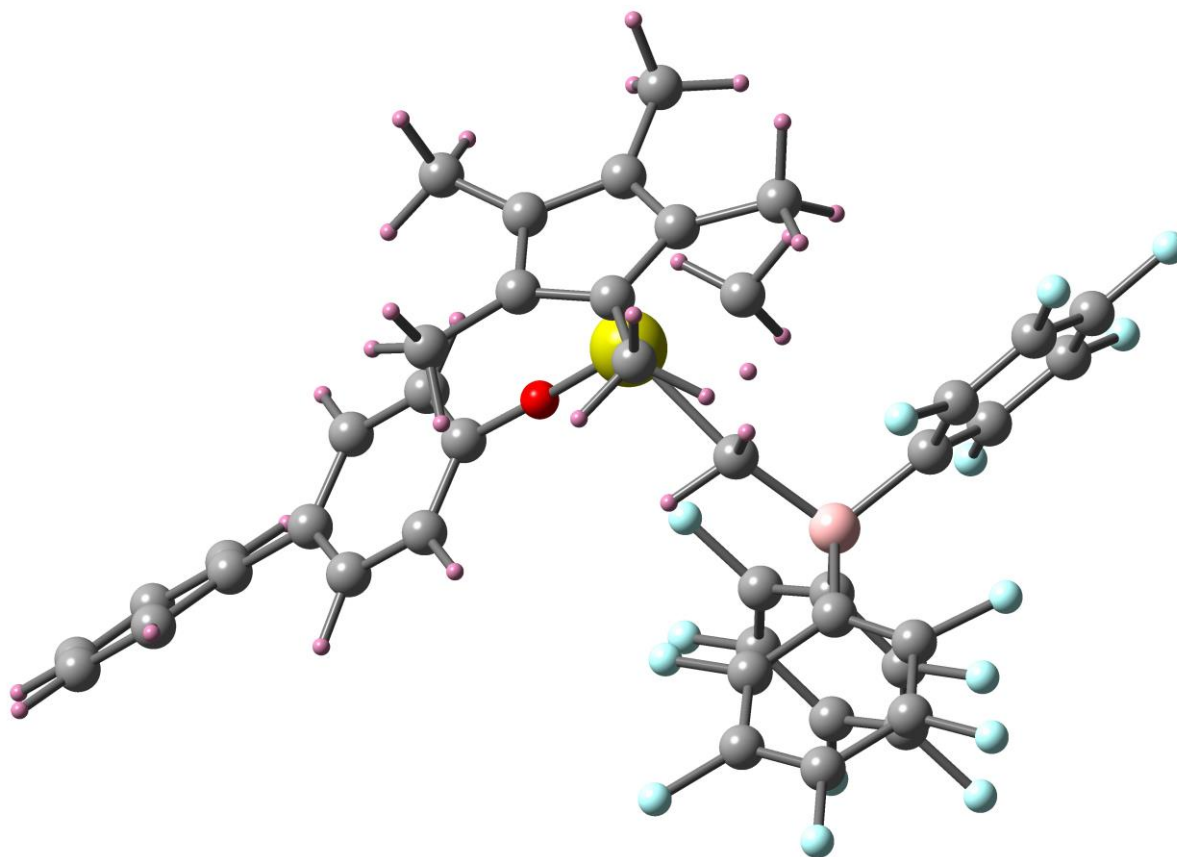
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C	-0.19379800	1.96538800	-2.16384500
H	0.01912100	1.07794900	-2.77696000
H	-1.19981600	2.30191800	-2.45730700
H	0.53869800	2.74508500	-2.39173900
O	-2.52840100	1.27603200	-0.15859500
C	-3.76694700	0.66350700	-0.13305000
C	-4.06469200	-0.27586000	0.88436200
C	-4.72088500	0.95412200	-1.13759800
C	-5.32033500	-0.91296800	0.90474800
C	-5.97645100	0.31533100	-1.11946100
C	-6.26973000	-0.60980600	-0.09482400
H	-5.54474100	-1.64012900	1.68489500
H	-6.70745000	0.53621800	-1.89718600
C	-0.11233500	3.66981000	1.71728200
C	0.34358500	4.20731800	0.46637800
C	-1.57024600	3.65439100	1.69810400
C	-0.82730500	4.53601700	-0.33267200
C	-2.00552200	4.23659900	0.44891500
F	-0.32538000	-5.51244300	-2.77211600

C	0.11383500	-4.34637000	-2.16196300
C	1.43432400	-4.23505100	-1.69366600
C	-0.74804900	-3.25045600	-2.00614200
C	1.84994300	-3.04134100	-1.07724800
F	2.31445900	-5.29899700	-1.85200200
C	-0.27488000	-2.07859000	-1.38232200
F	-2.05787900	-3.32555700	-2.47164400
C	1.02882600	-1.90377500	-0.87751800
F	3.19006600	-3.00286500	-0.67681700
F	-1.21247200	-1.03427800	-1.30684600
B	1.61912700	-0.57149400	-0.06322500
C	2.12162400	-1.19902700	1.42161100
C	2.82145300	0.22109200	-0.90730100
C	0.49313600	0.63511800	0.30997200
C	3.45669500	-1.38761400	1.85649900
C	1.17065500	-1.66282800	2.36258800
C	3.12041200	0.04452400	-2.27844900
C	3.60244300	1.23695400	-0.30730500
H	-0.38525000	0.15006500	0.78943600
H	1.02361600	1.29359300	1.01730900
H	0.22028700	1.28536600	-1.07389400
C	3.81697900	-1.93429700	3.10589000
F	4.53498700	-1.05406400	1.03476400
C	1.47507300	-2.21557500	3.62036400
F	-0.20828500	-1.61708800	2.05906300
C	4.12719800	0.74810100	-2.97425500
F	2.38587800	-0.85188200	-3.06747400
C	4.61320500	1.97029100	-0.94982100
F	3.38231200	1.57691400	1.04152400
C	2.81933400	-2.34701700	4.00347400
F	5.15439000	-2.07588800	3.45637400
F	0.46194400	-2.63066900	4.48073400
C	4.89015200	1.71673100	-2.30378300
F	4.35752800	0.50352400	-4.32317400
F	5.32833500	2.94956900	-0.26592800
F	3.15347800	-2.88285500	5.23892300
F	5.87769900	2.42877700	-2.96894000
C	-0.80585400	5.29152800	-1.64198000
H	-0.88316700	6.37520600	-1.44663900
H	0.12560900	5.13279000	-2.19986700
H	-1.64282200	5.02331700	-2.30183900
C	1.77106300	4.52379200	0.08258400
H	2.07161000	4.06611800	-0.87076900
H	1.89194400	5.61363600	-0.03404400
H	2.48487000	4.19393500	0.84409700
C	0.73684700	3.31097600	2.91660500
H	1.75229300	3.00271500	2.64247100
H	0.82900900	4.19085500	3.57660900
H	0.29257800	2.50578200	3.51864800
C	-2.45711100	3.28365300	2.86702200
H	-2.07145800	2.42346700	3.43291700
H	-2.52041500	4.12907600	3.57410300
H	-3.48094000	3.04430700	2.55197100
C	-3.43086700	4.57309200	0.07447000
H	-4.15122300	3.83455000	0.44862400
H	-3.70706600	5.54818700	0.51232200
H	-3.56934300	4.65801500	-1.01190900

H	-3.31802100	-0.51902100	1.64036900
H	-4.47973400	1.66080900	-1.93161200
Br	-8.02153000	-1.49524300	-0.06472800

Frequencies	--	-1068.2338	6.5137	11.3833
Frequencies	--	18.0512	20.6984	23.5537
Frequencies	--	28.3207	29.4352	32.5881
Frequencies	--	36.8055	41.7561	46.9142
Frequencies	--	48.4832	53.7581	61.8256
Frequencies	--	65.9921	80.0269	91.7950
Frequencies	--	97.0195	102.7614	104.8699
Frequencies	--	109.0424	111.9713	115.8934
Frequencies	--	119.9545	124.5987	125.8733
Frequencies	--	129.6255	134.6726	138.2530
Frequencies	--	142.9861	143.2377	146.3409
Frequencies	--	155.6002	158.6236	161.1676
Frequencies	--	161.9048	166.9520	172.0870
Frequencies	--	183.3685	200.9988	211.9082
Frequencies	--	215.4188	219.4220	223.6116
Frequencies	--	231.2722	233.6584	240.5200
Frequencies	--	248.4651	262.1887	264.2977
Frequencies	--	264.5627	265.3706	274.4158
Frequencies	--	275.6017	278.2518	282.2968
Frequencies	--	288.3153	292.0006	301.1352
Frequencies	--	302.2189	302.7303	306.9500
Frequencies	--	322.3347	325.4954	330.4188
Frequencies	--	339.8286	350.8951	361.1729
Frequencies	--	371.6796	377.4016	378.5210
Frequencies	--	381.1342	382.3218	390.7119
Frequencies	--	395.7796	402.2177	412.2246
Frequencies	--	428.5112	431.4612	432.2299
Frequencies	--	433.6386	444.5322	451.7934
Frequencies	--	456.4782	464.0363	487.3224
Frequencies	--	506.1853	531.4547	535.2714
Frequencies	--	536.3646	537.4246	544.8695
Frequencies	--	553.8693	555.4583	570.9728
Frequencies	--	581.7417	593.9835	600.3486
Frequencies	--	603.6831	612.0856	627.5286
Frequencies	--	634.8031	635.7906	638.1997
Frequencies	--	643.0437	654.4576	670.7994
Frequencies	--	691.6735	695.9870	698.7997
Frequencies	--	718.5859	723.2623	733.4544
Frequencies	--	746.4761	748.7552	761.8777
Frequencies	--	771.3430	799.8192	803.4299
Frequencies	--	817.5811	830.5170	842.4519
Frequencies	--	871.6522	879.1351	883.8229
Frequencies	--	903.3500	912.4854	919.5899
Frequencies	--	925.8775	953.6131	967.5347
Frequencies	--	968.8096	969.1632	1005.6852
Frequencies	--	1017.4107	1018.5257	1028.6609
Frequencies	--	1038.3318	1040.0381	1042.9092
Frequencies	--	1044.1978	1046.4511	1049.8987
Frequencies	--	1052.7608	1053.3504	1057.1541
Frequencies	--	1064.4706	1085.6425	1088.2620
Frequencies	--	1094.5359	1116.3848	1123.5754
Frequencies	--	1170.3070	1174.2361	1192.5119
Frequencies	--	1209.8601	1213.3386	1216.4006
Frequencies	--	1252.5919	1265.2761	1303.4852
Frequencies	--	1307.0797	1316.5178	1320.4401
Frequencies	--	1326.1734	1337.6199	1343.5185
Frequencies	--	1345.2330	1349.5420	1352.0144
Frequencies	--	1407.4849	1408.1168	1411.5679

Frequencies --	1413.3236	1419.8134	1422.0084
Frequencies --	1422.9578	1425.9587	1428.1533
Frequencies --	1430.0078	1435.7097	1450.7459
Frequencies --	1451.5835	1463.2939	1467.6680
Frequencies --	1469.0024	1470.5965	1471.6124
Frequencies --	1479.6120	1481.6560	1488.0344
Frequencies --	1488.9998	1494.1923	1498.2884
Frequencies --	1500.2580	1504.7882	1505.5182
Frequencies --	1510.1850	1514.2649	1526.4195
Frequencies --	1577.9294	1594.0610	1596.0741
Frequencies --	1597.5038	1598.9597	1617.4087
Frequencies --	1620.5516	1622.7249	1821.7454
Frequencies --	2941.7293	3008.5320	3010.7002
Frequencies --	3012.2886	3014.8215	3020.7829
Frequencies --	3032.2180	3088.0524	3095.9691
Frequencies --	3097.9162	3099.0717	3102.5667
Frequencies --	3103.0581	3128.7469	3136.9762
Frequencies --	3141.4515	3145.9554	3154.5815
Frequencies --	3170.4650	3190.8038	3192.3695
Frequencies --	3193.5038	3209.3081	3213.3457

Catalyst 8:

vacuum	toluene-like solvent	D3 dispersion
-3273.3085715	-3273.3224593	-0.62631293

Imaginary frequency corresponding to vibration along the reaction coordinate: -970 cm^{-1} .

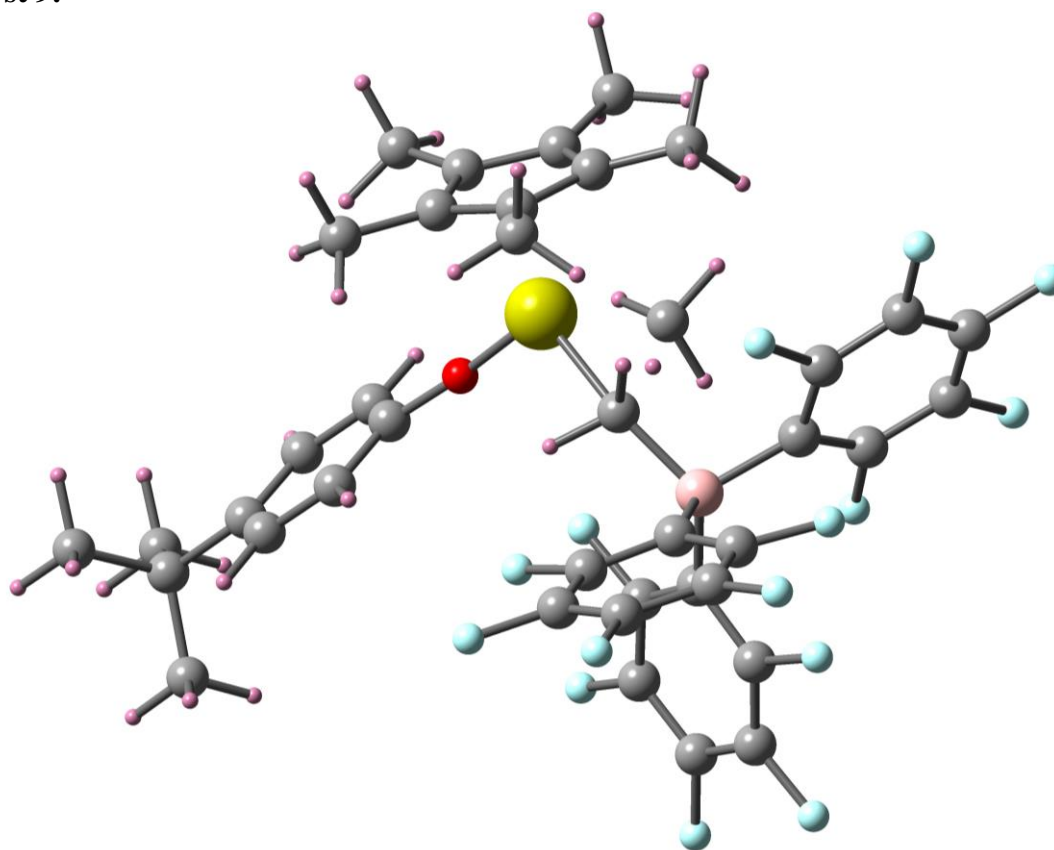
Ti	-0.57012200	2.26243200	0.02429300
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H	0.25346600	1.11409100	-2.78755700
H	-0.81054200	2.46664900	-2.43734800
H	0.96830900	2.71257900	-2.42073400
O	-2.18949200	1.54443700	-0.12378300
C	-3.47932600	1.04376000	-0.10060900
C	-3.87210200	0.15615500	0.92980100
C	-4.39354000	1.38991600	-1.12356800
C	-5.17476400	-0.37097500	0.93345900
C	-5.69175100	0.85052200	-1.10775400
C	-6.11613800	-0.03865300	-0.08109400
H	-5.44846100	-1.08184800	1.71388500
H	-6.39040300	1.14296600	-1.89264200
C	0.33288500	3.73165000	1.76225300
C	0.92051600	4.20182700	0.53803500
C	-1.11309300	3.88360500	1.65743300
C	-0.15499800	4.64498800	-0.33282000
C	-1.40507000	4.48440000	0.37588400

F	-0.71182600	-5.40005300	-2.68571200
C	-0.14708900	-4.27797700	-2.09584000
C	1.18191900	-4.29899200	-1.63933800
C	-0.88757900	-3.09552400	-1.95023200
C	1.72598000	-3.14690400	-1.04361800
F	1.94440200	-5.45181100	-1.78865100
C	-0.28877900	-1.97138600	-1.34707700
F	-2.20171600	-3.03863100	-2.40698500
C	1.03003000	-1.92732400	-0.85253600
F	3.06668600	-3.24494300	-0.65457200
F	-1.10882300	-0.83270100	-1.28559400
B	1.76050100	-0.65130800	-0.06105500
C	2.22356800	-1.31477400	1.42226400
C	3.02399100	0.00880100	-0.93230100
C	0.77097900	0.66800200	0.31859600
C	3.53991900	-1.63146400	1.83975100
C	1.24615600	-1.67665200	2.38106800
C	3.27431000	-0.20610700	-2.30784200
C	3.92165200	0.93929100	-0.35623400
H	-0.12985600	0.28346100	0.84876600
H	1.39199500	1.28519000	0.98823600
H	0.52261200	1.32674900	-1.09669900
C	3.86405400	-2.19899700	3.08973900
F	4.63355000	-1.41711000	0.99847200
C	1.51419700	-2.24580900	3.63988500
F	-0.12594600	-1.50120500	2.09644600
C	4.33595300	0.38134900	-3.02917300
F	2.43306700	-1.02400500	-3.07559300
C	4.99214300	1.55581600	-1.02516200
F	3.76918000	1.31128100	0.99292200
C	2.84474100	-2.50414800	4.00566500
F	5.18667600	-2.46763100	3.42269600
F	0.47845700	-2.55388800	4.51842500
C	5.21260500	1.26577800	-2.38213900
F	4.51089500	0.10549700	-4.38070100
F	5.82363500	2.45532300	-0.36361000
F	3.14379000	-3.05867000	5.24216400
F	6.25834600	1.86157400	-3.07244800
C	0.02930700	5.37516800	-1.64371900
H	-0.01106800	6.46498700	-1.47419000
H	1.00052100	5.15653300	-2.10479300
H	-0.75243200	5.13778600	-2.37927500
C	2.39711900	4.35218300	0.24765600
H	2.73464800	3.74738200	-0.60545900
H	2.63056000	5.40286300	0.01182600
H	3.00825900	4.06199300	1.10923700
C	1.08129000	3.28635900	3.00043200
H	1.90226400	2.59160100	2.77952500
H	1.52468400	4.16367800	3.50116100
H	0.42093300	2.79807700	3.72890700
C	-2.10817300	3.62861600	2.76874000
H	-1.86544600	2.73157200	3.35631800
H	-2.11546700	4.48091600	3.47025800
H	-3.13051800	3.50880600	2.38839500
C	-2.75756900	4.96727600	-0.09670800
H	-3.58105900	4.33740900	0.26299900
H	-2.93896000	5.98846600	0.28189600

H	-2.82377500	5.01564000	-1.19240200
H	-3.15424300	-0.13802100	1.69588900
H	-4.08602400	2.06683600	-1.92108400
C	-7.49636200	-0.61269800	-0.07492400
C	-8.19795800	-0.82618000	1.14395200
C	-8.14879200	-0.96767900	-1.28815800
C	-9.49816500	-1.37081000	1.15042600
H	-7.73722300	-0.54004700	2.09129100
C	-9.44807800	-1.51431900	-1.28328400
H	-7.62545900	-0.85130100	-2.23882800
C	-10.13103000	-1.71828700	-0.06368400
H	-10.01819800	-1.51699900	2.10009000
H	-9.92104600	-1.79140500	-2.22833000
H	-11.13750900	-2.14272700	-0.05938700

Frequencies --	-969.8636	5.9919	8.2329
Frequencies --	10.7438	17.1850	19.2947
Frequencies --	27.5830	29.0336	31.9207
Frequencies --	36.5015	40.2018	45.2021
Frequencies --	47.8675	50.5592	60.3199
Frequencies --	66.3972	69.5973	85.0221
Frequencies --	88.9071	91.5553	98.7034
Frequencies --	104.9404	107.6831	112.2731
Frequencies --	114.6627	115.5476	122.9386
Frequencies --	125.3624	128.4599	130.7315
Frequencies --	138.1021	139.9713	143.4745
Frequencies --	143.6886	145.2534	156.1956
Frequencies --	157.6800	161.3343	162.7168
Frequencies --	164.7984	168.7978	175.7036
Frequencies --	189.6987	203.6633	209.4976
Frequencies --	215.0576	219.4423	223.9401
Frequencies --	224.8934	239.7614	248.4647
Frequencies --	264.3557	264.6750	265.0187
Frequencies --	271.8780	274.6015	276.1036
Frequencies --	279.7178	281.6990	285.7809
Frequencies --	291.1256	301.7650	302.1049
Frequencies --	302.9731	307.4216	320.1139
Frequencies --	326.2903	329.7640	334.8873
Frequencies --	342.6994	359.7392	370.0273
Frequencies --	375.5973	377.7886	379.0831
Frequencies --	381.7945	390.6523	395.0321
Frequencies --	400.6032	406.2975	413.7143
Frequencies --	415.7699	427.6560	431.3686
Frequencies --	432.2740	433.6977	450.4704
Frequencies --	456.6901	457.1864	463.8685
Frequencies --	478.7450	510.0260	532.2260
Frequencies --	536.0918	537.2808	539.1664
Frequencies --	544.5209	553.2966	554.5205
Frequencies --	557.7640	576.6451	581.7091
Frequencies --	593.1759	599.1076	603.1436
Frequencies --	616.0307	622.0890	635.2434
Frequencies --	636.3811	638.2668	638.8043
Frequencies --	642.8266	644.0534	655.7661
Frequencies --	669.3633	694.1789	706.5397
Frequencies --	718.6710	722.1254	722.7551
Frequencies --	733.4368	746.0733	747.4865
Frequencies --	749.5268	762.2026	770.8878
Frequencies --	773.0137	801.5749	804.2639
Frequencies --	827.0825	841.2429	845.6350
Frequencies --	858.2260	872.3117	885.0210
Frequencies --	889.8305	903.9358	913.1708

Frequencies --	920.0130	928.5520	931.5711
Frequencies --	960.0217	968.5464	970.5990
Frequencies --	973.4583	985.9251	1000.0603
Frequencies --	1005.5958	1009.4983	1018.8281
Frequencies --	1022.2749	1028.7310	1038.9175
Frequencies --	1040.1706	1043.6878	1045.2928
Frequencies --	1047.4343	1049.6245	1049.8872
Frequencies --	1051.9256	1054.1447	1057.4243
Frequencies --	1061.8740	1087.2942	1088.6117
Frequencies --	1095.8197	1097.5841	1123.8342
Frequencies --	1129.1621	1170.3727	1174.9719
Frequencies --	1184.5232	1199.2618	1209.3957
Frequencies --	1211.4834	1213.0973	1216.0644
Frequencies --	1252.2869	1267.9810	1298.3164
Frequencies --	1300.7453	1315.5814	1316.2550
Frequencies --	1319.3303	1325.6532	1326.1899
Frequencies --	1337.2354	1343.3112	1348.2681
Frequencies --	1351.0656	1357.5635	1375.0022
Frequencies --	1410.1580	1411.1137	1413.0747
Frequencies --	1419.2171	1421.8779	1424.0166
Frequencies --	1425.0285	1425.6875	1428.0833
Frequencies --	1429.8764	1434.1284	1449.6973
Frequencies --	1451.9176	1453.4794	1461.9310
Frequencies --	1464.6521	1467.3139	1468.9897
Frequencies --	1471.5269	1482.4539	1487.6086
Frequencies --	1488.5428	1490.8401	1493.2983
Frequencies --	1499.0375	1500.2216	1503.8003
Frequencies --	1506.3483	1511.1159	1515.3263
Frequencies --	1517.5970	1520.6148	1571.8078
Frequencies --	1593.8913	1595.8678	1598.3222
Frequencies --	1599.5725	1617.1869	1618.3524
Frequencies --	1619.7834	1622.5871	1624.8443
Frequencies --	1814.7234	2925.6089	3009.5067
Frequencies --	3010.4201	3012.8591	3018.6061
Frequencies --	3025.3903	3031.6349	3094.6532
Frequencies --	3097.9922	3098.5080	3100.8940
Frequencies --	3106.0929	3110.2432	3128.7973
Frequencies --	3138.6334	3142.7060	3144.9150
Frequencies --	3146.7929	3154.6792	3160.2670
Frequencies --	3161.1949	3174.1867	3177.1307
Frequencies --	3181.3395	3183.8684	3187.1100
Frequencies --	3195.0489	3198.7501	3204.3505

Catalyst 9:

vacuum	toluene-like solvent	D3 dispersion
-3199.5142883	-3991.524761*	-0.62232474

*SCF energy in toluene equals LANL2DZ vacuum energy plus 6-311++G** solvation energy, because PCM calculation did not converge with LANL2DZ basis sets.

Imaginary frequency corresponding to vibration along the reaction coordinate: -975 cm^{-1} .

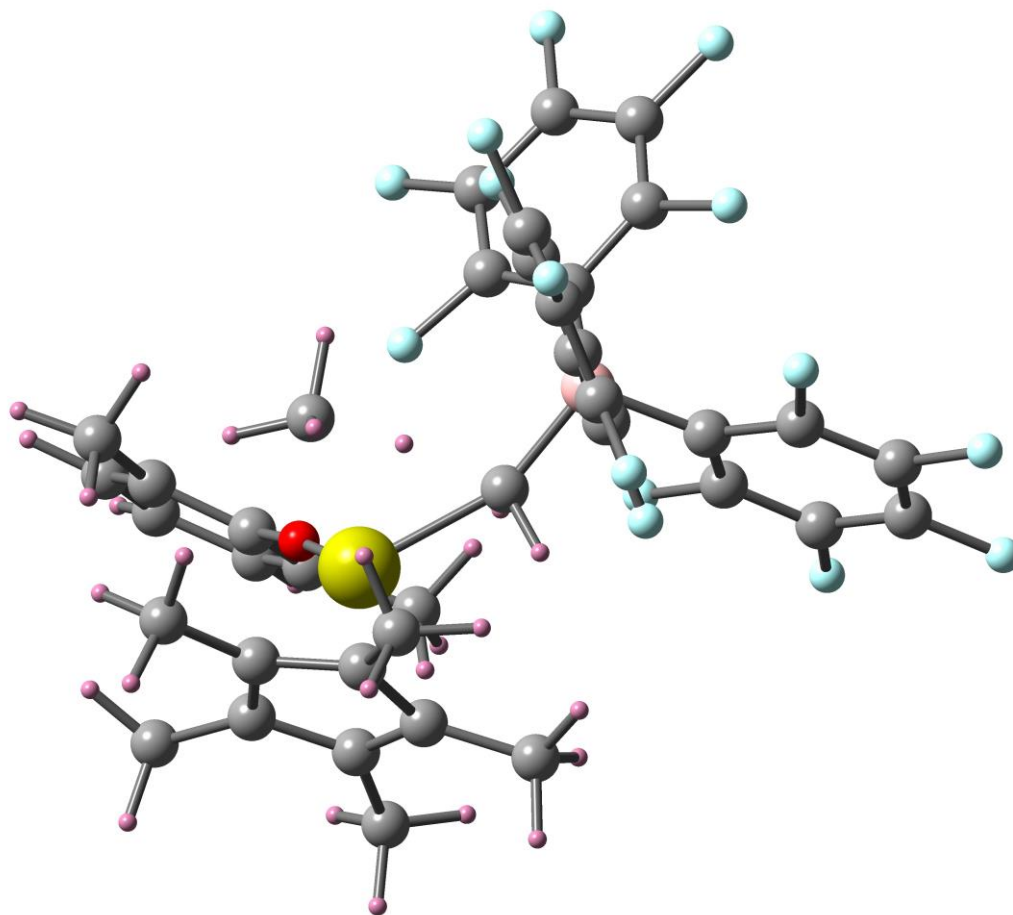
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C	-0.22254700	1.97902900	-2.16920000
H	-0.02866900	1.09332600	-2.79105400
H	-1.22971400	2.32671400	-2.44395700
H	0.51472200	2.75274700	-2.40316300
O	-2.54063400	1.28982000	-0.14769200
C	-3.78414800	0.67721400	-0.13026900
C	-4.10256700	-0.23985800	0.89936500
C	-4.72147700	0.93766200	-1.15268800
C	-5.35365300	-0.87895300	0.89523700
C	-5.96958800	0.28170500	-1.13960700
C	-6.32264800	-0.64183000	-0.12111200
H	-5.56586400	-1.58492200	1.69834300
H	-6.66371800	0.49913900	-1.94917100
C	-0.20871500	3.67268000	1.76902700
C	0.33071900	4.20277600	0.54733100
C	-1.66256300	3.69456200	1.66812600
C	-0.78234400	4.55544800	-0.31750500
C	-2.01073000	4.27817200	0.39256700

F	-0.42510200	-5.50736700	-2.71071800
C	0.03130400	-4.33934400	-2.11569300
C	1.35532400	-4.23822700	-1.65569200
C	-0.81645200	-3.23136900	-1.96859300
C	1.78790000	-3.04274500	-1.05425900
F	2.22243200	-5.31437600	-1.80731300
C	-0.32663300	-2.05815600	-1.36037300
F	-2.12924500	-3.29640500	-2.42887100
C	0.98078400	-1.89407900	-0.86132000
F	3.13105400	-3.01644400	-0.66245400
F	-1.24738100	-1.00030100	-1.29785700
B	1.58726600	-0.55926300	-0.06111000
C	2.09869100	-1.18532600	1.42305400
C	2.79238700	0.21185300	-0.92363300
C	0.48055500	0.66375000	0.31789300
C	3.43538000	-1.38629700	1.84779700
C	1.15129400	-1.63686100	2.37396600
C	3.06463200	0.02651100	-2.29936800
C	3.60457600	1.21346800	-0.34004800
H	-0.38947300	0.19620900	0.83215600
H	1.03542300	1.32535000	1.00265100
H	0.19002900	1.31438900	-1.09478200
C	3.80089500	-1.92911800	3.09737900
F	4.51075700	-1.07193700	1.01455800
C	1.46114200	-2.18567900	3.63223900
F	-0.22895600	-1.58375200	2.08076000
C	4.07270600	0.70797800	-3.01489000
F	2.29998000	-0.85789700	-3.07385800
C	4.61897000	1.92418700	-1.00290800
F	3.41734100	1.56367000	1.01019700
C	2.80703200	-2.32710900	4.00555400
F	5.14006800	-2.08260700	3.43741700
F	0.45136900	-2.58828500	4.50291500
C	4.86708800	1.66208000	-2.36071900
F	4.27442100	0.45530200	-4.36729300
F	5.36771800	2.88876200	-0.33417800
F	3.14632100	-2.85945300	5.24154400
F	5.85801000	2.35149200	-3.04493900
C	-0.66734300	5.30640800	-1.62460100
H	-0.80943500	6.38671700	-1.45000700
H	0.32009500	5.18221900	-2.08670000
H	-1.42311400	4.99989800	-2.36183200
C	1.78725600	4.48444400	0.25382500
H	2.17354700	3.91377500	-0.60201300
H	1.92641400	5.55219400	0.02005200
H	2.42422500	4.24734700	1.11295900
C	0.57994200	3.28981900	3.00329400
H	1.44911500	2.65707700	2.78009700
H	0.96066600	4.19992400	3.49695500
H	-0.03730500	2.75766900	3.73883200
C	-2.62991900	3.35097300	2.78016200
H	-2.30979600	2.47763200	3.36620000
H	-2.71058800	4.19828000	3.48323000
H	-3.63858700	3.14382500	2.40047400
C	-3.40448900	4.64157900	-0.06799300
H	-4.15519000	3.89750000	0.22801400
H	-3.70427200	5.60415400	0.38198400

H	-3.46341100	4.76435800	-1.15799900
H	-3.37081400	-0.46061100	1.67716200
H	-4.47073300	1.63017000	-1.95709200
C	-7.68621800	-1.38810700	-0.08807000
C	-8.45446400	-1.01223300	1.22197100
H	-9.42455300	-1.53293500	1.25577700
H	-7.89313500	-1.29521300	2.12421200
H	-8.64646200	0.07124000	1.26917100
C	-8.59454600	-1.02533100	-1.29948400
H	-9.54231700	-1.57988500	-1.22690400
H	-8.84186600	0.04740800	-1.32358400
H	-8.12711000	-1.29698600	-2.25848400
C	-7.43643400	-2.93211600	-0.12112800
H	-6.89392800	-3.22351600	-1.03362700
H	-6.84894200	-3.27519400	0.74237400
H	-8.39669900	-3.47179600	-0.10657300

Frequencies --	-975.0104	8.2091	12.9820
Frequencies --	15.5484	19.6093	23.8788
Frequencies --	27.9669	29.1331	32.2023
Frequencies --	37.1944	41.1865	46.8987
Frequencies --	49.1491	52.4276	53.9220
Frequencies --	67.4096	74.2037	76.8236
Frequencies --	94.0647	96.5869	97.4963
Frequencies --	102.7228	109.2690	112.0818
Frequencies --	113.4388	116.8692	121.0858
Frequencies --	125.0451	126.7380	132.0475
Frequencies --	137.9508	142.3900	143.5026
Frequencies --	145.1185	155.8141	157.8861
Frequencies --	161.4305	162.1984	167.8365
Frequencies --	171.7933	176.8543	187.8385
Frequencies --	205.7310	212.1320	215.4248
Frequencies --	217.0138	223.6079	224.2607
Frequencies --	227.9263	242.4617	246.1946
Frequencies --	251.0282	261.5141	264.2672
Frequencies --	264.5609	265.2552	274.0508
Frequencies --	275.4205	276.9658	280.9410
Frequencies --	285.6048	290.3341	297.4442
Frequencies --	299.4804	302.0120	302.4644
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Frequencies --	325.8491	329.7838	331.2123
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Frequencies --	379.6989	381.2839	387.8121
Frequencies --	395.5155	400.3280	411.7945
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Frequencies --	432.1661	433.5371	448.5220
Frequencies --	451.6301	456.7160	463.9548
Frequencies --	475.1562	482.2613	531.8982
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Frequencies --	544.6575	552.1557	554.1456
Frequencies --	558.3206	561.2850	576.8835
Frequencies --	581.8229	593.7208	601.5084
Frequencies --	602.1565	617.8850	634.9461
Frequencies --	635.9738	638.1656	638.7313
Frequencies --	642.8130	655.1210	669.8986
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Frequencies --	770.6800	802.1905	804.2001
Frequencies --	825.8620	834.8475	840.1016

Frequencies --	840.5568	873.3726	882.8444
Frequencies --	892.1584	903.8792	912.7232
Frequencies --	920.0408	924.0561	933.5298
Frequencies --	935.5866	957.5451	964.0372
Frequencies --	969.0816	969.2917	981.0996
Frequencies --	1005.2394	1018.5616	1022.8822
Frequencies --	1028.2352	1037.7704	1038.1746
Frequencies --	1039.4022	1042.2272	1043.5457
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Frequencies --	1052.0436	1055.1413	1057.3963
Frequencies --	1086.2965	1089.1888	1096.2217
Frequencies --	1120.7457	1123.7797	1133.4679
Frequencies --	1170.7520	1174.4533	1204.2531
Frequencies --	1209.1446	1212.8493	1214.4276
Frequencies --	1215.8068	1222.2744	1251.3740
Frequencies --	1267.1979	1274.7089	1304.3414
Frequencies --	1315.9601	1319.7899	1326.2022
Frequencies --	1327.0500	1337.0012	1343.0319
Frequencies --	1345.6352	1351.7768	1352.0483
Frequencies --	1399.2184	1401.4585	1409.3134
Frequencies --	1411.0976	1414.2481	1419.2258
Frequencies --	1422.0501	1422.5614	1422.8959
Frequencies --	1424.4581	1428.0185	1428.8057
Frequencies --	1430.2139	1434.2477	1449.9628
Frequencies --	1452.6771	1463.0388	1467.3385
Frequencies --	1468.5145	1470.4838	1471.2713
Frequencies --	1482.6601	1482.8673	1488.1048
Frequencies --	1488.8138	1489.8026	1490.0555
Frequencies --	1493.5971	1499.0644	1499.6909
Frequencies --	1501.4947	1504.5199	1505.6347
Frequencies --	1508.1311	1511.5369	1512.5319
Frequencies --	1514.6327	1520.7212	1521.0405
Frequencies --	1579.7508	1594.0630	1596.0626
Frequencies --	1599.1962	1616.9992	1618.6296
Frequencies --	1619.8002	1622.2966	1812.7879
Frequencies --	2929.5983	3008.4555	3008.6028
Frequencies --	3009.9105	3010.6783	3013.0825
Frequencies --	3016.9210	3018.3935	3027.1479
Frequencies --	3033.5862	3088.8956	3097.4148
Frequencies --	3098.3080	3101.2961	3109.0657
Frequencies --	3109.3394	3109.3578	3112.7372
Frequencies --	3115.5528	3122.9212	3125.6335
Frequencies --	3129.7672	3129.8201	3137.3498
Frequencies --	3140.8320	3143.6102	3145.3989
Frequencies --	3161.0681	3181.4398	3183.2040
Frequencies --	3189.5864	3202.0299	3212.4785

Catalyst 10:

vacuum	toluene-like solvent	D3 dispersion
-3120.9432301	-3120.9546399	-0.59403760

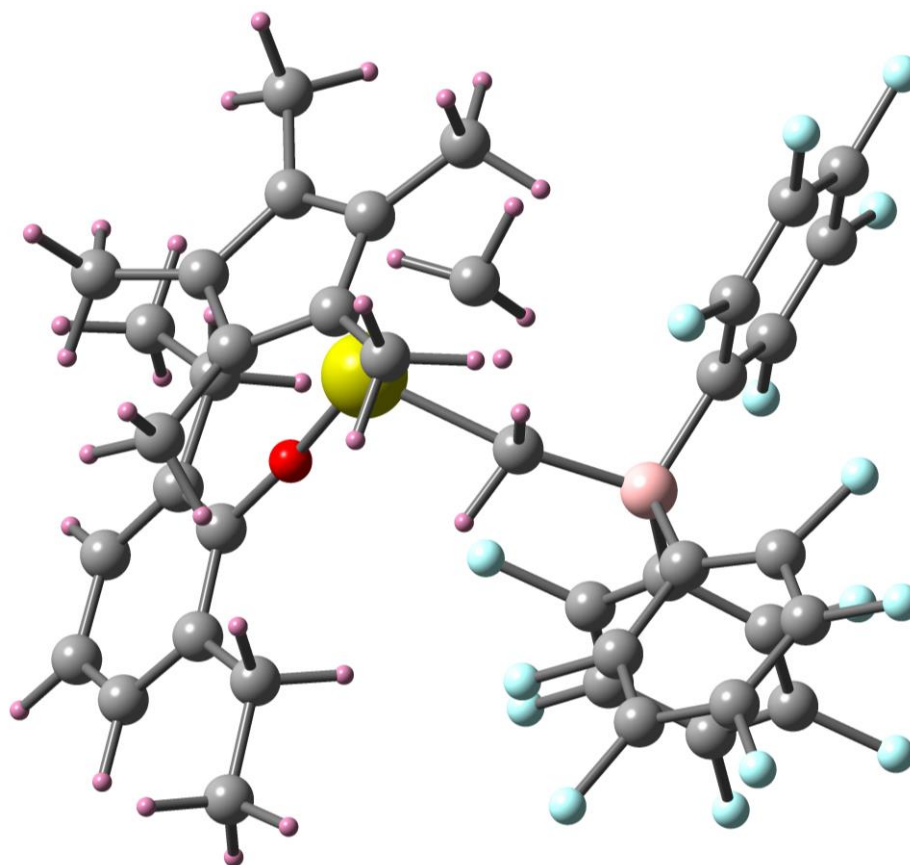
Imaginary frequency corresponding to vibration along the reaction coordinate: -1008 cm^{-1} .

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H	0.90895800	-0.62182300	-2.65784200
H	2.48624300	-1.31105700	-2.30384300
H	1.03453400	-2.35715800	-2.23945500
O	3.25365400	0.28336700	-0.02434200
C	4.15774700	1.34610200	-0.06301900
C	4.21416500	2.24975200	1.03987100
C	4.97914200	1.50620200	-1.21882300
C	5.15941500	3.30057900	0.97923000
C	5.90186400	2.57739100	-1.22775800
C	6.00212000	3.46506700	-0.13770800
H	5.22007600	4.00251200	1.81304300
H	6.53848900	2.71875500	-2.10322400
H	6.72139800	4.28569200	-0.16464000
C	3.19902000	-2.32934100	1.94042800
C	1.91174100	-2.99461300	1.78474400
C	3.98744100	-2.59300600	0.75732100
C	1.88958500	-3.61610500	0.49267500

C	3.16362300	-3.34496600	-0.15965000
F	-1.48923400	5.52252600	-2.74395900
C	-1.42962300	4.27555700	-2.13812800
C	-2.60338000	3.61407700	-1.73848700
C	-0.19674800	3.64346000	-1.91941400
C	-2.51054000	2.35143100	-1.12578500
F	-3.83984100	4.20873300	-1.96159700
C	-0.16559200	2.37717400	-1.30155600
F	0.98327000	4.26643600	-2.31781000
C	-1.29912900	1.66412100	-0.86274300
F	-3.73117100	1.74796600	-0.80329000
F	1.12071900	1.82728500	-1.16198100
B	-1.31485100	0.19396500	-0.06911700
C	-2.16240700	0.50771900	1.35871400
C	-1.99858200	-1.02168100	-0.99082900
C	0.19720700	-0.40920600	0.40685800
C	-3.47619800	0.08422500	1.67927800
C	-1.59194100	1.31779100	2.36947400
C	-2.26261600	-0.96090300	-2.37877400
C	-2.30216300	-2.28717100	-0.43606200
H	0.75412600	0.40536300	0.91730000
H	-0.03816200	-1.22896800	1.10445500
H	0.76916100	-0.89847900	-0.95410600
C	-4.13804400	0.38517800	2.88788300
F	-4.23430000	-0.66275600	0.77511900
C	-2.20706200	1.65025100	3.59080200
F	-0.31581000	1.88983300	2.18058400
C	-2.82374200	-2.01365300	-3.13341300
F	-1.94090300	0.18156300	-3.12596300
C	-2.85721000	-3.36990400	-1.13732600
F	-2.04512700	-2.52767300	0.92762100
C	-3.49799900	1.16964600	3.86039200
F	-5.42571200	-0.08234000	3.12408000
F	-1.55144000	2.44739700	4.52577300
C	-3.13382100	-3.23098800	-2.50773600
F	-3.05463100	-1.86243000	-4.49617500
F	-3.11939200	-4.57703300	-0.49438100
F	-4.13070200	1.47318900	5.05756600
F	-3.67574500	-4.28400500	-3.23078800
C	3.27036800	2.14380400	2.22362900
H	2.24749400	2.42982000	1.93774300
H	3.22173900	1.12684000	2.63394000
H	3.58501700	2.81610600	3.03332700
C	4.85290300	0.59800400	-2.42874800
H	4.96838200	-0.46364000	-2.16517600
H	3.86787800	0.71730400	-2.90675000
H	5.61756400	0.84127500	-3.17887500
C	0.82454700	-4.54582300	-0.04032600
H	1.15258900	-5.59161100	0.09312200
H	-0.12880400	-4.43713300	0.48634700
H	0.63586600	-4.41138200	-1.11441300
C	0.87117500	-3.11896700	2.87549000
H	-0.12061900	-3.37359300	2.48630300
H	1.16549800	-3.91939200	3.57622000
H	0.77055600	-2.19789200	3.46803400
C	3.71225500	-1.71683400	3.22541700
H	4.12411200	-2.50987700	3.87420500

H	4.51795600	-0.99205300	3.05161000
H	2.92079200	-1.21592000	3.79995400
C	5.45011200	-2.25478600	0.58161200
H	5.71352400	-1.28313400	1.01970600
H	6.06787800	-3.01873500	1.08542700
H	5.75389300	-2.24062700	-0.47287800
C	3.62662600	-3.96506000	-1.45877200
H	4.38341000	-3.35581600	-1.97201700
H	4.08568400	-4.94899900	-1.25928100
H	2.80010000	-4.13454800	-2.16037200
Frequencies --	-1007.6984	8.8966	20.7159
Frequencies --	22.8867	26.0413	28.9605
Frequencies --	29.8866	33.0126	38.8758
Frequencies --	40.7285	44.3971	49.2733
Frequencies --	50.6001	66.3296	71.6940
Frequencies --	90.4926	93.3012	102.3967
Frequencies --	108.5301	111.3736	113.7508
Frequencies --	114.9758	117.9948	120.5763
Frequencies --	122.1799	125.9196	130.0922
Frequencies --	137.5353	141.7941	142.0288
Frequencies --	145.2418	145.9285	155.7587
Frequencies --	158.0796	161.0068	161.8955
Frequencies --	164.4464	170.5847	172.2052
Frequencies --	174.0619	186.0767	189.6530
Frequencies --	195.9703	208.7190	215.1389
Frequencies --	217.9467	220.6364	220.8717
Frequencies --	223.5448	236.1242	255.6193
Frequencies --	261.2927	264.5329	264.8499
Frequencies --	265.1937	275.3133	276.5246
Frequencies --	278.5885	284.0283	290.0359
Frequencies --	295.1120	302.8517	302.9630
Frequencies --	303.3672	308.0391	317.3155
Frequencies --	326.2395	329.5677	334.0809
Frequencies --	335.0471	343.1469	357.5008
Frequencies --	363.5754	373.5437	376.7111
Frequencies --	377.7418	380.0746	381.4444
Frequencies --	393.2493	399.0038	401.7508
Frequencies --	431.9455	432.8571	434.4480
Frequencies --	451.4345	456.9876	464.0794
Frequencies --	487.0601	493.5470	511.4569
Frequencies --	529.9016	533.0382	533.7081
Frequencies --	538.9633	545.0223	547.5201
Frequencies --	550.2960	553.8472	555.1023
Frequencies --	563.8463	575.5194	584.1257
Frequencies --	595.6745	601.3678	606.2260
Frequencies --	615.0913	634.5914	635.7800
Frequencies --	637.9868	642.0015	655.0467
Frequencies --	672.6378	702.6195	716.9857
Frequencies --	721.5956	733.2921	735.6002
Frequencies --	741.9142	744.8218	747.7705
Frequencies --	760.7141	769.5546	785.8756
Frequencies --	800.5635	804.0431	842.1759
Frequencies --	868.8834	879.3382	885.2943
Frequencies --	903.4707	910.1181	912.0861
Frequencies --	918.6533	921.9282	927.5403
Frequencies --	966.5988	972.0943	987.1718
Frequencies --	1003.1291	1007.2497	1017.8230
Frequencies --	1027.4690	1038.8292	1041.0644
Frequencies --	1043.9740	1045.5630	1046.4727
Frequencies --	1048.0130	1049.1874	1049.8786
Frequencies --	1053.0702	1055.8275	1056.8269

Frequencies --	1059.5715	1086.5988	1088.1147
Frequencies --	1090.6500	1111.4730	1125.5075
Frequencies --	1171.1741	1174.5280	1193.5399
Frequencies --	1197.4123	1209.7905	1212.5073
Frequencies --	1215.6336	1264.4989	1279.4597
Frequencies --	1282.2263	1304.0951	1317.6087
Frequencies --	1319.5798	1325.1664	1337.4522
Frequencies --	1344.0848	1350.4225	1358.5152
Frequencies --	1360.0975	1408.9248	1410.8916
Frequencies --	1413.9753	1417.5149	1419.0528
Frequencies --	1421.4621	1422.5038	1424.1111
Frequencies --	1425.4515	1427.0117	1428.6159
Frequencies --	1429.0712	1435.5792	1450.6403
Frequencies --	1452.6448	1465.3180	1467.8530
Frequencies --	1468.9714	1470.3656	1471.6815
Frequencies --	1472.8109	1482.8099	1488.7114
Frequencies --	1491.7787	1493.3726	1494.1144
Frequencies --	1498.4497	1500.7704	1503.1894
Frequencies --	1506.1035	1507.6030	1510.4136
Frequencies --	1511.1312	1512.4320	1515.7144
Frequencies --	1528.0115	1594.5808	1596.5130
Frequencies --	1598.5455	1604.3776	1606.9104
Frequencies --	1617.3500	1620.2380	1622.4844
Frequencies --	1823.1007	2952.4524	3008.0040
Frequencies --	3010.2804	3011.4738	3012.8528
Frequencies --	3013.9351	3019.5565	3035.9689
Frequencies --	3047.9625	3095.3864	3096.0860
Frequencies --	3097.2524	3099.0565	3099.8996
Frequencies --	3103.0631	3107.7411	3127.6745
Frequencies --	3131.9226	3139.0037	3140.4323
Frequencies --	3142.2323	3147.6602	3148.2133
Frequencies --	3160.1267	3163.9615	3172.3056
Frequencies --	3175.1086	3195.6298	3197.1725

Catalyst 11:

vacuum	toluene-like solvent	D3 dispersion
-3199.5139592	-3199.5248465	-0.62981350

Imaginary frequency corresponding to vibration along the reaction coordinate: -964 cm^{-1} .

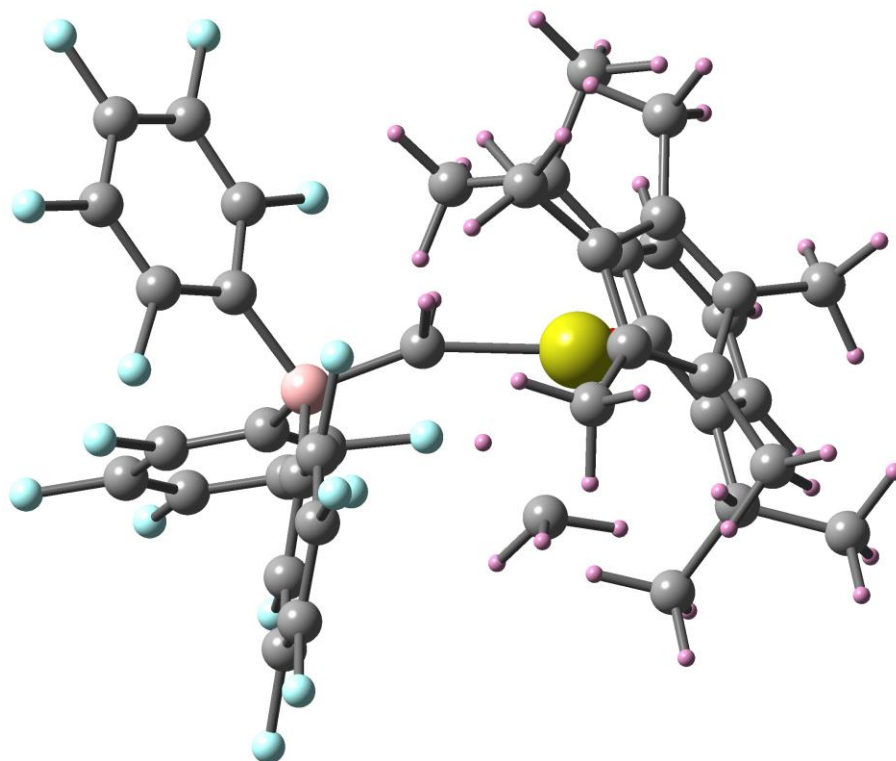
Ti	-1.94129900	1.26592400	0.38725800
C	-1.23572900	1.78613200	-1.78416600
H	-0.87137900	1.08101800	-2.54434000
H	-2.30531100	1.93194000	-1.98212600
H	-0.71707900	2.74463900	-1.88778400
O	-3.08584000	-0.04874700	0.02494300
C	-4.07283800	-1.03127300	-0.10007200
C	-4.10447100	-2.10359500	0.84565000
C	-4.99547700	-0.93027800	-1.18663300
C	-5.15622000	-3.04010100	0.72132800
C	-6.01417700	-1.90707300	-1.26476200
C	-6.10782900	-2.94009800	-0.31242700
H	-5.22807300	-3.86382500	1.42941600
H	-6.73747700	-1.86715700	-2.07757500
H	-6.90865900	-3.67843800	-0.38717200
C	-1.59709100	2.77762600	2.30833700
C	-1.49453300	3.61966400	1.15088900
C	-2.93583300	2.20614600	2.33332400
C	-2.76826100	3.57639300	0.44957100
C	-3.66888400	2.73392100	1.20494300

F	1.26728000	-5.34319900	-3.11647100
C	1.29855400	-4.12867400	-2.44581400
C	2.52086600	-3.55142300	-2.06193200
C	0.11122100	-3.44568800	-2.14357100
C	2.52039000	-2.32201400	-1.37841300
F	3.71414900	-4.19528200	-2.36842000
C	0.17333900	-2.21568800	-1.45878400
F	-1.11565900	-3.98296900	-2.52530600
C	1.35889700	-1.59063100	-1.02460100
F	3.78401300	-1.80121600	-1.07812200
F	-1.07226900	-1.60220000	-1.24265000
B	1.48154500	-0.17444100	-0.14526800
C	2.38488100	-0.61790000	1.21480000
C	2.17912700	1.05797900	-1.03428600
C	0.02998800	0.46985000	0.45642200
C	3.73503600	-0.28368200	1.48795900
C	1.82396800	-1.45620400	2.20794900
C	2.33936300	1.06456000	-2.43991400
C	2.61048100	2.26471000	-0.43520500
H	-0.54439400	-0.35178600	0.93926400
H	0.35294500	1.21026100	1.20419500
H	-0.57824000	1.15347300	-0.82318100
C	4.43868100	-0.68660100	2.64213200
F	4.48877300	0.46957200	0.58574600
C	2.47957700	-1.88818100	3.37584200
F	0.51203900	-1.95406000	2.05620400
C	2.91795400	2.12104800	-3.17537400
F	1.88509100	-0.00587900	-3.22397000
C	3.18986000	3.34880800	-1.11574700
F	2.47166200	2.44327700	0.95524000
C	3.80604500	-1.49033300	3.60372400
F	5.76052800	-0.30163000	2.83443600
F	1.82789800	-2.70279300	4.29897100
C	3.35721800	3.27510500	-2.50874600
F	3.04077100	2.03636100	-4.55774900
F	3.58664600	4.49263100	-0.42854400
F	4.47948200	-1.89297900	4.74827100
F	3.92074900	4.33049200	-3.21127200
C	-3.00679200	-2.24057400	1.90152500
H	-2.04016600	-2.27641600	1.37874800
C	-4.83333900	0.15569900	-2.25088800
H	-3.92086000	-0.07527000	-2.82937900
C	-3.08586600	-3.45509500	2.85357200
H	-3.88630500	-3.34568300	3.60301900
H	-3.25204400	-4.39703100	2.31022100
H	-2.13098000	-3.55601400	3.39191700
C	-6.00653800	0.33980200	-3.24062100
H	-6.96477000	0.49241900	-2.71951900
H	-5.82341100	1.22359900	-3.87211400
H	-6.11680500	-0.52460300	-3.91286000
H	-4.63777600	1.11873000	-1.75710700
H	-2.97564000	-1.32513000	2.51392600
C	-0.57051700	2.63452400	3.41003800
H	0.45633900	2.53270200	3.03531000
H	-0.59123100	3.53075300	4.05395300
H	-0.77594100	1.76872300	4.05356800
C	-0.33134800	4.52556100	0.81848500

H	-0.28929300	5.35524700	1.54534600
H	0.63503000	4.01398100	0.86879900
H	-0.42811100	4.97608200	-0.17747600
C	-3.52433200	1.41181700	3.48015700
H	-2.91597700	0.54005400	3.75933900
H	-3.59991700	2.05103900	4.37589000
H	-4.53310600	1.04925800	3.24761100
C	-3.15297900	4.45955300	-0.71692600
H	-3.33159400	5.48856400	-0.36091000
H	-2.37082200	4.51941100	-1.48506200
H	-4.07635800	4.12270600	-1.20573500
C	-5.14919000	2.54892500	0.95757000
H	-5.49416000	1.53593200	1.20194900
H	-5.71868300	3.25170400	1.59045100
H	-5.43176300	2.75355700	-0.08274400

Frequencies --	-964.4268	-20.0284	10.5592
Frequencies --	21.0622	21.8799	23.8921
Frequencies --	27.4868	28.6886	30.8361
Frequencies --	32.6357	37.6437	38.0266
Frequencies --	47.5817	48.4963	51.7017
Frequencies --	55.3168	58.8523	64.4353
Frequencies --	69.1843	84.1496	89.7997
Frequencies --	97.1423	100.2247	110.4468
Frequencies --	112.8397	114.3688	118.4455
Frequencies --	122.9385	125.0501	128.3335
Frequencies --	137.9610	141.9278	143.0653
Frequencies --	144.9723	146.0254	155.6096
Frequencies --	159.9685	160.9766	165.3882
Frequencies --	168.1200	175.6453	176.1749
Frequencies --	182.2536	189.2518	192.4583
Frequencies --	199.1169	214.6253	218.4000
Frequencies --	219.3669	223.7729	232.8033
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Frequencies --	274.8386	275.1506	275.7949
Frequencies --	277.8474	284.7097	288.2491
Frequencies --	291.3205	299.9798	301.8330
Frequencies --	305.9479	306.8260	309.3072
Frequencies --	324.6172	326.4288	328.7030
Frequencies --	331.6879	334.7747	346.3892
Frequencies --	361.1348	364.9962	372.4450
Frequencies --	376.9251	378.0016	379.9880
Frequencies --	380.8116	391.6540	392.2698
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Frequencies --	434.5062	447.2021	456.7788
Frequencies --	463.6758	472.0356	504.1485
Frequencies --	528.9348	532.5360	533.0895
Frequencies --	534.4165	539.1415	544.3974
Frequencies --	547.7064	553.1125	556.9156
Frequencies --	575.3659	578.3316	582.6939
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Frequencies --	604.1350	619.3456	634.4576
Frequencies --	635.8610	637.9314	640.5783
Frequencies --	655.0830	670.0334	696.7760
Frequencies --	713.5157	715.9607	721.2445
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Frequencies --	853.0874	867.1497	880.4713

Frequencies --	888.4228	903.2839	912.1509
Frequencies --	918.5909	919.6599	929.7318
Frequencies --	964.8982	973.2711	990.2739
Frequencies --	995.4602	1006.5060	1016.8604
Frequencies --	1026.5509	1027.3324	1036.8665
Frequencies --	1040.1204	1042.5732	1044.4636
Frequencies --	1047.1603	1048.9654	1049.4992
Frequencies --	1053.6584	1056.0893	1057.0519
Frequencies --	1083.3405	1086.9689	1089.1345
Frequencies --	1090.1988	1098.6546	1100.3321
Frequencies --	1123.0575	1123.3712	1170.9443
Frequencies --	1175.8183	1185.9653	1203.7537
Frequencies --	1209.0673	1212.1891	1215.4539
Frequencies --	1257.7412	1260.4962	1276.1175
Frequencies --	1285.8253	1290.7115	1291.7525
Frequencies --	1316.3601	1319.2883	1325.4363
Frequencies --	1325.5890	1336.0162	1342.3613
Frequencies --	1343.2676	1350.5808	1352.8851
Frequencies --	1381.4420	1409.6251	1410.2560
Frequencies --	1412.9214	1415.2024	1416.8845
Frequencies --	1418.2039	1421.7747	1422.5806
Frequencies --	1423.8109	1427.0312	1430.8778
Frequencies --	1433.5409	1434.1829	1450.7129
Frequencies --	1451.6756	1465.9598	1467.6720
Frequencies --	1469.1955	1469.6174	1470.7565
Frequencies --	1471.9777	1479.1500	1484.5103
Frequencies --	1489.3145	1494.4438	1496.2049
Frequencies --	1498.5406	1498.6360	1499.0509
Frequencies --	1501.4587	1504.5878	1507.5247
Frequencies --	1508.5126	1509.8499	1511.5535
Frequencies --	1513.7617	1520.1611	1525.6482
Frequencies --	1594.0378	1595.9931	1598.9458
Frequencies --	1600.1069	1608.3348	1617.1980
Frequencies --	1619.5259	1622.5356	1812.0635
Frequencies --	2937.0717	3011.5757	3012.3364
Frequencies --	3013.3969	3014.4695	3015.1639
Frequencies --	3015.5969	3016.0023	3018.1598
Frequencies --	3040.1632	3043.2601	3077.3418
Frequencies --	3089.8531	3100.4290	3103.2826
Frequencies --	3104.5305	3105.8330	3106.5975
Frequencies --	3113.3565	3116.9507	3118.8928
Frequencies --	3123.3424	3124.7179	3138.7934
Frequencies --	3140.9663	3144.0160	3145.5916
Frequencies --	3149.4470	3170.4427	3174.2074
Frequencies --	3185.6139	3202.8782	3211.9442

Catalyst 12:

vacuum	toluene-like solvent	D3 dispersion
-3278.0926055	-3278.1031327	-0.67102025

Imaginary frequency corresponding to vibration along the reaction coordinate: -1004 cm^{-1} .

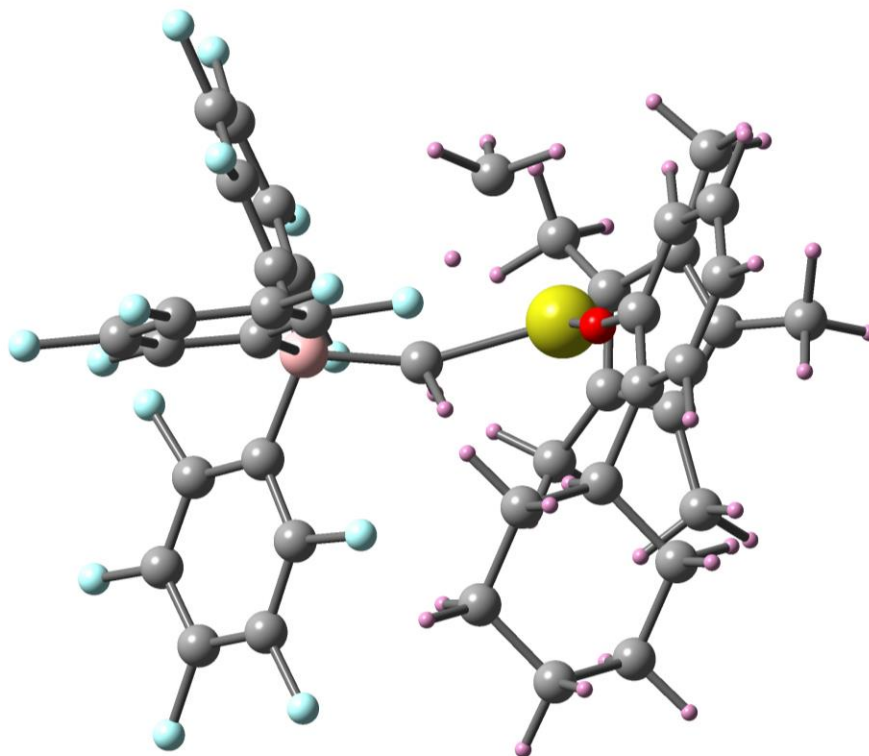
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C	-1.08285100	1.86836700	-1.67558700
H	-0.72742800	1.18575700	-2.45976200
H	-2.14795900	2.03790100	-1.87368000
H	-0.54953300	2.82070900	-1.74419900
O	-2.98288300	0.02323400	0.13157200
C	-4.03103100	-0.89575200	-0.02844200
C	-4.12752000	-2.01013900	0.86559200
C	-4.96155500	-0.70039900	-1.10156100
C	-5.20956200	-2.90351700	0.67919100
C	-6.01272100	-1.63639400	-1.23531400
C	-6.14786500	-2.72202900	-0.35106000
H	-5.30819800	-3.76241300	1.34311400
H	-6.73235000	-1.51903800	-2.04534500
H	-6.97022600	-3.42939300	-0.47427300
C	-1.20615800	2.87171600	2.32838800
C	-1.29617600	3.69144000	1.15638700
C	-2.49907300	2.23107700	2.52643300
C	-2.64902900	3.57579700	0.62710300
C	-3.40417600	2.71610900	1.50680100
F	1.25802100	-5.26808300	-3.28125200
C	1.32598900	-4.07409000	-2.57755700

C	2.56336700	-3.55535600	-2.15990500
C	0.16179800	-3.35268700	-2.27498800
C	2.59988400	-2.34570400	-1.44250900
F	3.73557200	-4.23605400	-2.46754300
C	0.26059100	-2.14506600	-1.55601600
F	-1.08000300	-3.83092300	-2.68718900
C	1.46207200	-1.58034000	-1.08380400
F	3.87870800	-1.88079300	-1.11687200
F	-0.96639300	-1.49077900	-1.34412000
B	1.61817800	-0.19168300	-0.16836600
C	2.55500500	-0.65629000	1.15942000
C	2.29625800	1.06595800	-1.03670000
C	0.17097300	0.41701300	0.48068100
C	3.90856400	-0.31626200	1.40474200
C	2.02129200	-1.50753800	2.15585200
C	2.47853200	1.10101700	-2.43879600
C	2.68964300	2.27067400	-0.40863300
H	-0.41148100	-0.43881500	0.88327800
H	0.49575000	1.09362800	1.28676500
H	-0.43182500	1.17676100	-0.73992700
C	4.64221900	-0.72878800	2.53625900
F	4.63467800	0.45359400	0.49315200
C	2.70781900	-1.95090500	3.30162800
F	0.70680100	-2.00356000	2.03146800
C	3.03589900	2.18817800	-3.14604900
F	2.07380000	0.03005900	-3.24801400
C	3.24477500	3.38399900	-1.06030400
F	2.54118700	2.40740600	0.98477300
C	4.03734400	-1.54872900	3.50220800
F	5.96599900	-0.33787800	2.70189600
F	2.08227000	-2.77900500	4.23097700
C	3.43061500	3.34237900	-2.45231300
F	3.18229200	2.13266800	-4.52754900
F	3.60006300	4.52523000	-0.34533600
F	4.74044900	-1.96198000	4.62498000
F	3.97104500	4.42759300	-3.12721600
C	-3.09516900	-2.31488300	1.96252500
H	-2.37932900	-1.48365000	2.01004500
C	-4.81121400	0.42790100	-2.13294500
H	-4.12925900	1.17781400	-1.71295400
C	-2.28168200	-3.59695200	1.61038500
H	-2.92606100	-4.48913200	1.60794500
H	-1.81921400	-3.51305600	0.61777200
H	-1.48196000	-3.75424800	2.34940500
C	-3.73977900	-2.45199200	3.37262600
H	-4.34660100	-1.57163400	3.63281000
H	-4.39146000	-3.33593700	3.43931300
H	-2.95313900	-2.56649100	4.13541200
C	-4.15553200	-0.11548400	-3.43969400
H	-4.80666400	-0.85640100	-3.92829100
H	-3.98031500	0.70483500	-4.15496500
H	-3.19306700	-0.60376500	-3.23007800
C	-6.14366900	1.16424000	-2.44901300
H	-6.85768300	0.52065500	-2.98353600
H	-6.63675400	1.52244700	-1.53192200
H	-5.94589400	2.03394600	-3.09657700
C	-0.05212400	2.79235300	3.30213700

H	0.90177300	3.08739800	2.85216700
H	-0.24070200	3.47277000	4.15068500
H	0.07408500	1.78485000	3.72499100
C	-0.24951700	4.65904700	0.65542400
H	-0.47380500	5.67009300	1.03888900
H	0.75852400	4.40149200	0.99535700
H	-0.22996200	4.73770000	-0.44004900
C	-2.88739200	1.42144700	3.74324900
H	-3.79178800	0.82636600	3.57250800
H	-2.09025900	0.73907300	4.07042100
H	-3.09594400	2.09899200	4.58977100
C	-3.21427900	4.41313000	-0.49836600
H	-3.55223400	5.38740700	-0.10427700
H	-2.47112200	4.62543500	-1.27821100
H	-4.08252000	3.94266400	-0.97949500
C	-4.89476800	2.47193400	1.46763300
H	-5.16096600	1.43730300	1.71929900
H	-5.39299700	3.12731900	2.20326400
H	-5.32811300	2.69928200	0.48651500

Frequencies --	-1003.5556	8.7910	16.9401
Frequencies --	21.9826	25.8498	27.7320
Frequencies --	28.6757	31.4973	33.1993
Frequencies --	37.2767	39.8486	43.8587
Frequencies --	47.7517	56.3308	60.1464
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Frequencies --	158.7998	159.3196	162.1151
Frequencies --	164.3657	166.3409	170.0736
Frequencies --	173.6520	185.7713	189.7602
Frequencies --	200.6134	206.3997	214.8325
Frequencies --	216.6198	219.4850	219.8663
Frequencies --	223.0639	225.6847	235.3282
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Frequencies --	264.2311	264.2655	265.0131
Frequencies --	274.8493	275.4116	276.6987
Frequencies --	277.4162	286.6715	287.9744
Frequencies --	292.6773	300.8716	302.3503
Frequencies --	302.7090	303.0415	304.3691
Frequencies --	307.4341	314.6397	321.7397
Frequencies --	326.5502	328.5677	335.0243
Frequencies --	342.4993	362.5878	370.9472
Frequencies --	373.4475	377.0910	377.9527
Frequencies --	380.9955	388.6068	396.5781
Frequencies --	399.8829	424.3932	426.8886
Frequencies --	431.4969	432.6737	434.0748
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Frequencies --	463.7965	475.4064	527.7731
Frequencies --	532.8219	534.3617	536.1288
Frequencies --	539.1476	543.4972	545.7078
Frequencies --	552.2389	554.8875	575.9102
Frequencies --	584.6738	593.2211	596.1656
Frequencies --	598.9202	607.2530	609.1707
Frequencies --	617.3151	629.7137	634.7475
Frequencies --	635.8497	638.2240	641.7123
Frequencies --	654.7302	671.6613	701.1640

Frequencies --	715.4303	721.2316	723.8190
Frequencies --	732.5781	743.7098	746.5772
Frequencies --	760.4096	760.8919	768.7364
Frequencies --	797.8189	801.5474	803.6225
Frequencies --	815.0289	842.0072	867.2112
Frequencies --	875.6209	878.6805	879.4239
Frequencies --	903.4074	911.8735	917.0493
Frequencies --	922.1889	927.0241	929.6996
Frequencies --	932.8972	940.8572	963.3118
Frequencies --	964.6027	968.0122	973.9921
Frequencies --	990.7420	1002.0565	1016.8772
Frequencies --	1026.5953	1037.9658	1040.2255
Frequencies --	1042.4370	1044.5764	1046.1821
Frequencies --	1049.1120	1049.5013	1053.1309
Frequencies --	1055.3856	1056.4417	1072.3966
Frequencies --	1084.0347	1087.4104	1090.4578
Frequencies --	1111.1867	1113.6133	1120.7786
Frequencies --	1125.8026	1165.9647	1172.6464
Frequencies --	1174.5195	1182.1306	1184.7318
Frequencies --	1206.3860	1209.6262	1212.2868
Frequencies --	1215.0940	1252.1343	1260.2172
Frequencies --	1278.2823	1290.9362	1303.5499
Frequencies --	1316.9882	1317.9390	1320.0505
Frequencies --	1322.1619	1325.6220	1332.8541
Frequencies --	1337.1473	1343.5482	1347.8313
Frequencies --	1350.0941	1377.7284	1401.2929
Frequencies --	1401.3803	1407.9399	1411.1182
Frequencies --	1414.4177	1418.2420	1419.9972
Frequencies --	1420.2406	1421.8909	1422.7185
Frequencies --	1426.5892	1427.4143	1429.7644
Frequencies --	1435.1120	1436.1923	1450.2437
Frequencies --	1453.4494	1467.1494	1467.8023
Frequencies --	1468.8114	1471.8608	1472.3378
Frequencies --	1474.4907	1482.7807	1485.4629
Frequencies --	1486.8946	1488.2664	1491.0394
Frequencies --	1492.2013	1495.9680	1499.1425
Frequencies --	1500.7767	1502.0466	1504.6825
Frequencies --	1507.3567	1508.3709	1508.8356
Frequencies --	1511.2417	1513.0130	1518.1364
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Frequencies --	1596.3531	1597.3963	1598.5451
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Frequencies --	1622.4460	1816.6225	2953.6835
Frequencies --	3008.9775	3009.7997	3010.7922
Frequencies --	3013.2516	3013.3121	3014.0170
Frequencies --	3014.6132	3015.2669	3025.5432
Frequencies --	3052.1174	3080.5576	3086.4325
Frequencies --	3096.3343	3099.1729	3100.4551
Frequencies --	3103.0417	3104.3884	3106.8376
Frequencies --	3111.5316	3113.6960	3114.5792
Frequencies --	3121.4197	3125.7389	3131.1065
Frequencies --	3135.0019	3139.4041	3145.5960
Frequencies --	3153.6692	3154.2546	3161.1323
Frequencies --	3163.1694	3166.9796	3173.0418
Frequencies --	3190.1629	3198.8361	3202.4028

Catalyst 13:**distal conformation**

vacuum	toluene-like solvent	D3 dispersion
-3276.8990185	-3276.9103375	-0.65947011

Imaginary frequency corresponding to vibration along the reaction coordinate: -1021 cm^{-1} .

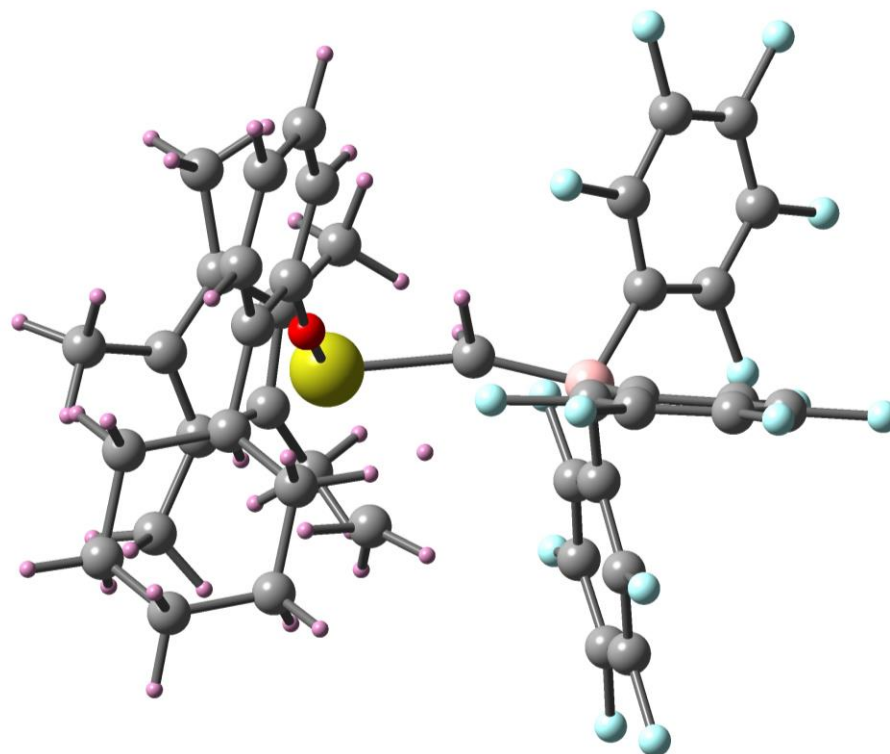
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H	0.03473000	1.75665100	-2.58810700
H	-1.31672700	2.78924300	-2.15383500
H	0.34552500	3.27874800	-1.69638100
O	-2.80445000	1.03718200	-0.53777300
C	-3.95654100	0.64036600	-1.21564600
C	-4.69238500	-0.51488600	-0.81793800
C	-4.34891600	1.42493200	-2.33049000
C	-5.84882700	-0.81779200	-1.58470200
C	-5.49467000	1.08751500	-3.06969100
C	-6.25332200	-0.04100800	-2.68741100
H	-6.44244400	-1.69241600	-1.31632600
H	-5.78652000	1.69133000	-3.93123300
H	-7.14686800	-0.31850100	-3.24982200
C	-0.88675100	3.15085900	2.25520200
C	-0.58000000	4.05177400	1.18327800
C	-2.30434400	2.82388300	2.17383100
C	-1.81044100	4.30767400	0.44360900
C	-2.88282100	3.59256300	1.09168500
F	0.60817500	-4.84643000	-3.94071400

C	0.81641700	-3.77836100	-3.07958400
C	2.05178800	-3.60884500	-2.43148100
C	-0.19879000	-2.83984300	-2.84302900
C	2.23067300	-2.52007700	-1.55905300
F	3.08247300	-4.51182300	-2.66511800
C	0.03874600	-1.76613100	-1.96203400
F	-1.43070100	-2.97413100	-3.47929400
C	1.24247700	-1.54862900	-1.26192900
F	3.50578300	-2.40477000	-0.99397000
F	-1.03535200	-0.86853300	-1.83017600
B	1.54670600	-0.34079000	-0.15084800
C	2.06195200	-1.16413100	1.23107400
C	2.65346000	0.77873200	-0.71031800
C	0.19562800	0.56086500	0.33118500
C	3.37800100	-1.21260800	1.75339600
C	1.15134500	-1.94873600	1.97838000
C	3.08605600	0.91431600	-2.05012200
C	3.20142300	1.76809000	0.13917300
H	-0.63835400	-0.14390100	0.53878100
H	0.52257200	1.07655500	1.25038100
H	-0.00525100	1.52368700	-0.87488500
C	3.74742100	-1.91769400	2.91775300
F	4.43255200	-0.56182700	1.10942800
C	1.46639500	-2.67405600	3.14235100
F	-0.18994500	-2.07061200	1.55555800
C	4.00697600	1.88557900	-2.49875500
F	2.58285300	0.08175900	-3.05974300
C	4.11616400	2.75950600	-0.25155500
F	2.82932700	1.79955900	1.49692500
C	2.78346400	-2.65157800	3.62746900
F	5.06249800	-1.89992000	3.36781500
F	0.48925200	-3.40745100	3.81140300
C	4.53633400	2.81588700	-1.59108400
F	4.38049300	1.94116100	-3.83675800
F	4.59609600	3.68909300	0.66774600
F	3.12611300	-3.34794300	4.77788200
F	5.43457600	3.78650900	-2.01087000
C	-1.96675000	5.33225000	-0.65812900
H	-2.11521800	6.33420400	-0.21920500
H	-1.08093900	5.39462300	-1.30394800
H	-2.83667300	5.13037800	-1.29811700
C	0.73171300	4.76725700	0.95750000
H	0.96507100	4.90530900	-0.10728100
H	0.67881500	5.77696200	1.40125900
H	1.57699400	4.25249800	1.42598100
C	0.03107700	2.72042400	3.37738100
H	1.09045000	2.80677000	3.11330700
H	-0.14244800	3.36150400	4.25905700
H	-0.15069800	1.68417700	3.69781100
C	-3.06645300	2.00515000	3.19314600
H	-2.48884500	1.14353200	3.55788600
H	-3.30245400	2.62749000	4.07408600
H	-4.01768500	1.62781900	2.79733200
C	-4.35777700	3.71720500	0.78816000
H	-4.90861900	2.78885600	0.98547600
H	-4.79792600	4.50132700	1.42903000
H	-4.55313200	4.00222300	-0.25310900

H	-3.74538200	2.28680900	-2.61448900
C	-4.27610900	-1.41058600	0.35234800
C	-5.33988900	-1.42759200	1.49623000
C	-3.96544900	-2.87006200	-0.11236800
H	-3.34553900	-1.00796700	0.77941900
C	-4.89844700	-2.32712600	2.67884800
H	-6.30169100	-1.79815600	1.10243600
H	-5.52419800	-0.39896400	1.85150700
C	-3.53010800	-3.76967900	1.07151700
H	-4.86181600	-3.30617300	-0.58506200
H	-3.18040200	-2.85075500	-0.88375400
C	-4.57631200	-3.76845300	2.21308400
H	-5.69227300	-2.34303100	3.44554500
H	-4.00257600	-1.89289700	3.15957900
H	-3.37174400	-4.79897700	0.70698400
H	-2.55911200	-3.42290700	1.46342100
H	-4.20610800	-4.36473600	3.06398300
H	-5.50510400	-4.25563100	1.86334000

Frequencies --	-1021.4003	12.2101	19.4789
Frequencies --	23.7853	26.1487	28.0241
Frequencies --	29.6422	30.8264	33.4551
Frequencies --	38.1766	42.1191	43.7809
Frequencies --	49.5644	50.9357	58.8458
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Frequencies --	120.8873	124.8435	127.6980
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Frequencies --	156.0498	158.8021	160.8756
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Frequencies --	1266.7605	1276.6777	1283.9692
Frequencies --	1293.3922	1299.3316	1316.8378
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Frequencies --	1483.0551	1484.2664	1485.2166
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Frequencies --	1529.0028	1586.8585	1594.2498
Frequencies --	1596.2178	1598.4762	1613.7302
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Frequencies --	1827.8962	2945.0216	2998.1677
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Frequencies --	3011.1843	3012.1009	3013.3553
Frequencies --	3014.3113	3019.6838	3026.6800
Frequencies --	3041.7534	3054.2582	3061.1608
Frequencies --	3069.3576	3078.7233	3079.7762
Frequencies --	3086.2052	3095.5243	3098.9490
Frequencies --	3099.0990	3101.6203	3104.7295
Frequencies --	3107.9595	3136.5250	3137.5998
Frequencies --	3142.6220	3152.4015	3162.5903
Frequencies --	3165.4813	3170.5246	3178.3893
Frequencies --	3192.6391	3197.5596	3204.7723

proximal conformation

vacuum	toluene-like solvent	D3 dispersion
-3276.8989632	-3276.9102304	-0.65858911

Imaginary frequency corresponding to vibration along the reaction coordinate: -1033 cm^{-1} .

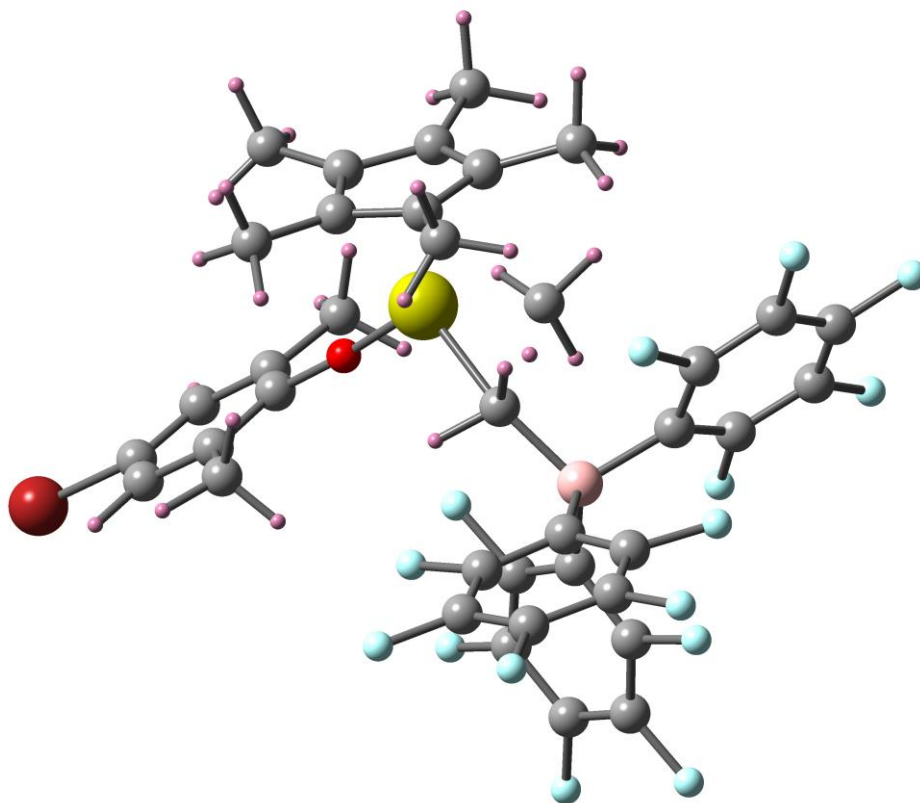
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C	1.34058800	-1.32810500	-1.69092600
H	1.06245700	-0.46691300	-2.31477100
H	2.43999900	-1.35520100	-1.68032200
H	0.95684900	-2.24586800	-2.14557500
O	2.66611200	-0.18603900	0.96992800
C	3.47887700	0.78702400	1.55001700
C	3.09540200	1.27857400	2.82374400
C	4.62677300	1.28562500	0.86663600
C	3.86567300	2.26687100	3.45958500
C	5.37961400	2.28126000	1.54220900
C	5.01945400	2.76629300	2.81498100
H	3.56317400	2.64775000	4.43690900
H	6.26324500	2.69415700	1.05400300
H	5.62562400	3.53686900	3.29510400
C	0.70287400	-3.44397000	1.89853500
C	0.87099300	-3.92421600	0.55678900
C	1.99930000	-2.97990300	2.37736400
C	2.27211200	-3.76674400	0.19631400
C	2.97434100	-3.22984400	1.33988300
F	-0.77531500	5.94490100	-1.82577800
C	-0.96888300	4.62133000	-1.45665000
C	-2.26213500	4.07490200	-1.39351900
C	0.12266100	3.79590600	-1.14895500

C	-2.42645000	2.73041200	-1.01393700
F	-3.36057400	4.86364500	-1.71529200
C	-0.10291900	2.45638000	-0.77519100
F	1.41904700	4.30182400	-1.22276300
C	-1.37037100	1.84971000	-0.67138200
F	-3.74350800	2.25836800	-1.02600000
F	1.06382400	1.71247100	-0.52904900
B	-1.69467500	0.29241600	-0.16393200
C	-2.79015100	0.49014600	1.10621400
C	-2.26283600	-0.68007000	-1.39761600
C	-0.38964200	-0.55671400	0.49787700
C	-4.17438600	0.18968500	1.08552100
C	-2.37180400	1.04932700	2.33803300
C	-2.20678500	-0.37893900	-2.77839800
C	-2.78367600	-1.97111400	-1.14391000
H	0.11282600	0.10986100	1.23197400
H	-0.85329000	-1.42301600	0.99680500
H	0.45743000	-0.93158800	-0.75904400
C	-5.04629500	0.37427400	2.17856400
F	-4.78610100	-0.30204400	-0.06965200
C	-3.19883500	1.25561200	3.45809100
F	-1.03636100	1.47481500	2.50856200
C	-2.66719500	-1.23440200	-3.80258800
F	-1.64196100	0.82079300	-3.23397100
C	-3.25371100	-2.86389000	-2.12089200
F	-2.85858800	-2.44094400	0.18153900
C	-4.55603900	0.90515100	3.38228000
F	-6.39221900	0.04245100	2.07399400
F	-2.68554100	1.80011000	4.63270300
C	-3.20484600	-2.48842300	-3.47409800
F	-2.57690700	-0.85275000	-5.13645600
F	-3.75347600	-4.11373000	-1.76451300
F	-5.39610300	1.08976200	4.47137300
F	-3.65546800	-3.34977300	-4.46428200
C	2.91207800	-4.31085000	-1.06118000
H	3.24691500	-5.34861300	-0.88947900
H	2.21300700	-4.33603900	-1.90666000
H	3.79539600	-3.73535900	-1.37183800
C	-0.17108000	-4.61107900	-0.29711800
H	-0.33010000	-4.11661300	-1.26655000
H	0.14620000	-5.64442500	-0.51416100
H	-1.14262300	-4.66321800	0.20517200
C	-0.55052700	-3.52699000	2.74143200
H	-1.46778200	-3.48364000	2.14318200
H	-0.56195000	-4.48474900	3.29009100
H	-0.60251800	-2.72729500	3.49363800
C	2.30244200	-2.53481900	3.79171000
H	1.48655500	-1.94452200	4.23258300
H	2.44394900	-3.41753600	4.43972300
H	3.21986600	-1.93583700	3.85165500
C	4.47043600	-3.06219000	1.47461300
H	4.74570600	-2.14907000	2.01858600
H	4.88906200	-3.91531200	2.03656800
H	4.97601000	-3.03846800	0.50049600
H	2.19008000	0.89565000	3.29471200
C	5.01426200	0.82107700	-0.53931600
C	4.84950900	1.96363600	-1.59303500

C	6.45609600	0.22877400	-0.61066500
H	4.32069500	0.01833200	-0.83083600
C	5.20152900	1.47781100	-3.02136900
H	5.50662300	2.80860400	-1.32465000
H	3.81761100	2.34590500	-1.56529700
C	6.80283300	-0.25962700	-2.04015300
H	7.19046900	0.99382300	-0.30700200
H	6.55523800	-0.60306300	0.10708600
C	6.62093500	0.86245900	-3.09203600
H	5.11949700	2.32285800	-3.72577900
H	4.45905000	0.72591800	-3.34765000
H	7.84085900	-0.63407200	-2.06059500
H	6.15447200	-1.11583600	-2.30600800
H	6.81319200	0.46685700	-4.10383300
H	7.37148100	1.65400800	-2.91399500

Frequencies --	-1032.8500	7.8769	11.9810
Frequencies --	22.1121	24.0842	26.8282
Frequencies --	27.5331	30.8852	31.8370
Frequencies --	33.6516	37.9680	41.2276
Frequencies --	45.2070	47.4759	51.0742
Frequencies --	69.9559	78.5138	86.2149
Frequencies --	98.9413	104.0066	105.5041
Frequencies --	110.1379	110.2360	114.2413
Frequencies --	116.7493	120.7163	121.7490
Frequencies --	125.3062	129.0828	136.0313
Frequencies --	141.0703	142.4898	144.9038
Frequencies --	145.4414	149.0065	152.1172
Frequencies --	155.8071	159.3669	161.3189
Frequencies --	163.0945	170.3866	174.5830
Frequencies --	176.3950	188.7453	208.9643
Frequencies --	215.4915	216.3661	222.3314
Frequencies --	223.2477	224.5133	227.2469
Frequencies --	245.8633	260.7446	264.6606
Frequencies --	264.8006	265.1542	274.7062
Frequencies --	275.2603	275.7332	283.1084
Frequencies --	283.5242	290.9103	296.6091
Frequencies --	299.1809	301.6689	302.1853
Frequencies --	306.7422	307.3173	325.0375
Frequencies --	326.5311	330.8105	336.8282
Frequencies --	341.9996	354.8536	364.7667
Frequencies --	372.8458	376.8670	378.5576
Frequencies --	379.2190	380.9929	393.5135
Frequencies --	397.7060	404.2067	431.3541
Frequencies --	431.9044	434.0741	435.2722
Frequencies --	439.7952	449.2952	456.4565
Frequencies --	463.8001	476.2793	490.6970
Frequencies --	496.8486	519.7451	531.1428
Frequencies --	535.6461	536.7891	537.8864
Frequencies --	544.6432	552.2369	554.5341
Frequencies --	557.6335	573.0040	582.3500
Frequencies --	594.9619	599.3691	606.0933
Frequencies --	612.8172	616.9249	635.1689
Frequencies --	635.9038	638.0014	643.4110
Frequencies --	655.7882	666.8583	674.3900
Frequencies --	701.3212	718.4116	723.2746
Frequencies --	733.8743	741.5020	747.0204
Frequencies --	748.1248	761.6649	765.1897
Frequencies --	767.5888	770.8932	790.8323
Frequencies --	802.3057	803.8652	820.4673
Frequencies --	843.0302	864.6097	867.0847

Frequencies --	871.2794	880.9278	884.8877
Frequencies --	889.6683	899.7820	903.3445
Frequencies --	912.5751	919.1070	924.0382
Frequencies --	937.7384	957.3708	968.7540
Frequencies --	973.3372	992.5683	997.0646
Frequencies --	1006.6689	1019.0000	1029.0769
Frequencies --	1038.6865	1042.0713	1043.5311
Frequencies --	1045.7869	1046.2617	1049.8922
Frequencies --	1052.0587	1052.7304	1053.2886
Frequencies --	1053.9659	1055.9305	1056.3419
Frequencies --	1082.3165	1087.4385	1089.6938
Frequencies --	1093.8425	1098.9094	1114.0143
Frequencies --	1125.7487	1153.1707	1170.4919
Frequencies --	1174.7939	1183.4559	1192.6522
Frequencies --	1197.3723	1209.4442	1212.7659
Frequencies --	1215.2579	1224.4201	1245.6984
Frequencies --	1269.4480	1276.4300	1280.9950
Frequencies --	1291.9813	1298.2138	1312.5688
Frequencies --	1316.5570	1319.3200	1325.7952
Frequencies --	1326.3506	1337.1822	1343.6357
Frequencies --	1345.2565	1349.2783	1351.5485
Frequencies --	1353.2927	1358.8787	1360.6411
Frequencies --	1370.4773	1384.9529	1409.3636
Frequencies --	1411.3593	1413.2447	1419.0838
Frequencies --	1422.2278	1423.2644	1426.1764
Frequencies --	1428.5868	1429.3968	1435.4220
Frequencies --	1444.9435	1450.7292	1452.5034
Frequencies --	1462.3342	1466.2104	1467.3529
Frequencies --	1469.2864	1471.6914	1480.3286
Frequencies --	1481.0968	1482.0695	1483.7625
Frequencies --	1486.3471	1488.4644	1491.3937
Frequencies --	1492.1055	1495.7581	1497.2708
Frequencies --	1500.0810	1502.7003	1505.5453
Frequencies --	1507.7249	1511.5079	1516.9759
Frequencies --	1527.8371	1585.8868	1594.0980
Frequencies --	1596.0420	1598.7695	1612.7786
Frequencies --	1617.0971	1620.2375	1623.0278
Frequencies --	1826.0041	2945.9129	2991.8612
Frequencies --	2999.0434	3004.8128	3008.3459
Frequencies --	3010.5755	3012.2728	3014.6068
Frequencies --	3014.7224	3021.9718	3022.1496
Frequencies --	3035.0353	3055.3946	3059.3892
Frequencies --	3066.3768	3074.3531	3083.9797
Frequencies --	3095.2246	3096.6933	3100.0986
Frequencies --	3100.2472	3103.0387	3103.5279
Frequencies --	3104.0656	3133.2054	3140.0170
Frequencies --	3142.4691	3146.8890	3156.3864
Frequencies --	3165.5998	3167.3974	3178.2077
Frequencies --	3192.0624	3193.0621	3204.9961

Catalyst 14:

vacuum	toluene-like solvent	D3 dispersion
-3133.5024764	-3133.514216	-0.60250211

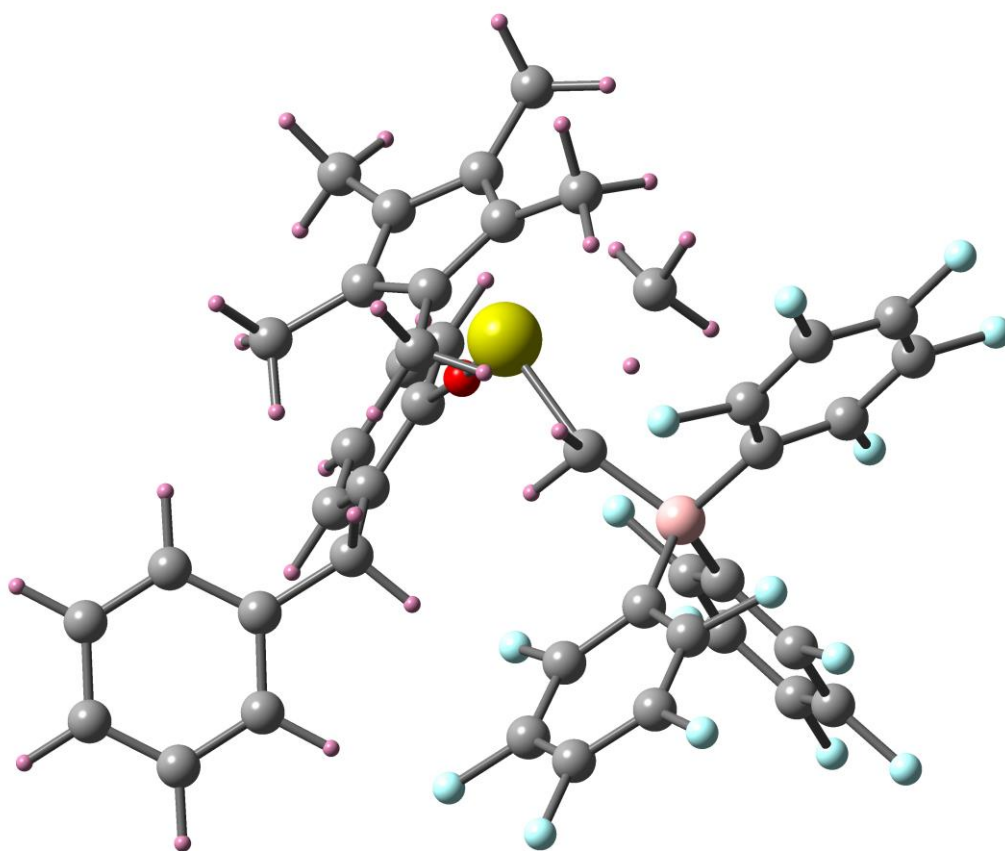
Imaginary frequency corresponding to vibration along the reaction coordinate: -1025 cm^{-1} .

Ti	-0.96141300	1.99845400	0.17929500
C	-0.20053700	1.91876000	-2.02719300
H	-0.01499900	1.03707400	-2.65675200
H	-1.20102700	2.28329100	-2.29309000
H	0.54157200	2.68951000	-2.25335300
O	-2.49090100	1.09406400	0.00295900
C	-3.72894600	0.45923200	-0.02208500
C	-4.11479300	-0.35678200	1.08285300
C	-4.56618600	0.62022700	-1.16589800
C	-5.38941100	-0.96842000	1.04749800
C	-5.83097000	-0.01110700	-1.16387400
C	-6.23525900	-0.78540300	-0.06109400
H	-5.70284600	-1.59306200	1.88306700
H	-6.48409600	0.10059700	-2.02851400
C	0.01590600	3.63454600	1.77132200
C	0.24877400	4.19895200	0.47376600
C	-1.42383700	3.50011200	1.95066900
C	-1.04424100	4.42333600	-0.15852500
C	-2.07532000	4.03561500	0.77575100
F	-0.05103200	-5.56521200	-2.70587700
C	0.35943800	-4.38141000	-2.11023000
C	1.70240800	-4.19060000	-1.74220700

C	-0.55496700	-3.34563600	-1.86851400
C	2.08815500	-2.98035500	-1.13849400
F	2.63336400	-5.19299800	-1.98711300
C	-0.10968900	-2.15410500	-1.26163900
F	-1.89047400	-3.49876100	-2.23164300
C	1.21531900	-1.89983100	-0.85598500
F	3.45074000	-2.86120400	-0.84404600
F	-1.10661700	-1.17665000	-1.09315100
B	1.78347800	-0.53810800	-0.07152300
C	2.45516900	-1.14672000	1.35482100
C	2.86974000	0.32703900	-1.00069800
C	0.60924400	0.58971400	0.40425600
C	3.83300700	-1.25509400	1.66894800
C	1.62428100	-1.68019000	2.36893000
C	3.07368300	0.17342500	-2.39179000
C	3.64251100	1.37737000	-0.45255900
H	-0.21039800	0.04198300	0.91594600
H	1.13507000	1.26351100	1.09962000
H	0.24853300	1.25124500	-0.95644600
C	4.33580000	-1.78836000	2.87415400
F	4.81417000	-0.84930700	0.76215900
C	2.07192900	-2.22357500	3.58733500
F	0.22505800	-1.72272700	2.18729500
C	3.98738300	0.93123100	-3.15557400
F	2.32849100	-0.75553400	-3.13244800
C	4.56265000	2.16546600	-1.16301600
F	3.51471900	1.69486500	0.91339600
C	3.44990000	-2.27188000	3.85002900
F	5.70541600	-1.84774700	3.10342900
F	1.16637300	-2.71170900	4.52575200
C	4.74853900	1.93450000	-2.53625100
F	4.12642300	0.70565400	-4.52041300
F	5.27554900	3.17769800	-0.52588700
F	3.92477700	-2.79611900	5.04356400
F	5.64488300	2.70041600	-3.26754600
C	-3.18888900	-0.62504400	2.25455100
H	-2.35709400	-1.27814500	1.95308200
H	-2.75100700	0.29621700	2.65976200
H	-3.72506600	-1.12857100	3.06998300
C	-4.12316300	1.40400800	-2.38816000
H	-3.81890800	2.42971200	-2.13403400
H	-3.26631900	0.91321300	-2.87561400
H	-4.93379700	1.46816300	-3.12618400
Br	-8.00544300	-1.63900600	-0.07807900
C	1.04446200	3.36769000	2.84753300
H	2.05521300	3.24286200	2.44416500
H	1.07248200	4.21998200	3.54836200
H	0.80996300	2.47364400	3.44377500
C	1.57842400	4.65423900	-0.08015600
H	1.70043200	5.73626100	0.10339900
H	2.42554400	4.14976900	0.39547700
H	1.66157900	4.50927700	-1.16596400
C	-2.10640400	3.11967300	3.24623800
H	-1.56136500	2.34180700	3.79911200
H	-2.16158200	4.00134600	3.90865100
H	-3.13446600	2.76915000	3.08941100
C	-1.26298800	5.16985700	-1.45522000

H	-1.27554200	6.25647600	-1.26125400
H	-0.46674600	4.98584800	-2.18779000
H	-2.22121000	4.91827100	-1.92978100
C	-3.56123800	4.26408100	0.61920900
H	-4.16027800	3.47481400	1.09175200
H	-3.84066400	5.21852800	1.09859700
H	-3.86741900	4.33113200	-0.43258000
Frequencies --	-1025.0706	7.0874	13.1810
Frequencies --	16.8902	26.4279	26.6510
Frequencies --	29.1260	31.0138	36.5708
Frequencies --	38.8094	40.2835	47.2078
Frequencies --	49.1404	59.2348	67.1894
Frequencies --	77.5989	97.4426	101.6879
Frequencies --	105.2074	110.9522	112.9684
Frequencies --	114.4703	118.1366	120.7905
Frequencies --	121.5895	126.1725	132.9277
Frequencies --	137.7251	140.8755	142.1337
Frequencies --	144.8598	146.4650	148.9879
Frequencies --	155.0891	156.6518	156.9821
Frequencies --	160.7785	161.1658	167.0178
Frequencies --	172.2820	173.1266	176.3704
Frequencies --	185.2732	191.4214	198.3767
Frequencies --	202.3684	213.3593	216.4202
Frequencies --	219.9164	221.7060	223.0807
Frequencies --	234.9228	241.5019	258.9730
Frequencies --	260.8729	264.3879	264.7664
Frequencies --	264.8761	274.9545	275.7494
Frequencies --	278.0829	285.9710	290.4086
Frequencies --	299.0510	302.0263	302.9621
Frequencies --	303.7969	307.3948	320.6548
Frequencies --	325.7352	331.1081	336.2807
Frequencies --	349.2641	357.3140	362.6594
Frequencies --	372.6967	376.9151	377.7116
Frequencies --	380.2965	390.0897	392.2410
Frequencies --	395.1953	405.2978	420.9208
Frequencies --	431.5097	432.7938	434.3540
Frequencies --	450.1429	456.8261	463.8529
Frequencies --	475.7806	501.2385	509.9294
Frequencies --	529.3321	532.6387	533.6648
Frequencies --	538.6987	544.6541	552.4790
Frequencies --	554.5921	563.7313	565.8794
Frequencies --	571.7631	575.7347	584.2415
Frequencies --	594.8086	600.3802	608.3244
Frequencies --	613.7991	634.3986	635.2439
Frequencies --	637.6923	641.4970	654.4569
Frequencies --	671.9894	698.7454	716.8830
Frequencies --	721.4268	729.6676	732.5128
Frequencies --	744.5125	747.3549	760.3837
Frequencies --	769.5221	798.9950	801.6146
Frequencies --	802.7238	840.7090	867.6713
Frequencies --	880.1516	882.5532	883.9715
Frequencies --	887.1840	902.8237	911.9753
Frequencies --	918.6846	925.9799	949.8476
Frequencies --	967.5086	972.1018	999.0808
Frequencies --	1008.6345	1017.5591	1027.5089
Frequencies --	1037.0636	1040.9182	1044.2666
Frequencies --	1044.5732	1046.5314	1048.3790
Frequencies --	1048.7605	1050.2240	1051.9641
Frequencies --	1054.9916	1056.4796	1058.7381
Frequencies --	1087.0675	1088.7709	1088.8509
Frequencies --	1124.6483	1125.5473	1171.2297

Frequencies --	1174.7385	1205.6429	1209.7839
Frequencies --	1212.8830	1215.8726	1263.5314
Frequencies --	1264.2807	1286.5390	1295.7437
Frequencies --	1317.3455	1320.6569	1325.0945
Frequencies --	1336.9272	1343.5599	1346.0797
Frequencies --	1351.4154	1353.7564	1408.7747
Frequencies --	1410.6023	1413.4081	1414.5192
Frequencies --	1418.4523	1419.5986	1421.9049
Frequencies --	1422.9470	1424.3342	1425.4825
Frequencies --	1427.4620	1429.9857	1431.1275
Frequencies --	1436.1642	1450.3660	1452.6541
Frequencies --	1465.2852	1467.7545	1469.1586
Frequencies --	1470.4973	1471.7806	1483.6800
Frequencies --	1487.4739	1490.5611	1492.0596
Frequencies --	1493.5591	1499.0264	1500.5786
Frequencies --	1501.4267	1506.2860	1507.1178
Frequencies --	1510.0981	1510.7141	1512.5927
Frequencies --	1516.5471	1527.8625	1587.3592
Frequencies --	1590.9146	1594.2402	1596.3699
Frequencies --	1598.6480	1617.6776	1620.3187
Frequencies --	1622.5175	1813.4615	2957.3916
Frequencies --	3008.9982	3011.3530	3012.8784
Frequencies --	3013.5784	3014.5754	3021.8410
Frequencies --	3039.5962	3046.2345	3094.2698
Frequencies --	3095.8506	3099.2054	3100.3267
Frequencies --	3102.1922	3105.5243	3110.9614
Frequencies --	3132.3979	3135.2860	3140.1672
Frequencies --	3142.8129	3145.0048	3145.8316
Frequencies --	3149.6607	3161.2015	3171.7776
Frequencies --	3195.5844	3200.6349	3202.5506

Catalyst 15:**distal conformation**

vacuum	toluene-like solvent	D3 dispersion
-3312.5928371	-3312.6060671	-0.64928325

Imaginary frequency corresponding to vibration along the reaction coordinate: -962 cm^{-1} .

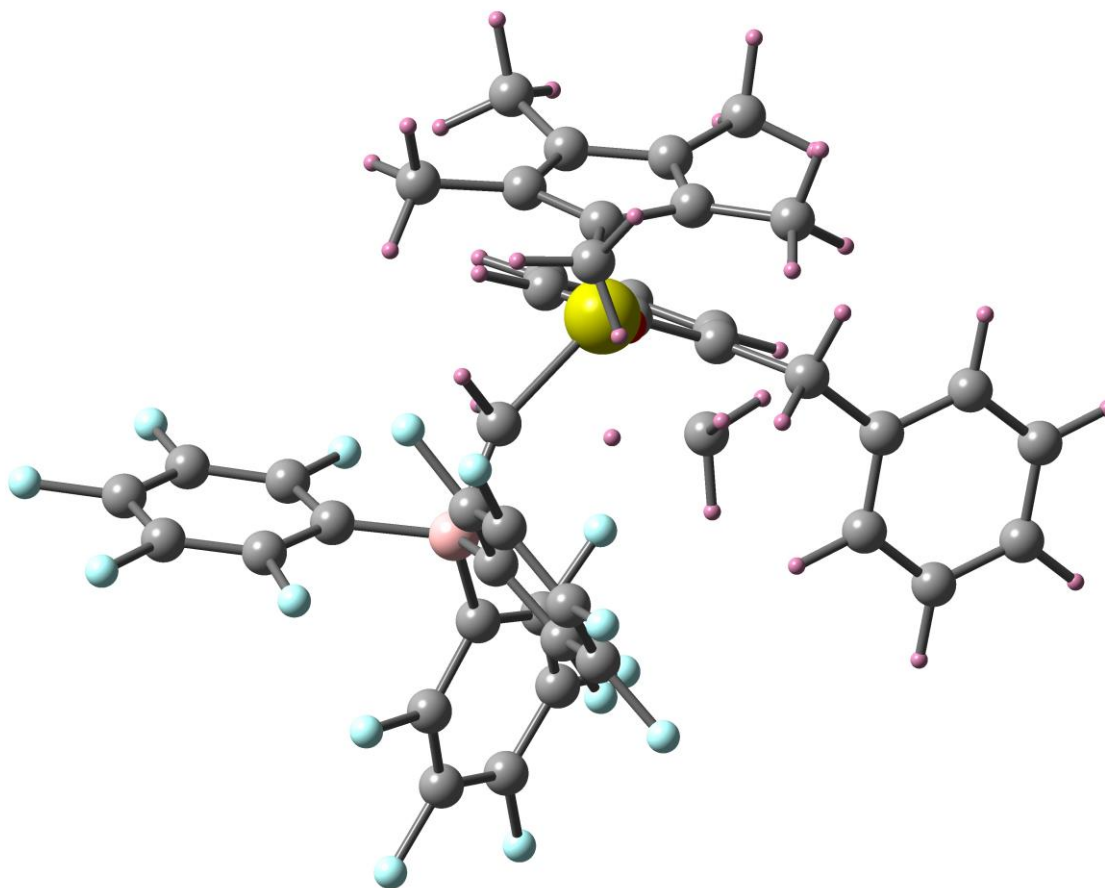
Ti	1.02574400	2.16818300	-0.00846900
C	-0.42612800	2.63719100	1.75734200
H	-0.79801900	1.97320700	2.55098000
H	0.43246600	3.17359900	2.18469200
H	-1.20840800	3.35274500	1.48715700
O	2.39466100	1.54842400	0.94257200
C	3.52878300	1.14464900	1.64136100
C	4.29642300	0.01983100	1.21840500
C	3.86230000	1.87459100	2.80901200
C	5.40414500	-0.33666100	2.02675700
C	4.96995100	1.49447800	3.58657700
C	5.74377000	0.38100600	3.19136800
H	6.00716000	-1.19682500	1.73504500
H	5.21839500	2.05304800	4.49111900
H	6.60125400	0.06830300	3.79016000
C	0.76843000	3.11620200	-2.26190700
C	0.00012000	3.98008100	-1.41122200

C	2.15621600	3.16608300	-1.81710500
C	0.90628700	4.57478600	-0.43901100
C	2.24223300	4.10545400	-0.72127100
F	-0.90587100	-4.29379400	4.61935300
C	-1.05869800	-3.38450000	3.58218400
C	-2.18705200	-3.43284000	2.74569300
C	-0.09258800	-2.39460900	3.34873800
C	-2.31194000	-2.49999300	1.70099800
F	-3.16698400	-4.39432200	2.96376200
C	-0.27283000	-1.48407500	2.28779700
F	1.03299800	-2.31724800	4.16491300
C	-1.37118200	-1.48192800	1.40513600
F	-3.48097000	-2.60041200	0.93851100
F	0.74586600	-0.52426300	2.16046000
B	-1.59851300	-0.48621800	0.08215300
C	-1.69020400	-1.57217600	-1.20971400
C	-2.94714800	0.48740100	0.24008400
C	-0.33428900	0.57830600	-0.28132400
C	-2.84859600	-1.93345600	-1.94172800
C	-0.54190300	-2.29141800	-1.62047900
C	-3.64011300	0.74480400	1.44594900
C	-3.46814000	1.22111100	-0.85182600
H	0.61755900	0.00454000	-0.28897100
H	-0.57678000	0.95754400	-1.28864000
H	-0.48456700	1.64652300	0.87968000
C	-2.86370400	-2.86850000	-2.99803400
F	-4.09640900	-1.38714900	-1.63440200
C	-0.50188900	-3.23545900	-2.66313200
F	0.68425400	-2.11115400	-0.94472500
C	-4.77002800	1.58317400	1.55654900
F	-3.20820800	0.18855000	2.65899300
C	-4.58673800	2.06917100	-0.80072600
F	-2.84609900	1.12812300	-2.11176300
C	-1.67938300	-3.52361300	-3.37109700
F	-4.04600600	-3.15620500	-3.67027300
F	0.68567900	-3.88401300	-2.99263300
C	-5.25831100	2.24693500	0.42045400
F	-5.39330800	1.77262600	2.78501400
F	-5.02343400	2.74376200	-1.93765900
F	-1.67401000	-4.44578100	-4.40797800
F	-6.36189000	3.08372100	0.50624900
C	0.54722400	5.68132600	0.52691100
H	0.70324900	6.66140900	0.04360700
H	-0.50458700	5.64190900	0.83704400
H	1.16665800	5.66937200	1.43474800
C	-1.45181800	4.36158500	-1.58534900
H	-2.00489600	4.39295300	-0.63604600
H	-1.51445300	5.37370300	-2.02130400
H	-1.98171400	3.68308600	-2.26124000
C	0.28267000	2.38995700	-3.49718000
H	-0.74707100	2.02360900	-3.40721100
H	0.31296500	3.07552600	-4.36156900
H	0.91703300	1.52887300	-3.74898700
C	3.32642100	2.51985700	-2.52621000
H	3.08724300	1.51694600	-2.90566300
H	3.62336800	3.13047300	-3.39658400
H	4.20631900	2.43115400	-1.87667700

C	3.51425200	4.59339900	-0.06704400
H	4.28275300	3.81250800	-0.00787800
H	3.93709500	5.42630400	-0.65557800
H	3.34402700	4.97100400	0.94991100
H	3.23918500	2.71948200	3.10311000
C	3.88967500	-0.81953700	0.00557300
H	3.16808500	-1.57742300	0.34948200
H	3.33039500	-0.18684700	-0.69897800
C	5.01193200	-1.52059900	-0.76391600
C	6.11591500	-0.79943000	-1.28900500
C	4.93307100	-2.90968800	-1.03063000
C	7.11005500	-1.44611700	-2.05222400
H	6.20497400	0.27234300	-1.09371700
C	5.92548100	-3.56234700	-1.79560800
H	4.08856300	-3.48562600	-0.64484300
C	7.01892500	-2.83291100	-2.30960200
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H	7.78734600	-3.33531800	-2.90168400

Frequencies --	-961.9099	6.3863	10.8413
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Frequencies --	52.6233	69.2114	75.7948
Frequencies --	82.2141	93.2930	97.3161
Frequencies --	102.8928	106.6123	112.7131
Frequencies --	114.8795	120.5231	124.4934
Frequencies --	126.2355	130.5023	133.1713
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Frequencies --	448.0705	456.7606	463.5914
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Frequencies --	552.1243	553.3455	572.1009
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Frequencies --	636.3255	638.0519	642.2945
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Frequencies --	1090.8199	1092.8346	1109.8526
Frequencies --	1122.9846	1170.4462	1174.1114
Frequencies --	1178.6951	1183.0478	1194.5978
Frequencies --	1205.0981	1209.2723	1212.7595
Frequencies --	1215.5836	1220.6947	1224.0012
Frequencies --	1240.5533	1264.2659	1290.8090
Frequencies --	1297.6283	1315.7456	1319.1161
Frequencies --	1320.2122	1325.1600	1336.5860
Frequencies --	1342.4897	1344.3535	1352.2652
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Frequencies --	1407.7506	1410.5817	1412.2965
Frequencies --	1419.3823	1422.1953	1423.1969
Frequencies --	1424.0147	1426.1652	1428.1498
Frequencies --	1433.7079	1445.5660	1449.3155
Frequencies --	1452.6600	1455.4160	1462.7961
Frequencies --	1467.2086	1467.2952	1469.5133
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Frequencies --	1511.0930	1514.9174	1524.0443
Frequencies --	1586.8811	1593.7481	1596.0854
Frequencies --	1599.3984	1604.0814	1615.9982
Frequencies --	1617.0964	1620.4397	1622.6375
Frequencies --	1626.9856	1788.6286	2951.0872
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Frequencies --	3096.1746	3099.3149	3100.6541
Frequencies --	3104.8809	3106.0707	3134.2637
Frequencies --	3140.0443	3142.3484	3147.3570
Frequencies --	3148.1062	3149.5637	3155.4898
Frequencies --	3166.1382	3167.1111	3170.3745
Frequencies --	3175.3357	3180.6494	3190.5332
Frequencies --	3191.8943	3194.4947	3204.3133

proximal conformation

vacuum	toluene-like solvent	D3 dispersion
-3312.593656	-3312.6064956	-0.64833272

Imaginary frequency corresponding to vibration along the reaction coordinate: -876 cm^{-1} .

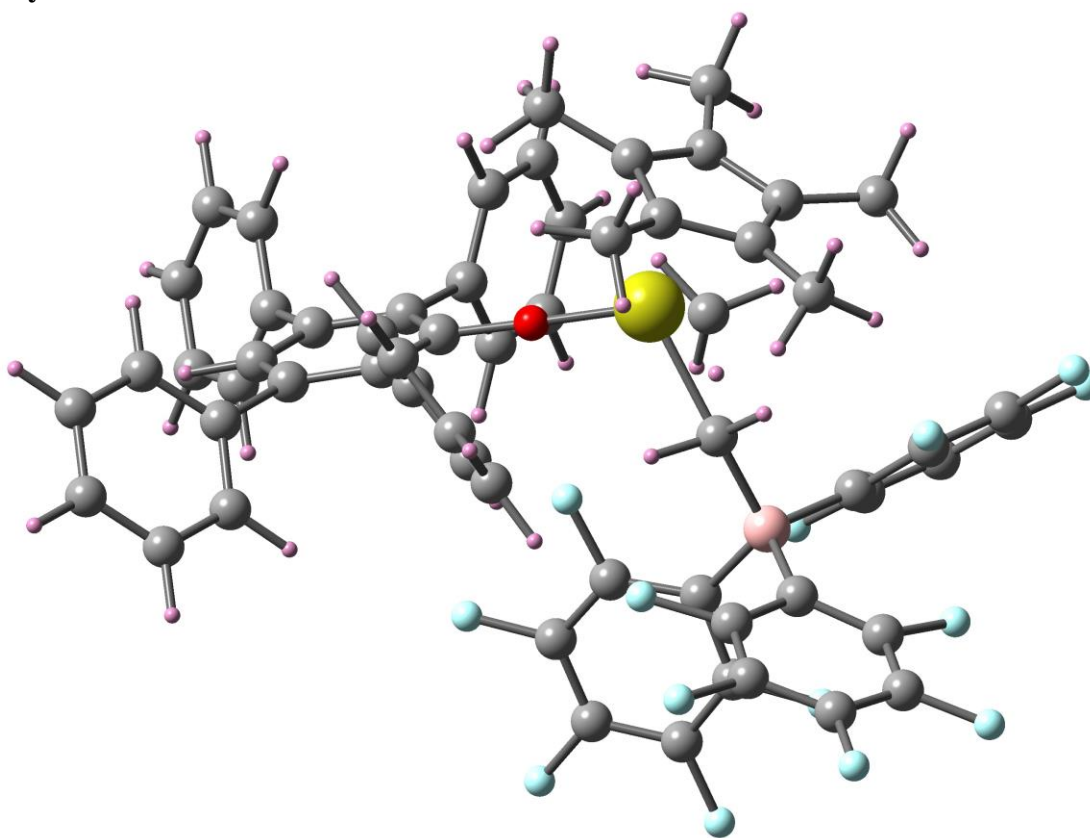
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H	2.10019700	-1.51339700	-1.95078700
H	0.51398500	-2.00247500	-2.62920800
O	2.39538400	-1.08693800	0.91947200
C	3.37259100	-0.47548200	1.70074200
C	3.10941200	-0.29804000	3.08076600
C	4.58372000	-0.01706900	1.10429700
C	4.07224600	0.31164900	3.90547700
C	5.53312000	0.58564500	1.96333700
C	5.29325700	0.74513800	3.34472300
H	3.86502600	0.45384400	4.96787100
H	6.46715400	0.95233700	1.53851000
H	6.04795100	1.22029100	3.97427500
C	-0.12470400	-4.02540100	1.06932900
C	-0.05376700	-4.19377400	-0.35489500
C	1.23716300	-3.95509400	1.58442100

C	1.34964900	-4.23190000	-0.73235400
C	2.14350800	-4.12417600	0.47100500
F	0.46012600	6.04558100	-0.42750700
C	-0.02428700	4.74673500	-0.36913900
C	-1.40547800	4.49099200	-0.41612600
C	0.85388000	3.65744800	-0.27393200
C	-1.86552200	3.16290200	-0.35443200
F	-2.29865100	5.54940600	-0.53339300
C	0.33560900	2.34895100	-0.21431700
F	2.23118400	3.87555300	-0.24783300
C	-1.03438800	2.02092700	-0.23732700
F	-3.25118400	3.00100900	-0.45904400
F	1.31020700	1.33734500	-0.15985600
B	-1.70289600	0.49602700	-0.10101800
C	-2.78352400	0.63232700	1.18985200
C	-2.41160800	-0.02144700	-1.52332600
C	-0.64037500	-0.74523800	0.34001400
C	-4.19832800	0.63606500	1.11844500
C	-2.30418400	0.81285100	2.51022900
C	-2.23653400	0.57461700	-2.79424100
C	-3.20824100	-1.19035000	-1.57810300
H	-0.07157700	-0.40344100	1.23433800
H	-1.30081100	-1.59118600	0.58983600
H	0.20280200	-0.96921700	-0.99819200
C	-5.05212800	0.75105700	2.23517600
F	-4.85672600	0.55218400	-0.11034900
C	-3.11045000	0.93542600	3.65724100
F	-0.91720700	0.91102300	2.75462200
C	-2.83077500	0.10769400	-3.98648500
F	-1.40753500	1.69350700	-2.95927000
C	-3.82094600	-1.70212400	-2.73394400
F	-3.43803700	-1.93381100	-0.40501400
C	-4.50696800	0.89444300	3.52100300
F	-6.43281200	0.73324100	2.07464600
F	-2.53867000	1.09529400	4.91688400
C	-3.63986000	-1.03851000	-3.95906600
F	-2.60836800	0.76435100	-5.19153600
F	-4.59286500	-2.85930500	-2.67867600
F	-5.32983600	1.00499400	4.63296300
F	-4.22862600	-1.52083900	-5.11902500
C	1.87576300	-4.57121600	-2.10896300
H	2.15270900	-5.63831800	-2.15282100
H	1.12594900	-4.39952200	-2.89089000
H	2.77575900	-3.99934500	-2.37774900
C	-1.21825100	-4.43174100	-1.28999200
H	-1.30711500	-3.66390800	-2.07175300
H	-1.10077300	-5.40043000	-1.80206900
H	-2.17059100	-4.45476000	-0.74935300
C	-1.38033500	-4.06390800	1.91411900
H	-2.17951500	-3.41805100	1.52834200
H	-1.77870600	-5.09219700	1.93852700
H	-1.18630700	-3.76749200	2.95297200
C	1.62197800	-3.93651600	3.04793800
H	0.96825100	-3.28940200	3.64975800
H	1.54069200	-4.95434900	3.46752100
H	2.65537900	-3.60190000	3.20175900
C	3.64480700	-4.27738200	0.56071300

H	4.08996000	-3.62900000	1.32689500
H	3.89622300	-5.31862100	0.82792900
H	4.14125000	-4.06162300	-0.39495500
H	2.15245200	-0.62036900	3.49092100
C	4.82061700	-0.18006000	-0.40282800
H	5.09983600	-1.22999300	-0.59975600
H	3.86062700	-0.01483900	-0.91162200
C	5.87038800	0.73940200	-1.02526600
C	7.14939700	0.25125300	-1.38937700
C	5.57282800	2.10411100	-1.27730400
C	8.10932300	1.09857300	-1.98748600
H	7.39926200	-0.79794900	-1.20827900
C	6.52805600	2.95390100	-1.87335600
H	4.59364300	2.50435000	-1.00528100
C	7.80098700	2.45445700	-2.23142800
H	9.08903800	0.70070600	-2.26298100
H	6.27758700	4.00059300	-2.06137000
H	8.53922200	3.11200000	-2.69642000

Frequencies --	-876.4607	9.5651	12.1609
Frequencies --	16.4316	25.3119	25.6788
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Frequencies --	33.0871	37.3821	39.3937
Frequencies --	42.2802	47.2801	49.6515
Frequencies --	50.8959	68.8943	78.7422
Frequencies --	85.2675	93.9979	100.3774
Frequencies --	107.0072	110.6600	113.0436
Frequencies --	116.6571	118.9972	122.9586
Frequencies --	125.5382	126.2883	133.6679
Frequencies --	138.5579	139.2346	142.7978
Frequencies --	144.4942	150.3306	154.8506
Frequencies --	156.8382	160.8459	161.7849
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Frequencies --	223.4377	229.4993	242.1470
Frequencies --	247.9619	259.0251	264.3956
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Frequencies --	468.0721	480.3103	490.4341
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Frequencies --	972.3422	990.2231	997.9020
Frequencies --	1006.2130	1008.5720	1019.8542
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Frequencies --	1048.9041	1050.4838	1051.4197
Frequencies --	1052.8976	1053.0991	1054.2395
Frequencies --	1056.0801	1088.1640	1089.3962
Frequencies --	1093.8516	1099.5275	1109.4079
Frequencies --	1124.9673	1170.1495	1175.5119
Frequencies --	1181.9906	1183.1301	1191.9016
Frequencies --	1203.7911	1206.6723	1209.5957
Frequencies --	1213.1522	1214.9043	1222.3700
Frequencies --	1241.2005	1276.2565	1287.0864
Frequencies --	1308.7563	1316.6312	1318.7896
Frequencies --	1319.4177	1325.9748	1337.2567
Frequencies --	1343.3546	1345.8172	1350.3434
Frequencies --	1352.7044	1375.5330	1380.2806
Frequencies --	1410.1726	1411.4884	1413.3873
Frequencies --	1419.4409	1421.1492	1425.0344
Frequencies --	1425.5276	1428.1989	1430.0727
Frequencies --	1434.2711	1445.7575	1450.1321
Frequencies --	1453.5036	1455.4793	1464.9103
Frequencies --	1467.4242	1469.0620	1471.4326
Frequencies --	1473.4771	1480.1294	1485.1635
Frequencies --	1491.7654	1493.3758	1494.6931
Frequencies --	1496.4764	1500.2447	1502.2171
Frequencies --	1503.8287	1507.6012	1508.3362
Frequencies --	1512.9926	1516.8485	1522.0137
Frequencies --	1588.2608	1594.4291	1596.3554
Frequencies --	1598.0094	1604.7117	1614.0888
Frequencies --	1617.1378	1620.0832	1622.7739
Frequencies --	1627.3916	1814.0980	2929.7475
Frequencies --	3010.1161	3011.0593	3014.3397
Frequencies --	3017.8112	3020.5061	3026.7947
Frequencies --	3038.8186	3095.5500	3096.8712
Frequencies --	3097.2642	3098.8567	3102.1849
Frequencies --	3107.2159	3112.5055	3135.7332
Frequencies --	3139.5786	3143.9841	3144.8520
Frequencies --	3145.6849	3148.9633	3157.2857
Frequencies --	3162.5412	3167.9286	3168.6412
Frequencies --	3179.8886	3183.6422	3191.5716
Frequencies --	3193.3926	3199.8166	3207.6805

Catalyst 16:

vacuum	toluene-like solvent	D3 dispersion
-3966.126723	-3966.1419353	-0.89084065

Imaginary frequency corresponding to vibration along the reaction coordinate: -995 cm^{-1} .

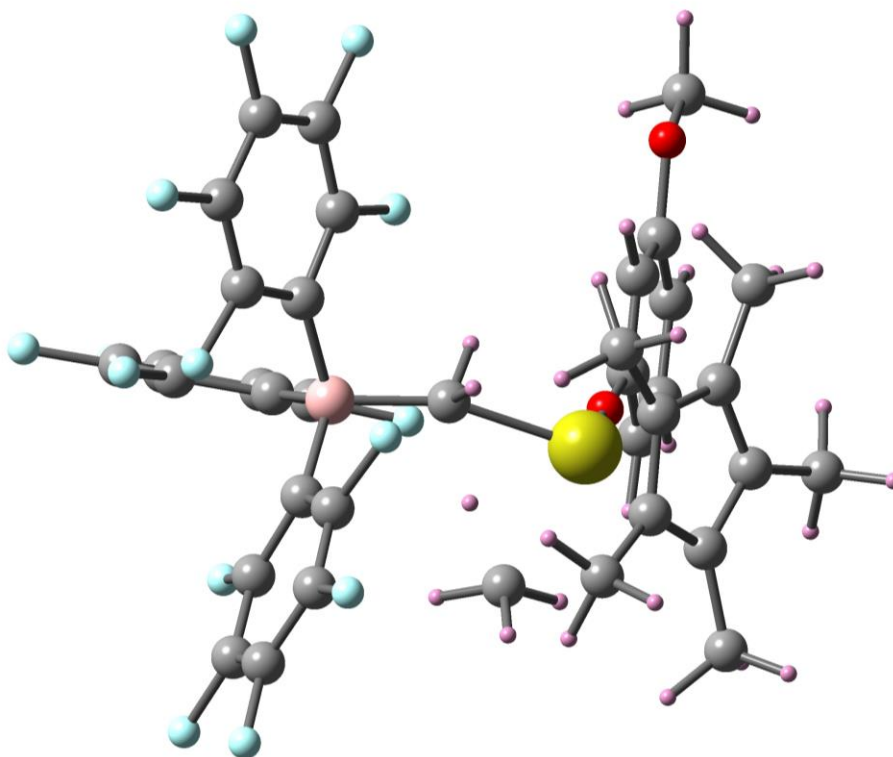
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C	0.66009200	-2.46676300	-1.00196700
H	0.68740600	-2.67492300	0.07470900
H	-0.30020800	-2.85554500	-1.35925700
H	1.47434900	-2.99736100	-1.50143700
O	-1.63849400	-0.26826500	-1.21870300
C	-2.89364200	-0.09376100	-0.62692200
C	-3.47227300	1.21781700	-0.57042100
C	-3.55204100	-1.24104500	-0.07478100
C	-4.73148700	1.37084700	0.08928500
C	-4.81586900	-1.05832400	0.55987000
C	-5.37143000	0.23578400	0.63057900
H	-6.32465000	0.36627700	1.14061500
C	1.27302700	0.14703300	-4.05084000
C	1.36774700	-1.28154500	-4.01497900
C	-0.13535100	0.50021700	-4.14022200
C	0.01994900	-1.82545000	-4.08410100
C	-0.90561700	-0.72436100	-4.20340400
F	0.36510300	0.00075600	6.12691600
C	0.87110900	0.02680200	4.83472600
C	2.25399700	0.13035400	4.60491600

C	0.01468200	-0.05473100	3.72735200
C	2.73561700	0.14939100	3.28343500
F	3.12839800	0.20021400	5.68336900
C	0.55456900	-0.02489600	2.42618900
F	-1.36231500	-0.17248800	3.91829100
C	1.92590800	0.07551800	2.12232700
F	4.12712200	0.21334800	3.15118700
F	-0.39830100	-0.12077100	1.39806400
B	2.61170000	0.16309300	0.59951100
C	3.45112700	1.63179900	0.63520300
C	3.60066800	-1.14851200	0.28462000
C	1.52749700	0.26069800	-0.71237500
C	4.85454700	1.82673900	0.67573600
C	2.73634500	2.85129600	0.69048400
C	3.62923600	-2.35808300	1.01694800
C	4.47161900	-1.17084100	-0.82966300
H	0.73899500	1.00202300	-0.47011100
H	2.14130100	0.60883400	-1.55475900
H	1.12652000	-1.23558200	-0.81115300
C	5.48355700	3.08963600	0.69751400
F	5.73478700	0.74379300	0.72854900
C	3.31044200	4.13526100	0.71266900
F	1.32928800	2.83589500	0.76424300
C	4.47123900	-3.45229700	0.72538100
F	2.76126600	-2.56843900	2.09908500
C	5.32950200	-2.22983800	-1.16949500
F	4.52087200	-0.06200900	-1.69389900
C	4.70814800	4.26006100	0.70475900
F	6.87025700	3.18802500	0.72074400
F	2.50667500	5.27407800	0.74511100
C	5.33994800	-3.38809500	-0.37473100
F	4.43260800	-4.60289800	1.50588700
F	6.15371300	-2.14856600	-2.28922200
F	5.30867200	5.51118500	0.71853800
F	6.17028800	-4.45510300	-0.68806800
C	-0.31075900	-3.28923700	-4.26344100
H	-0.19242500	-3.56572700	-5.32600700
H	0.35370800	-3.94541300	-3.68609600
H	-1.34338900	-3.52358900	-3.97895300
C	2.63434200	-2.09937800	-4.10068300
H	2.60461400	-3.00568300	-3.48050400
H	2.77799700	-2.43823800	-5.14191700
H	3.52389400	-1.52506000	-3.82361900
C	2.40903500	1.13790200	-4.16400400
H	3.36069300	0.73385400	-3.80400100
H	2.54754900	1.41895900	-5.22255300
H	2.20992900	2.06851600	-3.61293600
C	-0.64814900	1.89208100	-4.41859100
H	-0.12989900	2.66024100	-3.83101900
H	-0.48461900	2.13372600	-5.48407200
H	-1.71787700	1.99131800	-4.21662600
C	-2.38409800	-0.82410800	-4.50241200
H	-2.95562900	0.00504200	-4.06640600
H	-2.54330600	-0.79455600	-5.59471400
H	-2.82141800	-1.76179300	-4.13683500
C	-5.42117600	2.69611300	0.28878100
C	-6.73339400	2.89659300	-0.21391500

C	-4.82999100	3.73432000	1.05430000
C	-7.42700100	4.10244500	0.02300300
H	-7.21091600	2.10803900	-0.79999900
C	-5.52387500	4.93732000	1.29950500
H	-3.83210700	3.59734000	1.47202500
C	-6.82380900	5.12963000	0.78133400
H	-8.43356900	4.23706100	-0.38039300
H	-5.05094500	5.71996000	1.89733500
H	-7.35973200	6.06272300	0.97016300
C	-5.59589300	-2.17735100	1.20314100
C	-6.24163500	-3.17810400	0.43363100
C	-5.76447100	-2.19797200	2.61203900
C	-7.02566200	-4.17429400	1.05310700
H	-6.14262800	-3.17285700	-0.65304900
C	-6.54222300	-3.19725900	3.23505600
H	-5.27641700	-1.43545300	3.22292900
C	-7.17686800	-4.19038300	2.45724200
H	-7.51861700	-4.93308900	0.44051100
H	-6.65073500	-3.19873600	4.32222500
H	-7.78183200	-4.96306600	2.93738600
C	-2.83204000	2.43453900	-1.18438800
C	-3.48489100	3.11457800	-2.24672200
C	-1.65393100	3.00872900	-0.64566000
C	-2.98714900	4.33671600	-2.74324000
H	-4.40321700	2.69956900	-2.66589600
C	-1.15191600	4.23298000	-1.13944200
H	-1.15648000	2.52750200	0.19439200
C	-1.81961400	4.90431600	-2.18676500
H	-3.51735700	4.84991200	-3.54901900
H	-0.25783000	4.66613600	-0.68819300
H	-1.44203900	5.86099200	-2.55507500
C	-2.94765400	-2.62174800	-0.07879500
C	-3.09041200	-3.48826700	-1.19074100
C	-2.32640300	-3.12582400	1.09257000
C	-2.63259000	-4.82307900	-1.13582100
H	-3.59522900	-3.12774100	-2.08943300
C	-1.86617600	-4.45763200	1.15090800
H	-2.21834300	-2.47754600	1.96280200
C	-2.01902800	-5.31336800	0.03757900
H	-2.77028100	-5.48097200	-1.99756500
H	-1.39755000	-4.82770500	2.06562100
H	-1.67343100	-6.34830000	0.08743000
Frequencies --	-994.8033	8.7306	11.2770
Frequencies --	15.3748	21.0442	27.0807
Frequencies --	28.2227	29.1790	31.0928
Frequencies --	33.6742	35.8290	38.2745
Frequencies --	42.0730	42.4939	44.2458
Frequencies --	49.3868	50.4280	52.7070
Frequencies --	56.0502	59.1281	63.3374
Frequencies --	70.4111	76.9876	81.8714
Frequencies --	87.1928	92.7146	102.6363
Frequencies --	104.2154	110.2881	112.9435
Frequencies --	115.4598	115.6839	118.6623
Frequencies --	120.7113	122.5695	125.0987
Frequencies --	126.5710	133.9838	136.7268
Frequencies --	140.3510	141.1388	143.5507
Frequencies --	144.7254	148.9238	156.3708

Frequencies --	158.7667	161.6421	168.4427
Frequencies --	169.9113	174.7092	182.0146
Frequencies --	191.4341	194.5202	204.1626
Frequencies --	209.0847	212.1099	215.0989
Frequencies --	218.2718	223.1864	223.4735
Frequencies --	232.2742	242.5019	246.9276
Frequencies --	252.8477	259.0832	263.1019
Frequencies --	264.0946	265.1008	265.1493
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Frequencies --	280.7429	285.6060	290.0515
Frequencies --	296.5080	302.5842	303.0984
Frequencies --	307.6446	308.4912	314.8388
Frequencies --	322.2091	325.8383	329.8256
Frequencies --	332.5828	338.0614	358.1490
Frequencies --	365.7957	372.7631	375.4776
Frequencies --	378.1847	381.1963	386.6904
Frequencies --	392.1628	397.4045	404.3071
Frequencies --	404.7518	405.9881	410.3514
Frequencies --	413.5432	416.1455	432.0069
Frequencies --	433.0218	433.4843	434.2964
Frequencies --	451.2300	456.8353	462.9697
Frequencies --	483.6650	498.5890	512.3047
Frequencies --	516.4711	528.1602	532.5108
Frequencies --	534.2876	539.7837	543.5516
Frequencies --	544.9785	550.8431	552.2832
Frequencies --	554.6746	576.7143	587.2953
Frequencies --	594.7475	598.6193	608.2783
Frequencies --	612.6705	616.2326	617.1522
Frequencies --	617.6678	620.4594	624.8935
Frequencies --	633.5205	633.7832	634.4553
Frequencies --	637.4554	640.8725	641.3508
Frequencies --	655.2992	655.4069	673.6085
Frequencies --	687.5469	697.3202	703.2709
Frequencies --	710.1155	710.9372	711.6624
Frequencies --	715.9099	717.9028	719.8103
Frequencies --	732.0037	736.3747	742.8894
Frequencies --	743.7112	747.6041	759.7257
Frequencies --	767.0427	773.1466	776.1772
Frequencies --	778.8618	793.0032	801.0123
Frequencies --	806.2492	807.1056	836.8559
Frequencies --	857.8148	859.6153	859.9296
Frequencies --	866.1940	868.7026	873.8256
Frequencies --	874.4325	889.0378	902.7024
Frequencies --	911.8352	912.6855	917.3640
Frequencies --	931.4190	938.1758	940.5544
Frequencies --	945.3418	959.9961	968.3650
Frequencies --	973.1176	986.1657	986.3239
Frequencies --	991.8204	994.2723	995.9375
Frequencies --	1004.3222	1004.8182	1006.5368
Frequencies --	1009.5023	1013.2571	1016.4473
Frequencies --	1016.5055	1020.4876	1024.7266
Frequencies --	1026.7833	1038.9972	1039.4033
Frequencies --	1039.4668	1042.7597	1045.8418
Frequencies --	1047.2840	1047.6710	1048.2628
Frequencies --	1049.5654	1051.4573	1052.2679
Frequencies --	1054.5185	1055.3446	1055.9957
Frequencies --	1082.2386	1087.0814	1088.9912
Frequencies --	1089.8956	1090.7925	1091.1956
Frequencies --	1091.5913	1123.2636	1125.6358
Frequencies --	1128.5246	1174.5413	1175.1501
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Frequencies --	1207.2582	1207.6798	1210.0577

Frequencies --	1212.1399	1213.9557	1226.6769
Frequencies --	1254.3506	1260.5207	1278.7827
Frequencies --	1296.1221	1303.5617	1318.1493
Frequencies --	1320.5121	1321.2996	1324.2968
Frequencies --	1328.8907	1330.5571	1332.0492
Frequencies --	1333.5519	1337.6335	1343.9838
Frequencies --	1351.8099	1367.2781	1367.5643
Frequencies --	1368.5040	1369.3043	1370.2344
Frequencies --	1378.2854	1408.9679	1410.5341
Frequencies --	1414.4662	1420.0135	1420.5848
Frequencies --	1422.1739	1426.3541	1428.4189
Frequencies --	1430.2605	1437.3909	1440.3091
Frequencies --	1443.3970	1444.9612	1447.5212
Frequencies --	1451.3084	1453.0794	1454.1646
Frequencies --	1467.0287	1467.8469	1469.2510
Frequencies --	1471.0425	1473.9022	1482.8017
Frequencies --	1491.4535	1493.8945	1497.1491
Frequencies --	1497.4698	1498.6355	1500.8205
Frequencies --	1502.9062	1505.8277	1508.4090
Frequencies --	1508.7263	1509.4361	1517.1543
Frequencies --	1520.7794	1525.2170	1531.7496
Frequencies --	1591.2351	1593.9912	1594.9460
Frequencies --	1595.6582	1596.9908	1597.2449
Frequencies --	1598.6997	1599.9550	1617.8493
Frequencies --	1620.5936	1622.2836	1622.4267
Frequencies --	1623.8283	1623.9408	1624.5130
Frequencies --	1808.2445	2977.8708	3009.6150
Frequencies --	3010.2812	3011.0826	3012.6433
Frequencies --	3014.4359	3058.8086	3097.3146
Frequencies --	3098.7451	3105.1572	3107.0241
Frequencies --	3115.2633	3124.9310	3147.7036
Frequencies --	3151.4775	3151.9149	3152.6733
Frequencies --	3154.8789	3155.5017	3159.5019
Frequencies --	3160.1892	3161.3014	3163.2186
Frequencies --	3167.9277	3169.9267	3172.5491
Frequencies --	3172.5821	3174.0827	3174.9523
Frequencies --	3182.1529	3182.2558	3184.0945
Frequencies --	3185.6066	3186.4897	3193.5611
Frequencies --	3194.7549	3195.1804	3198.1992
Frequencies --	3199.7669	3205.2082	3220.9942

Catalyst 17:**distal conformation**

vacuum	toluene-like solvent	D3 dispersion
-3156.8316642	-3156.8441568	-0.57036226

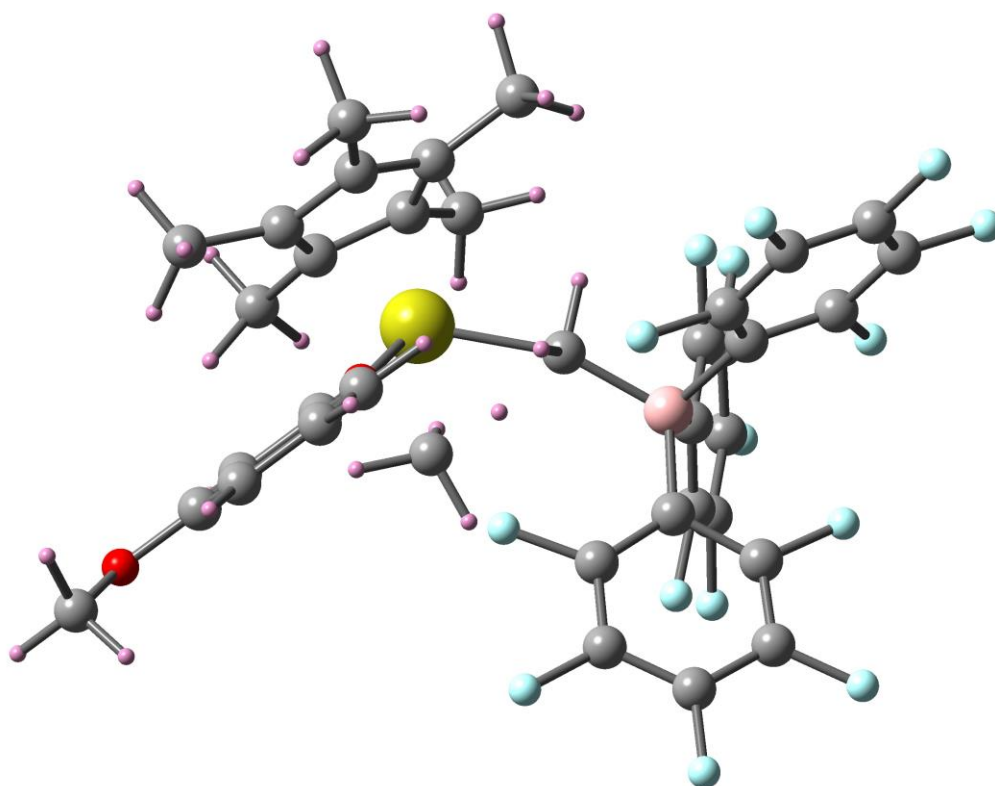
Imaginary frequency corresponding to vibration along the reaction coordinate: -1048 cm^{-1} .

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H	-0.26040200	1.20470400	-2.79500200
H	-1.68985600	2.18849500	-2.52190400
H	-0.06331900	2.88828100	-2.22466900
O	-3.02580300	0.74809400	-0.45636200
C	-4.14889700	-0.04206600	-0.64842800
C	-4.62191600	-0.83762000	0.41309000
C	-4.78045600	-0.05548000	-1.91751400
C	-5.75265300	-1.66469200	0.20952300
C	-5.89961600	-0.88687800	-2.10111600
C	-6.39844600	-1.69165200	-1.05251800
H	-6.38980500	-0.91737700	-3.07638800
H	-7.26440200	-2.32572700	-1.23133400
C	-1.18717400	3.38978500	1.78097600
C	-0.84849400	4.10024800	0.58072900
C	-2.60506200	3.05433000	1.72011400
C	-2.05403100	4.21768200	-0.22725100
C	-3.14572300	3.61420300	0.50137800
F	0.39800600	-5.43601800	-3.13693600
C	0.60382100	-4.25163000	-2.44319100

C	1.84350200	-3.97928300	-1.83996400
C	-0.41818200	-3.29668500	-2.33714400
C	2.02076800	-2.77161700	-1.14118300
F	2.87980800	-4.89985900	-1.94717800
C	-0.18282500	-2.10339500	-1.62524300
F	-1.65185400	-3.53160200	-2.93913400
C	1.02677200	-1.77437300	-0.98088600
F	3.29940600	-2.56358700	-0.61140000
F	-1.26364800	-1.20603900	-1.61255900
B	1.33348500	-0.41662700	-0.05870100
C	1.83464100	-1.03687600	1.42932000
C	2.44350400	0.60973100	-0.76957700
C	-0.00435000	0.55934600	0.28308300
C	3.14817200	-1.01852000	1.95901100
C	0.91467900	-1.70693300	2.27195900
C	2.87693900	0.55374700	-2.11474400
C	2.98453700	1.71445600	-0.07077200
H	-0.82871500	-0.09758600	0.63883800
H	0.34238400	1.23742300	1.08189100
H	-0.26266100	1.27939700	-1.07099500
C	3.50971700	-1.56209200	3.20920500
F	4.20770300	-0.46348400	1.23755500
C	1.22264600	-2.26820600	3.52533100
F	-0.42497100	-1.87813000	1.86333200
C	3.79388100	1.45515700	-2.69761100
F	2.38002800	-0.41873500	-2.99389700
C	3.89463700	2.64415300	-0.59958500
F	2.60775600	1.94251900	1.26721900
C	2.53888400	-2.18806300	4.00719900
F	4.82358500	-1.49127300	3.65826600
F	0.24077800	-2.89792000	4.28570300
C	4.31684600	2.50918900	-1.93282000
F	4.16982400	1.31922600	-4.02930400
F	4.36720900	3.70004400	0.17576000
F	2.87393400	-2.72532500	5.24224600
F	5.21107800	3.41404500	-2.48702600
C	-2.19004400	5.04151600	-1.48743700
H	-2.44400000	6.08345500	-1.22558900
H	-1.26112300	5.07665100	-2.07065400
H	-2.98785500	4.67318700	-2.14741200
C	0.47577600	4.75891500	0.27046800
H	0.72853300	4.72412400	-0.79827800
H	0.43037200	5.82621700	0.54960200
H	1.30634200	4.31418500	0.82834900
C	-0.29666500	3.15373200	2.98026700
H	0.76897700	3.18905800	2.72824500
H	-0.48208400	3.93746900	3.73506400
H	-0.49316300	2.18862500	3.46944700
C	-3.39933300	2.41884400	2.84086300
H	-2.82004800	1.66419600	3.39193400
H	-3.69775000	3.18963900	3.57285900
H	-4.31816300	1.93870100	2.48107300
C	-4.60289100	3.64362600	0.10199000
H	-5.16592900	2.79634100	0.51249200
H	-5.07393200	4.56690400	0.48263400
H	-4.73934700	3.63647200	-0.98798700
H	-4.12054300	-0.85006300	1.37900600

H	-4.38523900	0.54804700	-2.73329200
O	-6.13766200	-2.40739200	1.33001000
C	-7.24716700	-3.35889700	1.20657300
H	-7.03231100	-4.12800500	0.44615300
H	-7.32432200	-3.82840400	2.19450500
H	-8.19342200	-2.84557400	0.96537200
Frequencies --	-1047.6404	7.8688	8.6553
Frequencies --	15.6352	22.8386	26.2622
Frequencies --	27.6205	29.2547	32.3732
Frequencies --	37.2594	40.2770	44.8019
Frequencies --	49.4473	53.8410	69.6819
Frequencies --	80.1304	93.9048	99.3311
Frequencies --	99.8145	104.5411	109.6029
Frequencies --	111.9342	112.9731	119.6589
Frequencies --	120.5961	124.5442	128.5299
Frequencies --	131.3060	136.8898	142.7120
Frequencies --	144.3104	146.3765	150.0824
Frequencies --	154.3519	157.4525	160.1702
Frequencies --	161.6417	163.4125	169.3100
Frequencies --	173.9888	186.1025	190.8985
Frequencies --	194.6546	210.6614	216.8427
Frequencies --	219.6168	224.0860	228.3178
Frequencies --	235.8687	252.0998	258.4590
Frequencies --	264.2231	264.8546	265.1535
Frequencies --	274.6815	275.7739	277.8678
Frequencies --	286.2832	289.6165	295.4820
Frequencies --	299.4818	302.1060	303.4312
Frequencies --	305.6729	308.1274	322.7906
Frequencies --	326.2883	328.1751	334.3194
Frequencies --	345.6170	362.1315	372.5233
Frequencies --	377.4187	378.6566	379.3855
Frequencies --	380.9109	391.1467	393.2273
Frequencies --	400.9152	410.5802	431.2473
Frequencies --	432.2387	433.8593	450.7023
Frequencies --	452.7864	456.8495	464.1857
Frequencies --	474.5633	486.0173	531.3942
Frequencies --	534.9518	536.8051	537.7342
Frequencies --	544.9997	554.3075	554.6634
Frequencies --	559.5133	570.7251	582.3280
Frequencies --	595.2934	599.8869	601.9893
Frequencies --	607.0243	610.6249	635.4733
Frequencies --	636.6933	638.7269	643.5085
Frequencies --	654.8697	655.2613	672.6199
Frequencies --	675.0586	702.4114	718.7131
Frequencies --	723.5256	734.2644	747.5861
Frequencies --	748.9756	756.9880	762.6486
Frequencies --	771.4095	783.7453	800.1171
Frequencies --	803.4456	828.9169	845.0389
Frequencies --	862.3110	871.6378	879.3921
Frequencies --	887.1044	904.0107	913.3982
Frequencies --	920.0982	953.1751	959.3806
Frequencies --	968.6933	969.9056	987.5685
Frequencies --	1014.8451	1019.7887	1025.4088
Frequencies --	1029.8089	1039.0279	1041.7149
Frequencies --	1044.9553	1045.5391	1046.2950
Frequencies --	1048.3305	1051.1271	1054.2957
Frequencies --	1057.5487	1087.6965	1087.9548
Frequencies --	1099.4656	1102.0647	1125.1250
Frequencies --	1126.5192	1165.5429	1170.9113
Frequencies --	1174.1023	1175.2779	1200.9154
Frequencies --	1209.8757	1212.8955	1215.9057

Frequencies --	1267.5734	1273.7402	1300.1425
Frequencies --	1302.9675	1317.3874	1319.9591
Frequencies --	1325.5393	1337.5751	1343.7938
Frequencies --	1350.0646	1352.5972	1386.4117
Frequencies --	1409.0831	1411.4267	1413.4388
Frequencies --	1419.3670	1422.2336	1422.8913
Frequencies --	1425.6568	1426.9544	1429.8487
Frequencies --	1435.7458	1446.2929	1448.9518
Frequencies --	1452.6287	1455.5183	1463.8503
Frequencies --	1467.0055	1468.6280	1469.9003
Frequencies --	1471.2804	1481.8628	1482.8914
Frequencies --	1484.7428	1487.8832	1488.3134
Frequencies --	1490.7046	1497.8500	1498.5217
Frequencies --	1499.3596	1503.9160	1509.0370
Frequencies --	1510.1567	1514.3594	1525.7680
Frequencies --	1591.0232	1594.2174	1596.2758
Frequencies --	1598.7254	1617.0597	1618.9019
Frequencies --	1620.3228	1622.4394	1830.4676
Frequencies --	2935.8071	2996.2978	3008.4394
Frequencies --	3010.2201	3011.5109	3013.2211
Frequencies --	3014.2703	3032.9085	3081.8719
Frequencies --	3095.6428	3096.2808	3098.9763
Frequencies --	3099.1419	3100.8957	3103.0454
Frequencies --	3129.0511	3139.3184	3141.3606
Frequencies --	3148.3098	3156.9608	3160.9585
Frequencies --	3169.3836	3173.8173	3193.3129
Frequencies --	3208.3955	3217.8762	3220.5804

proximal conformation

vacuum	toluene-like solvent	D3 dispersion
-3156.8319503	-3156.8446291	-0.57062786

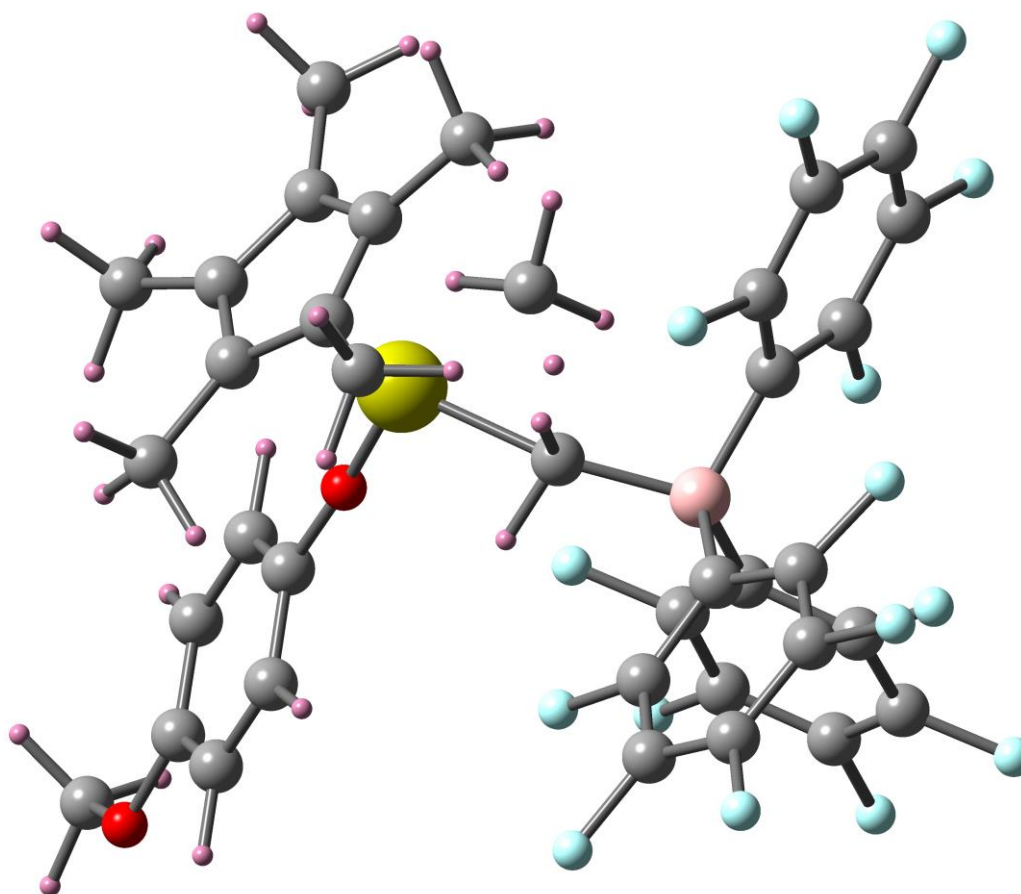
Imaginary frequency corresponding to vibration along the reaction coordinate: -1066 cm^{-1} .

Ti	1.73228300	-1.66971000	0.14009400
C	1.11266500	-1.59832200	-2.09773700
H	0.72462600	-0.76853300	-2.70573700
H	2.18711600	-1.66175000	-2.32665900
H	0.61111700	-2.52505100	-2.39168300
O	3.04867800	-0.47794200	0.14088900
C	4.06618900	0.44271200	0.34118500
C	3.99329400	1.33144300	1.44410600
C	5.13569600	0.49534700	-0.57303500
C	5.01943500	2.27782500	1.61088200
C	6.15814100	1.45674500	-0.38822700
C	6.10457500	2.35273700	0.70929500
H	4.97267700	2.97537900	2.44962100
H	6.87809200	3.10159500	0.86679100
C	1.08898600	-3.50998200	1.63799600
C	1.00090800	-4.06286800	0.31611300
C	2.46939100	-3.09606300	1.86237900
C	2.32551300	-4.00148000	-0.28458800
C	3.23806200	-3.45126900	0.69134900
F	-0.31995600	5.79052000	-2.35664000
C	-0.55235800	4.51852800	-1.85231600
C	-1.84841000	4.11719100	-1.48605600

C	0.50009300	3.60262300	-1.70635000
C	-2.05185600	2.82306100	-0.97409900
F	-2.91307000	4.99772000	-1.64106500
C	0.23598800	2.31829700	-1.18989600
F	1.79222700	3.96592900	-2.07673300
C	-1.03252400	1.85726100	-0.78375500
F	-3.37958800	2.49389700	-0.67848300
F	1.35465900	1.47165000	-1.12292100
B	-1.38590400	0.37855200	-0.09337200
C	-2.14562500	0.77702800	1.36137100
C	-2.30394800	-0.59705100	-1.08983800
C	-0.05669800	-0.57394400	0.34009600
C	-3.52129400	0.63268700	1.66724100
C	-1.41196500	1.37126500	2.41664200
C	-2.52932500	-0.38794900	-2.47037700
C	-2.87193500	-1.80607400	-0.62367800
H	0.64271300	0.06414900	0.92367300
H	-0.48173800	-1.37702400	0.96574100
H	0.47428500	-1.07169300	-1.02885000
C	-4.10499900	0.99064400	2.90027900
F	-4.41956400	0.13409400	0.72155800
C	-1.94404500	1.74888100	3.66359000
F	-0.03804100	1.65615800	2.25440700
C	-3.28314000	-1.24921000	-3.29675400
F	-1.97279800	0.71437800	-3.13402200
C	-3.62552600	-2.70181100	-1.39957600
F	-2.69475600	-2.18387000	0.72177900
C	-3.31056600	1.54825200	3.91478100
F	-5.46501200	0.80435400	3.11982300
F	-1.13250100	2.31621600	4.64303500
C	-3.84526600	-2.41660600	-2.75765500
F	-3.45939600	-0.96032900	-4.64528400
F	-4.14179500	-3.86877400	-0.84195400
F	-3.86468300	1.90320500	5.13662200
F	-4.58105000	-3.28379900	-3.55262200
C	2.72379500	-4.62458100	-1.60351300
H	3.06731400	-5.66054600	-1.43847100
H	1.88821600	-4.67348100	-2.31293300
H	3.54813100	-4.08674700	-2.09310200
C	-0.20566300	-4.73453000	-0.29823200
H	-0.29259800	-4.54857100	-1.37775700
H	-0.12371900	-5.82824000	-0.17147000
H	-1.14417900	-4.42447800	0.17352200
C	0.00354600	-3.49017000	2.69096500
H	-1.00213100	-3.56081800	2.26205500
H	0.13326700	-4.35169700	3.36863800
H	0.03777000	-2.58613200	3.31631900
C	3.02376800	-2.57989500	3.17270500
H	2.30774100	-1.94031600	3.70839000
H	3.25854100	-3.42673500	3.84116200
H	3.94957600	-2.00524700	3.03763400
C	4.73933400	-3.35851300	0.54765300
H	5.16690300	-2.53032300	1.12627300
H	5.20365700	-4.29034000	0.91560500
H	5.05360400	-3.23262700	-0.49721800
H	3.14646800	1.29243100	2.12785900
H	5.18012400	-0.17420000	-1.42966300

O	7.17051200	1.42259800	-1.35372000
C	8.24493700	2.41933500	-1.28977900
H	8.88336500	2.19929900	-2.15380600
H	7.84633300	3.44398500	-1.37421200
H	8.83139300	2.31991800	-0.36076800
Frequencies --	-1066.4401	8.7735	14.9745
Frequencies --	15.7474	22.6927	25.6137
Frequencies --	28.7138	29.8157	32.3210
Frequencies --	36.8228	41.4474	48.4255
Frequencies --	49.9273	59.3630	67.7066
Frequencies --	80.4365	97.5373	101.1891
Frequencies --	109.9840	113.4556	114.3556
Frequencies --	117.2946	121.4944	124.3903
Frequencies --	125.3128	126.3354	130.8726
Frequencies --	136.8798	137.9650	140.0863
Frequencies --	143.0020	144.8679	148.3838
Frequencies --	154.9405	157.0767	160.4035
Frequencies --	161.7025	164.9272	172.8730
Frequencies --	175.7154	184.9016	193.9858
Frequencies --	196.6925	212.3460	217.9350
Frequencies --	218.3245	224.1526	228.1377
Frequencies --	235.4797	256.6135	258.4770
Frequencies --	264.5431	264.5885	265.2383
Frequencies --	274.4971	275.6323	277.5452
Frequencies --	283.6039	288.6945	291.9718
Frequencies --	295.6260	302.3357	304.0973
Frequencies --	305.0806	306.0042	320.7237
Frequencies --	326.7350	327.1074	333.8060
Frequencies --	349.6549	359.8575	370.4020
Frequencies --	377.1229	378.0205	378.6838
Frequencies --	380.9802	393.1433	394.6442
Frequencies --	400.5094	410.1881	431.3821
Frequencies --	431.9692	433.8855	450.6591
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Frequencies --	472.7215	481.6114	531.7154
Frequencies --	535.0015	537.2645	537.2983
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Frequencies --	593.8298	599.0154	601.4290
Frequencies --	607.0683	610.7049	635.0953
Frequencies --	636.3711	638.4434	643.2486
Frequencies --	654.3549	657.6017	671.2675
Frequencies --	675.3431	697.3422	718.7595
Frequencies --	723.1183	733.7193	746.8161
Frequencies --	749.2656	759.1729	762.4522
Frequencies --	771.4213	780.9689	800.8822
Frequencies --	802.8503	831.8280	844.0385
Frequencies --	865.3288	870.2823	876.8270
Frequencies --	886.4897	904.2696	913.7170
Frequencies --	919.5858	952.4669	963.6877
Frequencies --	968.0169	969.8069	988.0913
Frequencies --	1018.1315	1019.6901	1023.9059
Frequencies --	1030.4114	1039.6564	1042.0238
Frequencies --	1043.9104	1045.6705	1046.2865
Frequencies --	1048.4707	1050.7362	1055.6365
Frequencies --	1058.8546	1087.0138	1087.8198
Frequencies --	1100.2287	1104.0996	1125.1530
Frequencies --	1126.5673	1162.7410	1170.5533
Frequencies --	1173.3178	1174.6876	1200.7209
Frequencies --	1209.4273	1213.1073	1215.9346
Frequencies --	1267.3973	1271.8099	1299.0287

Frequencies --	1302.3732	1316.4894	1320.4485
Frequencies --	1326.0058	1337.4717	1344.2085
Frequencies --	1350.0686	1354.0189	1386.5706
Frequencies --	1409.0218	1411.5674	1412.9511
Frequencies --	1419.8992	1422.3064	1423.6193
Frequencies --	1425.9799	1426.7569	1428.6622
Frequencies --	1434.5767	1447.4973	1449.6916
Frequencies --	1452.0022	1456.7011	1464.6983
Frequencies --	1467.1381	1467.8764	1469.5380
Frequencies --	1471.2149	1481.4529	1483.8662
Frequencies --	1484.8335	1485.2910	1488.1161
Frequencies --	1490.8308	1496.1886	1498.9555
Frequencies --	1499.8040	1505.1185	1508.1910
Frequencies --	1509.7223	1513.1857	1526.6334
Frequencies --	1590.3481	1594.1699	1596.3760
Frequencies --	1598.5514	1617.0683	1620.0177
Frequencies --	1620.4982	1622.4425	1821.3304
Frequencies --	2938.8400	2996.9302	3006.5659
Frequencies --	3010.0920	3011.7987	3013.1107
Frequencies --	3014.5477	3032.7257	3084.6536
Frequencies --	3094.6652	3096.6941	3098.3658
Frequencies --	3098.8866	3102.1710	3103.3412
Frequencies --	3128.8193	3134.5378	3142.1511
Frequencies --	3148.6384	3156.9569	3160.2309
Frequencies --	3166.0427	3175.4164	3191.4106
Frequencies --	3209.4785	3218.3557	3221.1433

Catalyst 18:

vacuum	toluene-like solvent	D3 dispersion
-3156.8305231	-3156.8435677	-0.57052281

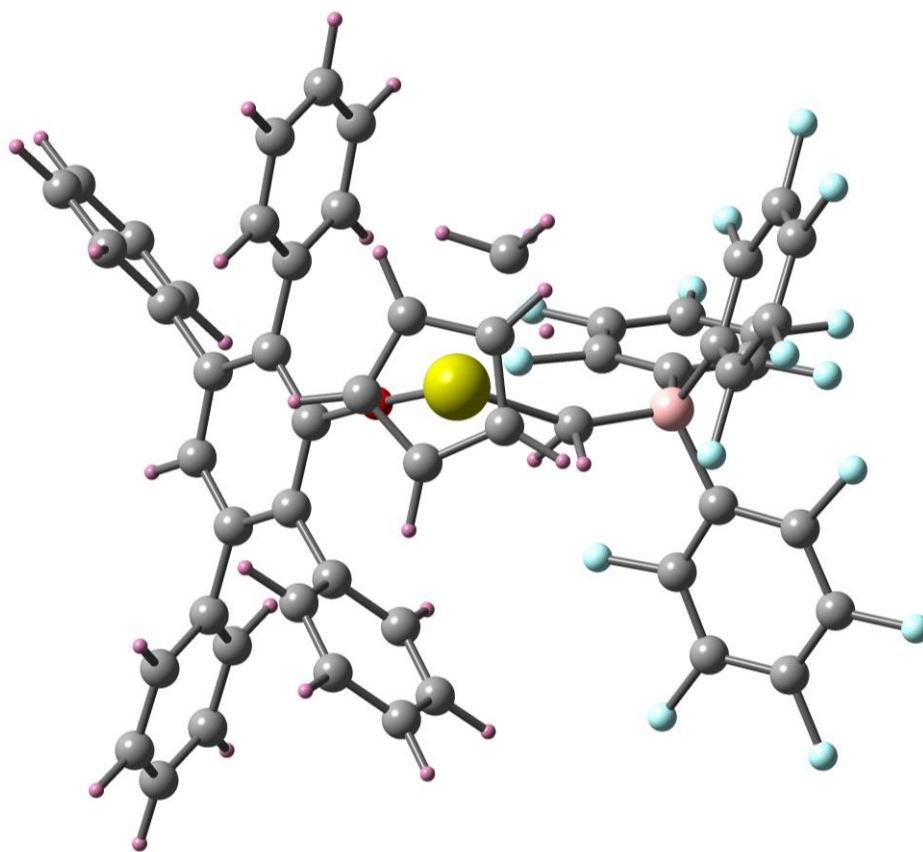
Imaginary frequency corresponding to vibration along the reaction coordinate: -912 cm^{-1} .

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C	-0.86382400	1.74614500	-2.15839300
H	-0.56557700	0.88878100	-2.77864600
H	-1.91733700	1.94661900	-2.40324500
H	-0.25102900	2.61363300	-2.42102200
O	-2.98929300	0.74515900	-0.06074900
C	-4.13191600	-0.03484900	-0.00344200
C	-4.31952200	-0.93421300	1.07807000
C	-5.09258800	0.04270700	-1.03561600
C	-5.46726900	-1.73655900	1.12331800
C	-6.24444700	-0.76769200	-0.99428000
C	-6.43886100	-1.66059100	0.09009500
H	-5.62667800	-2.43890700	1.94105300
H	-6.96564000	-0.69834600	-1.80680600
C	-0.99298100	3.51501600	1.73510700
C	-0.61056500	4.09606000	0.47876600
C	-2.43328000	3.28704900	1.70930600
C	-1.80835600	4.23294200	-0.33273200
C	-2.93674500	3.77185400	0.44428200

F	0.02179500	-5.73267100	-2.47403300
C	0.32072100	-4.48901400	-1.93525500
C	1.62626800	-4.18361900	-1.51446300
C	-0.67181200	-3.50596200	-1.80854300
C	1.89746500	-2.91538100	-0.97021300
F	2.63393500	-5.13212300	-1.64844600
C	-0.34133400	-2.25201600	-1.25668500
F	-1.97094100	-3.77308000	-2.23360800
C	0.93952500	-1.88533100	-0.79721500
F	3.23277500	-2.68275800	-0.62154900
F	-1.40320700	-1.33365200	-1.21253300
B	1.36830900	-0.44590000	-0.06710700
C	2.03870500	-0.92086200	1.40914300
C	2.39828500	0.47027900	-1.01146600
C	0.09678200	0.59568200	0.32829500
C	3.40728200	-0.88123000	1.77285100
C	1.22065500	-1.47405600	2.42414000
C	2.65794600	0.26241500	-2.38637600
C	3.04661500	1.62192700	-0.50489800
H	-0.67408400	0.00253500	0.86918200
H	0.55529400	1.34870200	0.99132900
H	-0.33306400	1.16995200	-1.09447000
C	3.91168300	-1.29547600	3.02314600
F	4.37849000	-0.43774000	0.87258000
C	1.67179900	-1.90444800	3.68584600
F	-0.16159000	-1.65718800	2.20120500
C	3.51517100	1.06524600	-3.16943100
F	2.03348800	-0.77697000	-3.09079400
C	3.90626100	2.45757300	-1.23716700
F	2.84767200	2.00117800	0.83616200
C	3.03743100	-1.80583900	3.99588400
F	5.27131500	-1.21072400	3.30083500
F	0.78168200	-2.42354600	4.62271700
C	4.15527000	2.17144900	-2.59006000
F	3.71744400	0.78028200	-4.51536000
F	4.50073000	3.56719000	-0.64193800
F	3.51305900	-2.21402600	5.23414400
F	4.99526000	2.98081900	-3.34170300
C	-1.88844100	4.95674900	-1.65796100
H	-2.21831500	5.99766100	-1.49822000
H	-0.91604400	5.00059900	-2.16390500
H	-2.60741500	4.49852000	-2.35228600
C	0.75935100	4.61823500	0.10769800
H	1.17177300	4.15080600	-0.79779300
H	0.70840900	5.70235200	-0.08534700
H	1.48446900	4.45954200	0.91312200
C	-0.09602300	3.30183600	2.93534300
H	0.88901900	2.89828000	2.66829600
H	0.07424200	4.26478800	3.44634000
H	-0.54466600	2.62105800	3.67088200
C	-3.26710900	2.81062700	2.87960300
H	-2.77344300	2.01281800	3.45299500
H	-3.44515600	3.64579300	3.57924000
H	-4.24889700	2.43383300	2.56499200
C	-4.38877700	3.88318800	0.03902000
H	-5.01465400	3.10611000	0.49526400
H	-4.79087700	4.85925800	0.36287200

H	-4.52265400	3.82622400	-1.05032000
H	-3.56366800	-1.01063800	1.86003300
H	-4.93249600	0.72084600	-1.87435500
O	-7.53625300	-2.51078000	0.25001500
C	-8.56736600	-2.54788400	-0.79231700
H	-8.14651100	-2.86576800	-1.76083500
H	-9.29248200	-3.29266300	-0.44333400
H	-9.06507300	-1.56930100	-0.90114800
Frequencies --	-911.6770	3.9781	13.1114
Frequencies --	16.5865	17.4751	20.0508
Frequencies --	27.3643	29.4915	31.2713
Frequencies --	36.3617	40.9339	47.3259
Frequencies --	48.9339	53.5520	67.8354
Frequencies --	75.0095	76.6738	94.8984
Frequencies --	99.3315	99.9177	108.7491
Frequencies --	110.6855	113.6747	116.6626
Frequencies --	118.2031	118.3742	119.4620
Frequencies --	123.4024	126.6131	128.8023
Frequencies --	138.7492	142.6545	142.9244
Frequencies --	145.9710	155.5971	158.1283
Frequencies --	159.5764	161.4846	169.8121
Frequencies --	173.6280	189.2303	191.8305
Frequencies --	204.9861	208.3774	215.7212
Frequencies --	217.6091	223.6042	226.4915
Frequencies --	227.2127	251.3374	264.4541
Frequencies --	264.5105	264.8913	270.4511
Frequencies --	274.9378	275.8397	278.1646
Frequencies --	280.1754	285.9417	290.8304
Frequencies --	293.0476	299.9836	302.7095
Frequencies --	304.6571	307.7311	325.3090
Frequencies --	326.4173	332.9542	341.0660
Frequencies --	359.6873	364.6337	372.6325
Frequencies --	377.2673	378.3771	381.0479
Frequencies --	390.5608	394.4176	397.2171
Frequencies --	408.5086	415.7397	420.8556
Frequencies --	431.3376	431.9155	434.2632
Frequencies --	449.8142	456.9957	464.0292
Frequencies --	473.2971	489.8302	516.8399
Frequencies --	531.9556	535.4042	536.6362
Frequencies --	539.5917	544.6861	554.8890
Frequencies --	557.0469	577.0624	580.1588
Frequencies --	583.7341	592.9534	600.0650
Frequencies --	600.4600	619.7601	635.0073
Frequencies --	635.7231	636.2518	638.5691
Frequencies --	643.0966	654.7526	670.2213
Frequencies --	694.5093	712.7743	718.7948
Frequencies --	722.9269	733.3874	746.8128
Frequencies --	748.9165	762.3299	767.7727
Frequencies --	771.2664	797.9266	801.0619
Frequencies --	803.2547	826.0200	844.1163
Frequencies --	872.6955	887.0939	902.1031
Frequencies --	906.8480	913.3456	921.3080
Frequencies --	926.7742	938.9847	966.9974
Frequencies --	968.0940	970.5300	991.6027
Frequencies --	1010.2466	1011.9619	1019.0123
Frequencies --	1029.1121	1039.5187	1039.8093
Frequencies --	1042.8644	1044.1625	1046.7394
Frequencies --	1048.8817	1051.0110	1053.9121
Frequencies --	1057.2356	1086.8087	1088.1603
Frequencies --	1098.5404	1120.4783	1123.5568
Frequencies --	1126.0591	1170.2531	1172.4589

Frequencies --	1174.4436	1184.0448	1209.2520
Frequencies --	1212.4605	1215.7909	1228.9250
Frequencies --	1261.4701	1268.9484	1300.2927
Frequencies --	1312.8246	1316.1362	1319.3426
Frequencies --	1325.7778	1337.1782	1343.3287
Frequencies --	1347.9617	1351.2115	1362.7609
Frequencies --	1409.5535	1411.1510	1412.6485
Frequencies --	1419.1725	1422.0048	1422.3747
Frequencies --	1424.5805	1427.5447	1429.4249
Frequencies --	1433.4873	1437.2982	1449.2559
Frequencies --	1452.3986	1454.8079	1462.7227
Frequencies --	1466.8892	1467.1821	1469.1891
Frequencies --	1471.4323	1481.6346	1484.5921
Frequencies --	1486.6922	1487.4326	1490.3320
Frequencies --	1494.1659	1498.0840	1499.7177
Frequencies --	1500.9518	1504.8087	1506.6158
Frequencies --	1508.7708	1515.5848	1521.7195
Frequencies --	1582.2174	1594.1405	1596.1105
Frequencies --	1598.6730	1616.9701	1619.6212
Frequencies --	1622.5813	1625.2210	1815.5450
Frequencies --	2933.5287	2995.9120	3008.2169
Frequencies --	3009.1096	3012.6402	3017.2207
Frequencies --	3024.3578	3033.5343	3086.6148
Frequencies --	3095.5363	3096.2243	3097.2985
Frequencies --	3099.5891	3105.3599	3109.1478
Frequencies --	3130.4617	3136.5423	3141.9369
Frequencies --	3144.9645	3146.4121	3161.4520
Frequencies --	3162.1024	3187.5425	3188.6607
Frequencies --	3192.2635	3211.9934	3215.4334

Catalyst 19:

vacuum	toluene-like solvent	D3 dispersion
-3769.6648687	-3769.6821422	-0.78806683

Imaginary frequency corresponding to vibration along the reaction coordinate: -1063 cm^{-1} .

Ti	-0.07072500	-0.54677400	-2.12594800
C	0.59701700	-2.57372500	-1.23455100
H	0.59021600	-2.82014000	-0.16549800
H	-0.34568400	-2.95902500	-1.64463100
H	1.43405500	-3.07761600	-1.72619600
O	-1.67744600	-0.32779600	-1.40697800
C	-2.95194000	-0.07408500	-0.90364100
C	-3.38453600	1.28441000	-0.81096900
C	-3.72276800	-1.17725400	-0.42489400
C	-4.60657500	1.54608400	-0.12567000
C	-4.94594900	-0.88769100	0.24896100
C	-5.34052000	0.46114900	0.40611300
H	-6.28004800	0.67145600	0.91574400
C	0.02407500	0.56833600	-4.20102600
C	1.36359800	0.05270700	-4.05738700
C	-0.87043500	-0.54808100	-4.35885900
C	1.28736100	-1.37076900	-4.07730700
C	-0.09344000	-1.74744700	-4.25045400
F	1.12433800	-1.70447900	5.89469400
C	1.45255300	-1.32455200	4.60108400

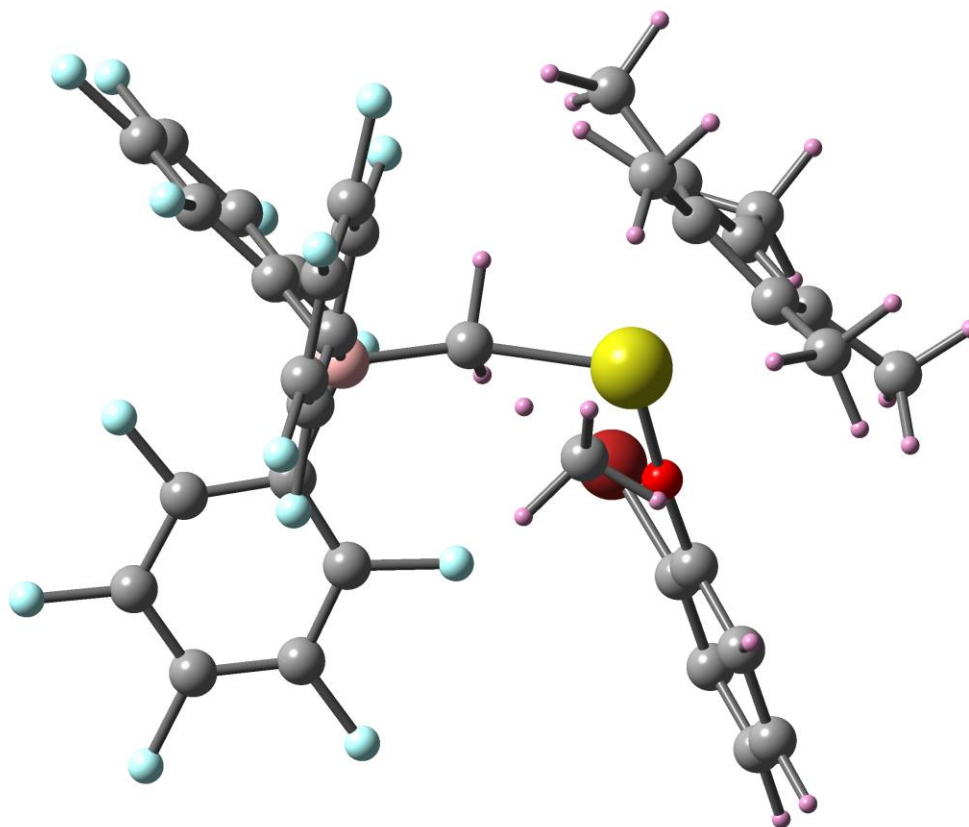
C	2.77966000	-1.01097100	4.25891200
C	0.46793100	-1.24626100	3.60558100
C	3.08032500	-0.63135400	2.93879700
F	3.77648400	-1.08667700	5.22415300
C	0.82661200	-0.85731700	2.29894300
F	-0.85692600	-1.55524100	3.91153700
C	2.13587000	-0.53429400	1.88634500
F	4.42716500	-0.35937700	2.67772100
F	-0.25073400	-0.81533800	1.39302700
B	2.61305500	0.00975600	0.37996600
C	3.20132500	1.55958700	0.68569900
C	3.72354300	-0.98233800	-0.37352500
C	1.35501000	0.17068200	-0.73908300
C	4.55314800	1.98174600	0.64751300
C	2.31734600	2.59248700	1.07787400
C	4.05561600	-2.30172600	0.00945600
C	4.37168700	-0.58108400	-1.56605700
H	0.50934400	0.69700000	-0.26428600
H	1.78238000	0.76382400	-1.57019300
H	1.06747500	-1.33314300	-0.97072000
C	4.98183300	3.29994000	0.91089500
F	5.58145900	1.08300000	0.35581400
C	2.69068000	3.92181900	1.34571500
F	0.94764900	2.31576200	1.25354600
C	4.97530500	-3.12499100	-0.67529900
F	3.44226100	-2.90672400	1.11544800
C	5.29012600	-1.35804800	-2.29156100
F	4.10491300	0.69163900	-2.10755800
C	4.04303400	4.28641400	1.25324700
F	6.32925700	3.63299300	0.83741500
F	1.73352900	4.87268800	1.69717800
C	5.60772800	-2.64863300	-1.83422700
F	5.24650000	-4.41160700	-0.22311400
F	5.87950500	-0.86878300	-3.45364500
F	4.44310500	5.59101200	1.50547200
F	6.50895500	-3.44300000	-2.52838200
C	-5.15839100	2.93357100	0.07847200
C	-5.64689500	3.71258300	-1.00101000
C	-5.25700500	3.46424000	1.39083200
C	-6.21077900	4.98609100	-0.77668100
H	-5.59883600	3.31992500	-2.01762100
C	-5.81312600	4.74113200	1.61723400
H	-4.88493000	2.88150300	2.23635800
C	-6.29288800	5.50788600	0.53298700
H	-6.58613900	5.56724300	-1.62238200
H	-5.86920700	5.13449600	2.63495900
H	-6.72542200	6.49601600	0.70608700
C	-5.85307600	-1.95111400	0.81002400
C	-6.50303900	-2.89609500	-0.02458100
C	-6.12819700	-1.98139800	2.20209200
C	-7.39470600	-3.84590400	0.51604600
H	-6.32295300	-2.88294900	-1.10034400
C	-7.01362000	-2.93559900	2.74649200
H	-5.63526600	-1.26564700	2.86357400
C	-7.65167300	-3.87248300	1.90455000
H	-7.88929700	-4.56064400	-0.14608600
H	-7.20188900	-2.94716200	3.82263300

H	-8.33988700	-4.61028600	2.32346900
C	-2.56960300	2.41125800	-1.39141300
C	-2.65629400	2.72619800	-2.77194200
C	-1.75465300	3.22324200	-0.56403000
C	-1.96087900	3.83105200	-3.30852300
H	-3.29277800	2.12109800	-3.42289800
C	-1.04936600	4.32272600	-1.09840000
H	-1.67437600	3.00144000	0.50047300
C	-1.15384300	4.63390400	-2.47175700
H	-2.05983100	4.07206600	-4.36989400
H	-0.42980000	4.93425600	-0.43957900
H	-0.62017600	5.49399900	-2.88255900
C	-3.24714300	-2.59571900	-0.59044400
C	-3.30873900	-3.23820200	-1.85382300
C	-2.78186000	-3.33903700	0.52373100
C	-2.93192400	-4.59123900	-1.99817100
H	-3.68479000	-2.68888300	-2.72055400
C	-2.40139600	-4.68993300	0.38203400
H	-2.72114800	-2.86063500	1.50225100
C	-2.47770100	-5.32292000	-0.87828800
H	-3.00867800	-5.07557400	-2.97496500
H	-2.05170500	-5.24667600	1.25434100
H	-2.19288200	-6.37199200	-0.98533200
H	2.12213900	-2.05612300	-3.97141200
H	2.26579200	0.64341300	-3.94248000
H	-0.25452800	1.61639700	-4.22782200
H	-1.94647500	-0.48832700	-4.49315200
H	-0.47211900	-2.76340400	-4.31051300

Frequencies --	-1063.1682	8.0514	10.0695
Frequencies --	13.9021	21.1879	22.7065
Frequencies --	25.8324	27.7555	28.7925
Frequencies --	30.5298	33.3189	35.1024
Frequencies --	38.1087	40.8690	42.3238
Frequencies --	44.9157	47.2624	54.2065
Frequencies --	54.6545	56.7434	61.0915
Frequencies --	61.8546	69.8341	78.3148
Frequencies --	86.5382	103.5449	108.8954
Frequencies --	111.2858	114.9571	120.8773
Frequencies --	124.3326	124.9955	130.6091
Frequencies --	137.3408	140.2367	142.6078
Frequencies --	144.3186	147.6329	153.9048
Frequencies --	156.1939	159.7664	162.5996
Frequencies --	171.7716	177.5156	193.5068
Frequencies --	208.2577	209.5970	210.7384
Frequencies --	216.8401	219.7682	224.3642
Frequencies --	226.4859	228.5160	237.6846
Frequencies --	246.3727	250.6284	256.2129
Frequencies --	264.3163	264.5005	265.0219
Frequencies --	269.0198	274.6704	275.9198
Frequencies --	279.2699	288.1872	301.6484
Frequencies --	303.5024	314.9717	317.5461
Frequencies --	323.8738	325.7887	329.4652
Frequencies --	333.2173	345.1280	361.2670
Frequencies --	366.6406	376.4279	377.7791
Frequencies --	379.1355	381.7082	396.7590
Frequencies --	402.8626	404.4440	406.2026
Frequencies --	407.8704	409.6611	416.6589
Frequencies --	431.1373	431.4469	432.5318
Frequencies --	433.5084	452.5848	456.3076

Frequencies --	463.6026	490.0644	498.5182
Frequencies --	518.4085	525.4483	531.1836
Frequencies --	538.7228	542.8564	543.9832
Frequencies --	550.0754	552.1431	568.4283
Frequencies --	570.5711	576.1950	600.9388
Frequencies --	606.0510	611.0193	616.3480
Frequencies --	617.6159	619.8262	624.3975
Frequencies --	632.1087	635.6942	635.8809
Frequencies --	637.4707	640.6961	643.3877
Frequencies --	654.2653	654.9846	674.9388
Frequencies --	689.8267	700.5697	709.3159
Frequencies --	709.7963	710.1870	713.8809
Frequencies --	716.2285	716.6661	723.3745
Frequencies --	735.8265	743.1931	745.1342
Frequencies --	747.0993	749.5536	760.4686
Frequencies --	766.6973	770.5180	775.1931
Frequencies --	783.0887	789.4976	796.3408
Frequencies --	799.8706	808.3070	817.9616
Frequencies --	840.9843	841.8401	846.2410
Frequencies --	858.3864	859.7244	860.3082
Frequencies --	866.9103	868.3096	872.5151
Frequencies --	873.5738	878.6945	890.9650
Frequencies --	901.5734	911.7127	912.0862
Frequencies --	913.6145	920.4233	933.6341
Frequencies --	934.6999	940.7158	944.8496
Frequencies --	971.0421	984.8312	985.2778
Frequencies --	991.3493	995.3328	997.2430
Frequencies --	1002.7278	1004.8989	1005.1323
Frequencies --	1010.0897	1011.7761	1015.8571
Frequencies --	1017.6508	1020.6078	1025.2693
Frequencies --	1027.0214	1031.0146	1037.4959
Frequencies --	1039.1435	1042.8137	1047.6185
Frequencies --	1049.8066	1050.2312	1050.9337
Frequencies --	1054.5375	1054.8448	1055.4591
Frequencies --	1088.6254	1089.4363	1089.8297
Frequencies --	1090.6458	1090.8368	1091.1596
Frequencies --	1095.3657	1128.5831	1129.2440
Frequencies --	1135.7319	1183.4413	1183.4777
Frequencies --	1184.2105	1184.7533	1204.2372
Frequencies --	1205.2226	1206.5103	1207.7388
Frequencies --	1209.5475	1212.9409	1214.6957
Frequencies --	1234.8949	1261.2429	1264.4490
Frequencies --	1279.3191	1286.5178	1291.5200
Frequencies --	1308.1113	1318.7554	1319.8835
Frequencies --	1322.5130	1324.1155	1327.4709
Frequencies --	1329.9988	1332.8503	1334.8283
Frequencies --	1338.8193	1344.4114	1348.2283
Frequencies --	1355.5406	1366.8755	1367.6491
Frequencies --	1369.2484	1370.9609	1380.0400
Frequencies --	1393.2555	1393.8451	1411.1713
Frequencies --	1420.0436	1421.8016	1439.9082
Frequencies --	1442.5574	1443.6591	1444.4338
Frequencies --	1445.5304	1456.1906	1458.2358
Frequencies --	1461.2940	1467.4105	1468.3673
Frequencies --	1470.6893	1496.7226	1496.7793
Frequencies --	1502.3044	1509.9572	1510.9818
Frequencies --	1530.7538	1589.9768	1593.7214
Frequencies --	1593.9230	1594.6795	1596.2303
Frequencies --	1597.1706	1597.4209	1599.4435
Frequencies --	1618.1303	1619.7575	1622.1014
Frequencies --	1622.8037	1623.4704	1624.2651
Frequencies --	1624.9143	1826.9052	2981.8557
Frequencies --	3052.0288	3088.2104	3146.5600

Frequencies --	3148.0718	3153.8616	3153.9651
Frequencies --	3156.5257	3160.2351	3160.4845
Frequencies --	3160.9883	3162.3582	3170.7753
Frequencies --	3173.5215	3173.7148	3175.9274
Frequencies --	3183.9341	3184.3249	3184.6345
Frequencies --	3186.6690	3192.2054	3195.3412
Frequencies --	3195.4838	3195.9480	3196.8229
Frequencies --	3202.9455	3241.3760	3251.1697
Frequencies --	3263.4716	3266.8136	3284.8608

Catalyst 20:**distal conformation**

vacuum	toluene-like solvent	D3 dispersion
-3054.9137792	-3054.9264532	-0.56541433

Imaginary frequency corresponding to vibration along the reaction coordinate: -1033 cm^{-1} .

Ti	-1.86372000	1.50493600	0.01990300
C	-0.93923300	1.81276700	-2.10483700
H	-0.48395800	1.06047100	-2.76461200
H	-1.97516700	1.93674300	-2.44921000
H	-0.40352700	2.76065600	-2.20750000
O	-3.09909600	0.30266600	-0.45441600
C	-4.11271900	-0.52938500	-0.86875900
C	-4.57562400	-1.60739700	-0.06707900
C	-4.69483900	-0.32566400	-2.14679500
C	-5.59871100	-2.45671600	-0.53491100
C	-5.71504700	-1.17347100	-2.61365100
C	-6.17024600	-2.23962600	-1.80671600
H	-5.93921700	-3.28509100	0.08634000
H	-6.14456300	-1.00751600	-3.60322300
H	-6.95723100	-2.90648000	-2.16218000
C	-1.51501500	3.17924400	1.80295300
C	-1.32449500	3.89617700	0.57552300
C	-2.87703200	2.65858800	1.81270000
C	-2.56851500	3.83251800	-0.18045700

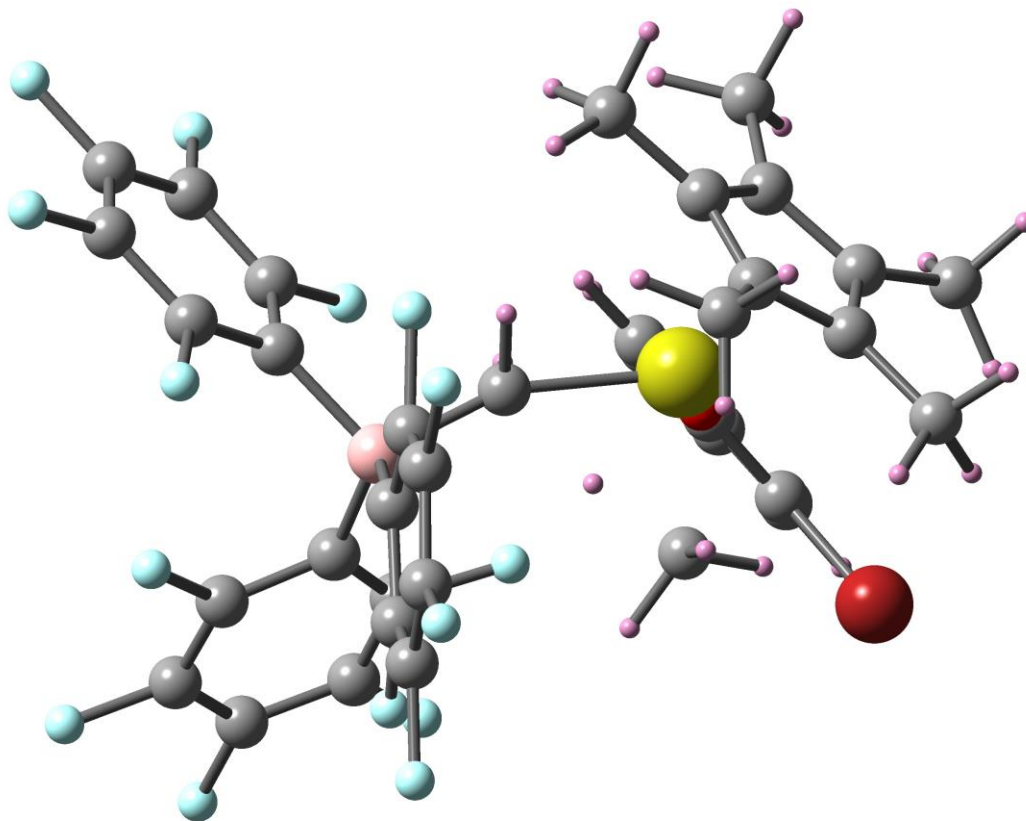
C	-3.53922000	3.11181200	0.60863300
F	1.18276600	-5.35964200	-3.16158800
C	1.22582800	-4.15599900	-2.47214900
C	2.43579700	-3.67429200	-1.94408700
C	0.06450300	-3.38944000	-2.29504200
C	2.44773800	-2.45287200	-1.24694500
F	3.60562600	-4.40334300	-2.12382300
C	0.13773200	-2.17159600	-1.58980500
F	-1.14651800	-3.83171200	-2.82135400
C	1.31039400	-1.63894600	-1.01799800
F	3.70229700	-2.02950100	-0.79458600
F	-1.07679100	-1.46964800	-1.50589200
B	1.43620400	-0.24586300	-0.10525600
C	2.11497400	-0.76844400	1.34982300
C	2.33264600	0.94135700	-0.86592300
C	-0.03230200	0.49628300	0.30152600
C	3.44066000	-0.54628900	1.79759200
C	1.36266200	-1.56620900	2.24574800
C	2.69842200	0.95306700	-2.23195700
C	2.74277300	2.11082600	-0.18417500
H	-0.73359200	-0.28695200	0.66371300
H	0.22652800	1.20775700	1.10439000
H	-0.42414200	1.18142000	-1.04043600
C	3.95795300	-1.02101600	3.02071400
F	4.35732600	0.16097900	1.01603100
C	1.83010900	-2.06588200	3.47573900
F	0.04501200	-1.94300800	1.91866300
C	3.44422600	1.97900300	-2.85147600
F	2.29914200	-0.07734600	-3.09529300
C	3.48180500	3.16332700	-0.74851900
F	2.40455400	2.27764100	1.17270400
C	3.14577000	-1.78311900	3.87528300
F	5.27107700	-0.74769800	3.38679100
F	1.00512400	-2.83401800	4.29301900
C	3.84997000	3.09452800	-2.10273400
F	3.76435700	1.90378100	-4.20243000
F	3.83731300	4.27383400	0.01284400
F	3.63529800	-2.25627100	5.08460000
F	4.57482900	4.12060300	-2.69189300
C	-2.86301000	4.60533500	-1.44647100
H	-3.21206200	5.62059600	-1.18942900
H	-1.97782200	4.72376600	-2.08451800
H	-3.65327900	4.13816000	-2.05053500
C	-0.12353000	4.73224900	0.20026600
H	0.11276200	4.68574600	-0.87160800
H	-0.33115200	5.79185200	0.43102100
H	0.77487500	4.45041600	0.75854600
C	-0.55376600	3.08877300	2.96684900
H	0.48712300	3.25661700	2.66982500
H	-0.81111300	3.85757700	3.71591100
H	-0.60417200	2.11703700	3.47909600
C	-3.53557500	1.97730500	2.99182500
H	-2.85348500	1.29821900	3.52169100
H	-3.86422700	2.73784100	3.72183500
H	-4.41948000	1.39758900	2.70045000
C	-5.00709800	2.95176800	0.28770600
H	-5.43309300	2.03766000	0.72027300

H	-5.57172300	3.80435800	0.70400100
H	-5.20206600	2.93157800	-0.79281200
H	-4.32295200	0.48972600	-2.76746400
Br	-3.78543700	-1.95638800	1.68816200

Frequencies --	-1033.1206	9.2612	18.4243
Frequencies --	20.2208	21.6352	26.0609
Frequencies --	28.0869	28.9165	32.2871
Frequencies --	39.4950	41.5922	44.6896
Frequencies --	50.0141	50.5762	67.5759
Frequencies --	91.1134	97.9349	102.1661
Frequencies --	106.5237	111.3136	112.2603
Frequencies --	114.5056	117.8184	119.4476
Frequencies --	124.6460	126.5736	134.3047
Frequencies --	138.9658	142.0737	145.0583
Frequencies --	151.4129	155.5114	155.9669
Frequencies --	159.6427	161.0421	164.6781
Frequencies --	169.9948	176.1649	178.6824
Frequencies --	181.5924	184.4358	203.3937
Frequencies --	210.3044	215.8028	220.9263
Frequencies --	223.6242	227.7662	242.3154
Frequencies --	254.6949	264.2970	264.6726
Frequencies --	264.8113	273.8857	274.5931
Frequencies --	276.1055	278.8762	285.8019
Frequencies --	288.7231	296.4917	301.2533
Frequencies --	302.0170	303.0252	305.7611
Frequencies --	315.4500	324.9704	325.6975
Frequencies --	331.4960	339.3341	355.2102
Frequencies --	364.1433	374.1514	377.2674
Frequencies --	378.0126	380.7619	384.7497
Frequencies --	393.6755	400.7582	407.6737
Frequencies --	431.6551	432.4972	433.8783
Frequencies --	442.8745	450.7537	456.8688
Frequencies --	464.0074	483.7974	491.0143
Frequencies --	531.4972	533.0806	534.5732
Frequencies --	537.8576	538.5471	545.0773
Frequencies --	553.5741	554.0519	573.2146
Frequencies --	582.9870	594.9241	599.4249
Frequencies --	605.5538	612.1395	633.6797
Frequencies --	635.1304	635.9766	637.9958
Frequencies --	642.5231	654.9118	671.4061
Frequencies --	682.5587	701.7677	704.6523
Frequencies --	717.9244	722.7994	733.6639
Frequencies --	745.4160	747.7868	761.1643
Frequencies --	761.5734	770.1334	800.5712
Frequencies --	801.1972	841.9629	857.9518
Frequencies --	870.8914	877.8273	882.6091
Frequencies --	903.7045	912.6134	919.6548
Frequencies --	932.6850	950.6541	966.3216
Frequencies --	969.5638	989.5344	1007.4278
Frequencies --	1018.8980	1028.7766	1029.5208
Frequencies --	1038.6674	1041.3718	1043.5747
Frequencies --	1044.4774	1046.2317	1048.5782
Frequencies --	1050.0956	1052.7697	1053.5973
Frequencies --	1057.0484	1085.5706	1088.5617
Frequencies --	1093.8048	1124.2331	1133.1134
Frequencies --	1171.4926	1173.9069	1183.1706
Frequencies --	1209.9870	1212.7961	1215.8582
Frequencies --	1255.2525	1260.6256	1275.2630
Frequencies --	1299.4949	1319.0242	1320.7897
Frequencies --	1326.5720	1337.5194	1343.8654
Frequencies --	1350.1954	1353.3009	1359.1423

Frequencies --	1407.0533	1411.6823	1413.5249
Frequencies --	1419.4065	1422.2816	1422.8658
Frequencies --	1426.6833	1427.9364	1428.5446
Frequencies --	1435.6025	1436.0439	1448.7679
Frequencies --	1452.8874	1465.2315	1466.1182
Frequencies --	1467.6091	1468.9721	1470.4848
Frequencies --	1472.0339	1482.5783	1488.4134
Frequencies --	1490.5681	1498.2857	1499.1299
Frequencies --	1502.2669	1506.7543	1508.9747
Frequencies --	1510.7449	1514.7200	1527.7439
Frequencies --	1580.8028	1594.4743	1595.9999
Frequencies --	1596.4301	1599.0630	1617.4840
Frequencies --	1620.2749	1622.8519	1813.3172
Frequencies --	2942.4131	3010.0897	3010.6996
Frequencies --	3011.9333	3014.1806	3015.4472
Frequencies --	3040.5654	3081.1752	3098.6091
Frequencies --	3099.3576	3102.9987	3103.3342
Frequencies --	3104.4044	3137.7537	3139.8993
Frequencies --	3144.7685	3152.5175	3161.0850
Frequencies --	3173.5877	3174.5372	3188.3826
Frequencies --	3194.9649	3201.5807	3211.2955

proximal conformation



vacuum	toluene-like solvent	D3 dispersion
-3054.9156274	-3054.9274942	-0.56488326

Imaginary frequency corresponding to vibration along the reaction coordinate: -1082 cm^{-1} .

Ti 1.84171500 -1.28654900 0.42351900

C	1.37882100	-1.41984700	-1.83493600
H	0.95071200	-0.66213900	-2.50678400
H	2.46872200	-1.36079300	-1.97164700
H	1.01794500	-2.40988300	-2.12830300
O	2.95560400	0.11257800	0.45401600
C	3.77112800	1.18651400	0.72344200
C	3.52487600	1.96574000	1.88432200
C	4.83156900	1.56305600	-0.14345700
C	4.32227200	3.08581500	2.17742800
C	5.62967100	2.68741000	0.14864700
C	5.37788000	3.44722600	1.31110200
H	4.11272300	3.67828500	3.06969300
H	6.43399100	2.97098500	-0.53016900
H	5.99764100	4.31900600	1.52628700
C	1.33735300	-3.12046400	1.99118500
C	1.41920100	-3.74704100	0.70158300
C	2.62959400	-2.50995200	2.27807300
C	2.76275700	-3.53545000	0.18452200
C	3.52125100	-2.81470100	1.18213600
F	-1.22561900	5.62970900	-2.59009600
C	-1.27671300	4.36196400	-2.02820900
C	-2.51093800	3.74828200	-1.75383300
C	-0.09808600	3.66249200	-1.72916900
C	-2.53114900	2.46388000	-1.18159900
F	-3.69396800	4.41172700	-2.05790800
C	-0.18013100	2.37625600	-1.15897200
F	1.13935900	4.23976800	-2.00046800
C	-1.38042100	1.70880300	-0.84424300
F	-3.80132500	1.91213800	-0.97999800
F	1.05904100	1.75602700	-0.92900800
B	-1.53760200	0.22162700	-0.10365300
C	-2.45025100	0.55402900	1.27878000
C	-2.21562400	-0.92726800	-1.10769200
C	-0.10913400	-0.48983600	0.46250900
C	-3.80634600	0.21129100	1.50493900
C	-1.89029700	1.29547700	2.34745700
C	-2.34820700	-0.81680800	-2.51184000
C	-2.64394200	-2.18436200	-0.62008700
H	0.44270500	0.27951700	1.04645000
H	-0.45242900	-1.31236700	1.10953000
H	0.58186900	-0.96222300	-0.84272500
C	-4.52156200	0.52542100	2.67956600
F	-4.55047700	-0.46160200	0.53428600
C	-2.55826100	1.63631200	3.53819900
F	-0.56645900	1.78129300	2.25926200
C	-2.90249200	-1.81329400	-3.34390000
F	-1.89289400	0.32103300	-3.19230800
C	-3.19760200	-3.21292800	-1.39997500
F	-2.52515300	-2.47613600	0.75263100
C	-3.89311600	1.23861400	3.71278000
F	-5.84939600	0.14064700	2.82298000
F	-1.91072200	2.35957400	4.53685900
C	-3.34097500	-3.02346700	-2.78460200
F	-3.00256100	-1.61361700	-4.71594300
F	-3.58869600	-4.41622900	-0.81877600
F	-4.57803200	1.55288200	4.87789600
F	-3.88018700	-4.02153600	-3.58323300

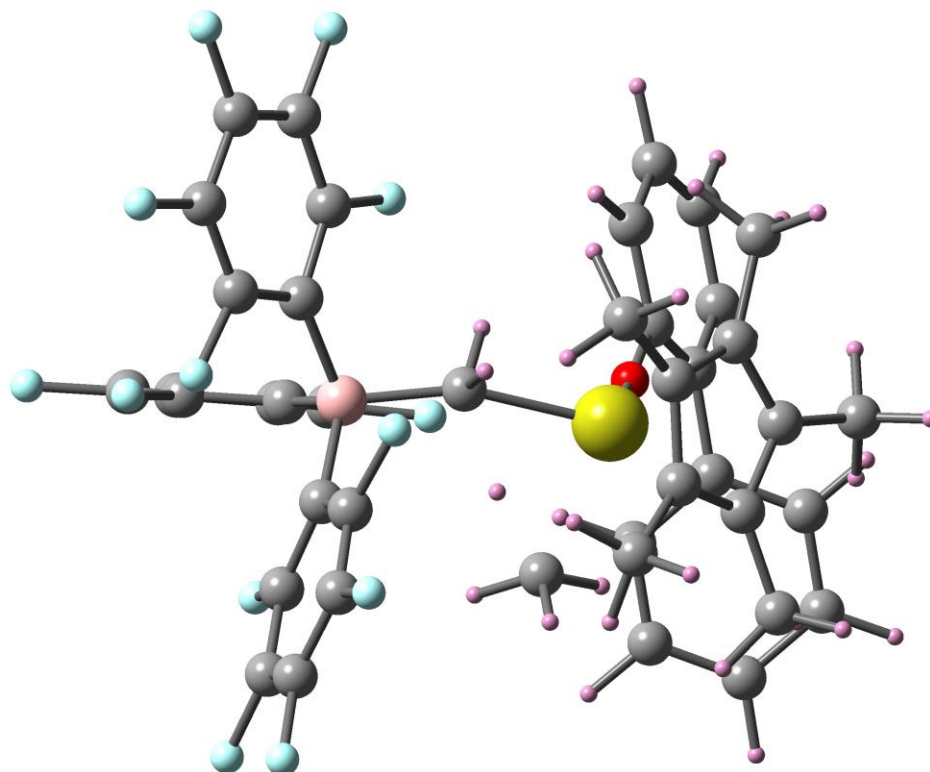
C	3.33311000	-4.16215200	-1.06771600
H	3.79355100	-5.13501700	-0.82241800
H	2.56509100	-4.35459100	-1.82747300
H	4.11458400	-3.54271100	-1.52954800
C	0.36114300	-4.60806100	0.05176100
H	0.27070100	-4.43110800	-1.02920900
H	0.62443500	-5.67263000	0.17699500
H	-0.62676000	-4.46259300	0.50076000
C	0.18782000	-3.19765800	2.97087300
H	-0.77207400	-3.40110900	2.48367100
H	0.37238600	-4.01601200	3.68815500
H	0.07468800	-2.27681700	3.56100300
C	3.01730200	-1.86131300	3.58916200
H	2.19030900	-1.29339300	4.03898100
H	3.30656700	-2.63638800	4.32031400
H	3.87263800	-1.18175600	3.48190000
C	5.00468000	-2.53270400	1.13836600
H	5.27539100	-1.62124100	1.68667100
H	5.55117500	-3.37041000	1.60630700
H	5.38297300	-2.42943000	0.11379600
H	2.69240500	1.69103200	2.53247600
Br	5.19303500	0.55429600	-1.78603300

Frequencies --	-1082.1134	8.8130	15.0055
Frequencies --	17.0749	18.7033	24.9224
Frequencies --	27.8429	29.3486	31.7687
Frequencies --	37.3653	39.3998	47.1966
Frequencies --	49.9494	54.0773	62.1371
Frequencies --	86.6906	91.7748	98.4465
Frequencies --	100.1685	107.2681	109.2825
Frequencies --	113.0536	115.1542	115.5602
Frequencies --	119.7805	122.2274	125.8813
Frequencies --	127.2928	134.0572	138.3662
Frequencies --	142.4153	145.2614	151.1426
Frequencies --	156.0891	159.0200	159.4038
Frequencies --	161.3701	168.3340	170.9349
Frequencies --	179.0942	184.1486	193.8379
Frequencies --	209.9264	213.9348	217.6804
Frequencies --	223.2530	225.7868	227.9076
Frequencies --	254.1470	264.6790	264.8922
Frequencies --	265.1438	274.8096	276.1607
Frequencies --	276.5557	279.2857	284.6749
Frequencies --	287.5636	293.4120	302.6724
Frequencies --	303.0087	304.3872	306.2558
Frequencies --	316.0122	324.5364	326.7296
Frequencies --	330.5720	336.6982	355.1418
Frequencies --	365.7188	373.8816	377.1612
Frequencies --	377.9880	380.3169	381.2193
Frequencies --	392.4484	397.2481	408.6784
Frequencies --	431.4823	432.0493	434.2820
Frequencies --	444.0943	449.7680	456.4593
Frequencies --	464.0677	477.0653	490.9405
Frequencies --	531.0119	533.8415	534.6340
Frequencies --	537.5354	538.0839	545.0471
Frequencies --	553.3928	553.8457	570.4835
Frequencies --	581.9389	594.1921	597.3406
Frequencies --	604.1863	610.5359	631.9834
Frequencies --	634.7737	635.9565	638.6027
Frequencies --	642.8906	654.4062	670.9569
Frequencies --	682.8432	699.1278	704.5154

Frequencies --	718.4669	723.0641	733.8515
Frequencies --	745.7270	748.4183	762.0168
Frequencies --	763.8478	770.9324	799.7394
Frequencies --	801.6477	841.3997	861.3229
Frequencies --	871.5480	880.3848	885.3036
Frequencies --	903.6472	913.0263	919.7512
Frequencies --	932.1759	953.9426	967.3585
Frequencies --	968.8271	991.8854	1007.2547
Frequencies --	1019.1595	1027.2815	1029.3158
Frequencies --	1039.2375	1040.4635	1043.2840
Frequencies --	1044.2691	1045.6834	1048.1716
Frequencies --	1050.9632	1053.2145	1053.5542
Frequencies --	1057.8645	1086.5064	1088.4257
Frequencies --	1096.0782	1124.5749	1134.6516
Frequencies --	1170.4579	1174.4104	1184.9776
Frequencies --	1209.5622	1213.8248	1216.5597
Frequencies --	1255.7284	1267.9480	1278.5188
Frequencies --	1300.1141	1316.0508	1320.7970
Frequencies --	1326.2865	1337.4624	1343.2128
Frequencies --	1344.9704	1351.9210	1359.2058
Frequencies --	1408.3363	1411.2426	1411.7778
Frequencies --	1419.7226	1422.7738	1422.8646
Frequencies --	1425.0979	1426.8107	1428.2913
Frequencies --	1434.3017	1435.8731	1449.5528
Frequencies --	1450.9722	1463.1174	1467.5354
Frequencies --	1468.2349	1468.3784	1470.2717
Frequencies --	1472.0475	1480.6770	1486.8764
Frequencies --	1490.2661	1497.0163	1498.1280
Frequencies --	1499.1559	1505.5058	1506.2906
Frequencies --	1509.6201	1512.6171	1526.1573
Frequencies --	1579.6011	1594.2849	1596.3992
Frequencies --	1596.7885	1598.9861	1617.3461
Frequencies --	1620.5728	1623.0630	1821.4320
Frequencies --	2939.9251	3007.9806	3010.7867
Frequencies --	3012.0019	3014.5776	3015.9897
Frequencies --	3033.5173	3095.6442	3099.6535
Frequencies --	3099.7443	3100.3861	3101.3729
Frequencies --	3106.9033	3130.6574	3137.5053
Frequencies --	3142.3425	3151.2351	3158.9144
Frequencies --	3170.0596	3175.9463	3189.2016
Frequencies --	3193.2125	3201.9048	3211.2593

Catalyst 21:**distal conformation**

Several attempts were made to locate a transition state for H transfer from counterion to methyl initiating group, but these structures always reverted to the contact ion pair. Thus, there does not seem to be a tendency for this conformation to decay by H transfer.

proximal conformation

vacuum	toluene-like solvent	D3 dispersion
-3273.306481	-3273.3189629	-0.63465835

Imaginary frequency corresponding to vibration along the reaction coordinate: -1056 cm^{-1} .

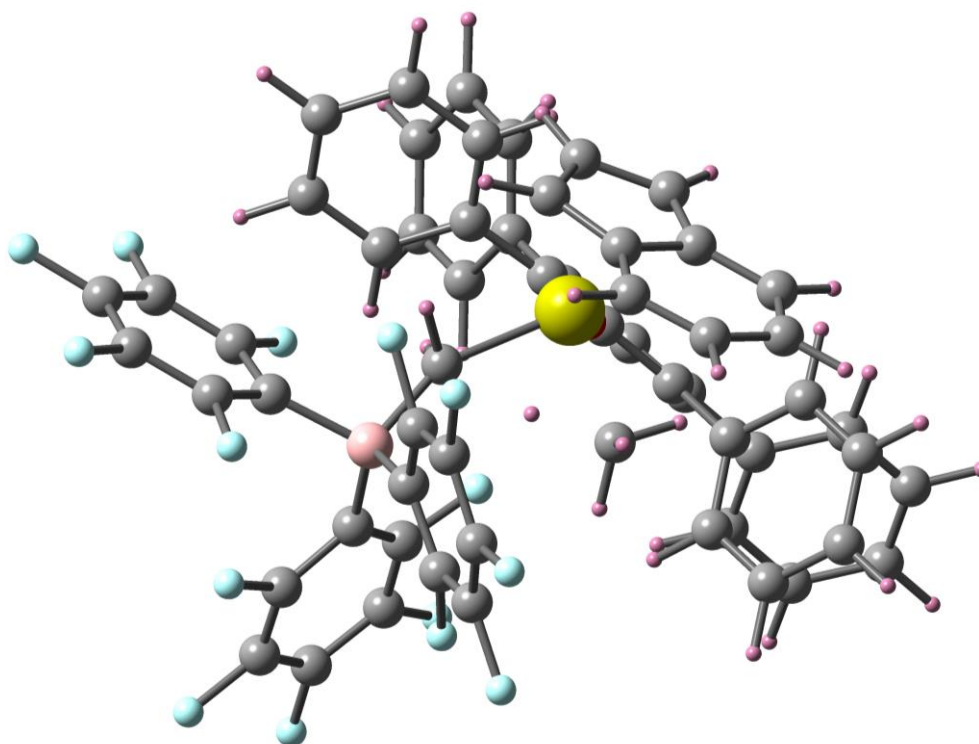
Ti	1.72157900	-1.16315300	0.68923100
C	1.39312100	-1.45547900	-1.58425200
H	0.96311700	-0.77679000	-2.33470900
H	2.48390500	-1.35320900	-1.67301800
H	1.09461100	-2.48170400	-1.81516400
O	2.79170500	0.26430000	0.73041100
C	3.56176600	1.35551900	1.11408100
C	3.13336200	2.10007800	2.24205300
C	4.75186400	1.70433900	0.40686900
C	3.89774000	3.18417600	2.70885800
C	5.50800800	2.79331500	0.91639600
C	5.09969000	3.52455200	2.04951100
H	3.55463500	3.75684800	3.57267200

H	6.41521600	3.08686400	0.38587900
H	5.70156000	4.36461600	2.40054500
C	1.15562500	-2.97137600	2.27475800
C	1.41090700	-3.64064500	1.03072800
C	2.37247800	-2.27031800	2.66672800
C	2.78559300	-3.36156400	0.64437900
C	3.39128600	-2.55918400	1.68338900
F	-1.32143200	5.49615700	-2.85869700
C	-1.37911300	4.25316200	-2.24473900
C	-2.61383400	3.62103900	-2.01784800
C	-0.20625300	3.59513300	-1.84610200
C	-2.64097200	2.36148700	-1.39237600
F	-3.79012700	4.24119300	-2.42236700
C	-0.29587900	2.33434500	-1.22368200
F	1.03490300	4.18540500	-2.07351200
C	-1.49696400	1.65112900	-0.95088900
F	-3.90848100	1.78598000	-1.24986800
F	0.94289000	1.75373600	-0.89715200
B	-1.66077500	0.19032800	-0.15808300
C	-2.70096500	0.54076400	1.12540500
C	-2.20998000	-1.02333100	-1.16576200
C	-0.25701000	-0.43105300	0.55505300
C	-4.05308200	0.13969500	1.25832800
C	-2.26636200	1.35820700	2.19676200
C	-2.24277400	-0.96920700	-2.57893900
C	-2.61450000	-2.28231000	-0.66296900
H	0.22081300	0.38778100	1.13597700
H	-0.61922400	-1.23213000	1.21886900
H	0.53412600	-0.95769500	-0.67158400
C	-4.87686200	0.46869300	2.35499300
F	-4.68242400	-0.61023800	0.26248100
C	-3.04614000	1.71841000	3.31142200
F	-0.96432500	1.90531500	2.18871600
C	-2.68315800	-2.02125300	-3.41061400
F	-1.79184500	0.16517400	-3.26942900
C	-3.05635300	-3.36487500	-1.44119000
F	-2.58836200	-2.51765000	0.72485600
C	-4.37026300	1.26004100	3.39827700
F	-6.19220500	0.02256500	2.41048700
F	-2.51908500	2.51958700	4.32134400
C	-3.10321100	-3.23207500	-2.83902100
F	-2.68690000	-1.87519500	-4.79332600
F	-3.43208000	-4.56543000	-0.84415300
F	-5.16317600	1.59096500	4.48802200
F	-3.53074600	-4.28400700	-3.63635100
C	3.52187600	-3.99430700	-0.51492900
H	3.96819600	-4.95212700	-0.19532700
H	2.86023100	-4.21631600	-1.36193200
H	4.34199000	-3.36358100	-0.88500900
C	0.48273200	-4.59943900	0.32166900
H	0.56121900	-4.53963600	-0.77266700
H	0.74332000	-5.63575100	0.59975300
H	-0.56686300	-4.44661000	0.59455200
C	-0.08083100	-3.09374000	3.13660800
H	-0.96319400	-3.40662000	2.56807400
H	0.09219400	-3.85204100	3.91990200
H	-0.33160600	-2.15589200	3.65307800

C	2.57848300	-1.55430500	3.98401900
H	1.67038300	-1.03854900	4.32739400
H	2.84772400	-2.28306700	4.76858500
H	3.38751100	-0.81420600	3.93673000
C	4.85268200	-2.18824700	1.77521700
H	5.01678900	-1.27860000	2.36608200
H	5.40757500	-3.00517000	2.26941700
H	5.30843700	-2.03334100	0.78934000
H	2.20187100	1.82726900	2.73790100
C	5.21392300	1.01766200	-0.84342700
C	6.52096000	0.46741600	-0.92295000
C	4.39580100	0.98054500	-2.00371700
C	6.99354100	-0.11426600	-2.11891600
H	7.16775400	0.48961800	-0.04307700
C	4.87068500	0.40808200	-3.20278600
H	3.40447200	1.43211800	-1.97604500
C	6.16887300	-0.14608200	-3.26531600
H	8.00198500	-0.53314900	-2.15638500
H	4.23268000	0.40893500	-4.08984000
H	6.53569500	-0.58494000	-4.19589400

Frequencies --	-1056.2213	11.4349	14.1246
Frequencies --	22.4327	25.5617	27.7659
Frequencies --	30.3138	32.4523	34.7645
Frequencies --	38.6463	41.2278	45.0844
Frequencies --	47.8716	52.3368	56.1505
Frequencies --	69.4216	79.6381	88.8811
Frequencies --	100.6632	105.5847	110.3479
Frequencies --	112.6863	114.9852	116.6186
Frequencies --	120.6419	122.2742	124.8935
Frequencies --	131.6527	134.9163	138.3132
Frequencies --	142.2017	143.4779	145.2165
Frequencies --	146.1232	152.7245	155.5595
Frequencies --	159.7779	161.5696	164.5131
Frequencies --	165.7945	173.6577	176.2361
Frequencies --	179.7723	194.3676	204.8825
Frequencies --	216.4489	220.0704	224.2091
Frequencies --	225.8211	248.8305	257.4017
Frequencies --	264.4156	264.5093	264.8193
Frequencies --	275.0223	276.0627	277.0259
Frequencies --	282.0979	290.5388	292.7903
Frequencies --	296.7559	303.0598	303.3697
Frequencies --	304.7506	305.9541	310.7036
Frequencies --	319.9744	327.1674	328.7957
Frequencies --	335.9850	348.5539	359.0477
Frequencies --	368.3952	375.1379	377.6295
Frequencies --	378.3303	380.8230	386.7807
Frequencies --	391.5636	399.2353	407.9152
Frequencies --	410.3159	431.4355	432.1377
Frequencies --	434.4563	451.4872	456.6516
Frequencies --	464.0764	472.1803	489.2210
Frequencies --	498.0075	530.5925	534.4013
Frequencies --	536.3057	537.8744	544.9920
Frequencies --	546.4035	553.9278	557.2842
Frequencies --	562.2907	573.1530	582.6126
Frequencies --	594.9980	599.4106	608.0985
Frequencies --	613.0108	614.9055	620.7837
Frequencies --	634.7846	636.1500	638.2526
Frequencies --	642.6717	655.2813	656.9849
Frequencies --	673.4312	703.5023	713.8255

Frequencies --	718.4393	723.2155	734.3514
Frequencies --	738.0894	742.5063	746.5300
Frequencies --	748.1397	761.3796	766.5320
Frequencies --	770.9220	779.8175	802.0308
Frequencies --	804.9183	843.8945	867.9034
Frequencies --	874.9980	875.7846	884.8722
Frequencies --	887.4500	904.2232	912.9187
Frequencies --	919.9581	923.9879	940.4027
Frequencies --	960.3879	969.9516	973.3718
Frequencies --	992.3347	993.6132	999.2183
Frequencies --	1009.2332	1012.3904	1019.5518
Frequencies --	1029.2527	1035.6224	1040.1758
Frequencies --	1041.7349	1044.0412	1045.2535
Frequencies --	1047.0457	1047.2231	1050.5753
Frequencies --	1052.2480	1054.0227	1056.7255
Frequencies --	1062.3854	1087.8103	1089.3067
Frequencies --	1091.0158	1098.7194	1126.5436
Frequencies --	1127.1611	1171.2746	1175.3278
Frequencies --	1184.4294	1186.8773	1208.7124
Frequencies --	1209.6637	1213.2021	1215.5128
Frequencies --	1224.6446	1265.7182	1274.4297
Frequencies --	1301.4907	1301.7706	1316.8114
Frequencies --	1320.6556	1325.7296	1336.2718
Frequencies --	1337.5869	1343.6711	1351.2499
Frequencies --	1356.9042	1357.8028	1370.3669
Frequencies --	1410.5693	1411.4721	1413.9031
Frequencies --	1419.6115	1422.0335	1425.1495
Frequencies --	1426.8970	1428.3930	1430.1574
Frequencies --	1434.0840	1435.4755	1450.9404
Frequencies --	1451.4106	1452.0070	1464.4818
Frequencies --	1467.2288	1469.0543	1470.6802
Frequencies --	1471.7138	1479.9790	1483.7811
Frequencies --	1489.1329	1492.5237	1498.9954
Frequencies --	1499.9786	1501.1270	1505.9655
Frequencies --	1508.6167	1509.7955	1512.1626
Frequencies --	1517.3073	1526.7846	1579.3313
Frequencies --	1594.1825	1595.5656	1596.2601
Frequencies --	1598.7739	1611.6251	1617.3117
Frequencies --	1620.6396	1623.0483	1623.6190
Frequencies --	1823.7546	2946.7341	3007.9290
Frequencies --	3010.8308	3011.8852	3013.4765
Frequencies --	3014.6583	3039.2572	3095.4841
Frequencies --	3098.5227	3099.0307	3100.5485
Frequencies --	3102.2118	3110.4371	3136.2269
Frequencies --	3140.2439	3142.3928	3154.5988
Frequencies --	3156.4247	3160.3257	3162.8578
Frequencies --	3167.5872	3168.6901	3175.3679
Frequencies --	3180.1169	3190.1635	3194.7117
Frequencies --	3195.6502	3206.5874	3208.8572

Catalyst 22:

vacuum	toluene-like solvent	D3 dispersion
-3923.2265199	-3923.2445784	-0.84828938

Imaginary frequency corresponding to vibration along the reaction coordinate: -993 cm^{-1} .

Ti	-0.05283200	-0.98499900	-1.77779300
C	0.64264500	-2.62715400	-0.38140600
H	0.55667800	-2.61981200	0.71150900
H	-0.24931500	-3.14432200	-0.76559500
H	1.51622800	-3.20030100	-0.70219500
O	-1.66229700	-0.54574100	-1.16525400
C	-2.94714800	-0.17611300	-0.76149500
C	-3.39146400	1.16846800	-0.97324900
C	-3.73775000	-1.15718400	-0.08437700
C	-4.68922800	1.52336600	-0.49220200
C	-5.01490500	-0.76484500	0.41079200
C	-5.45724300	0.55876400	0.19731600
H	-6.44938300	0.83750900	0.54961800
C	1.38816300	-0.87182300	-3.82512700
C	1.45083900	-2.28056000	-3.54145300
C	0.01870600	-0.53383700	-4.07587300
C	0.08277500	-2.80301600	-3.56850900
C	-0.80147800	-1.70020100	-3.87853300
F	0.33321300	1.49935500	5.97559500
C	0.83304800	1.21837200	4.71152600
C	2.19035800	1.42792300	4.41209500
C	-0.00300800	0.70943200	3.70689100
C	2.66720400	1.13322300	3.12183900
F	3.04566000	1.91155900	5.39532900

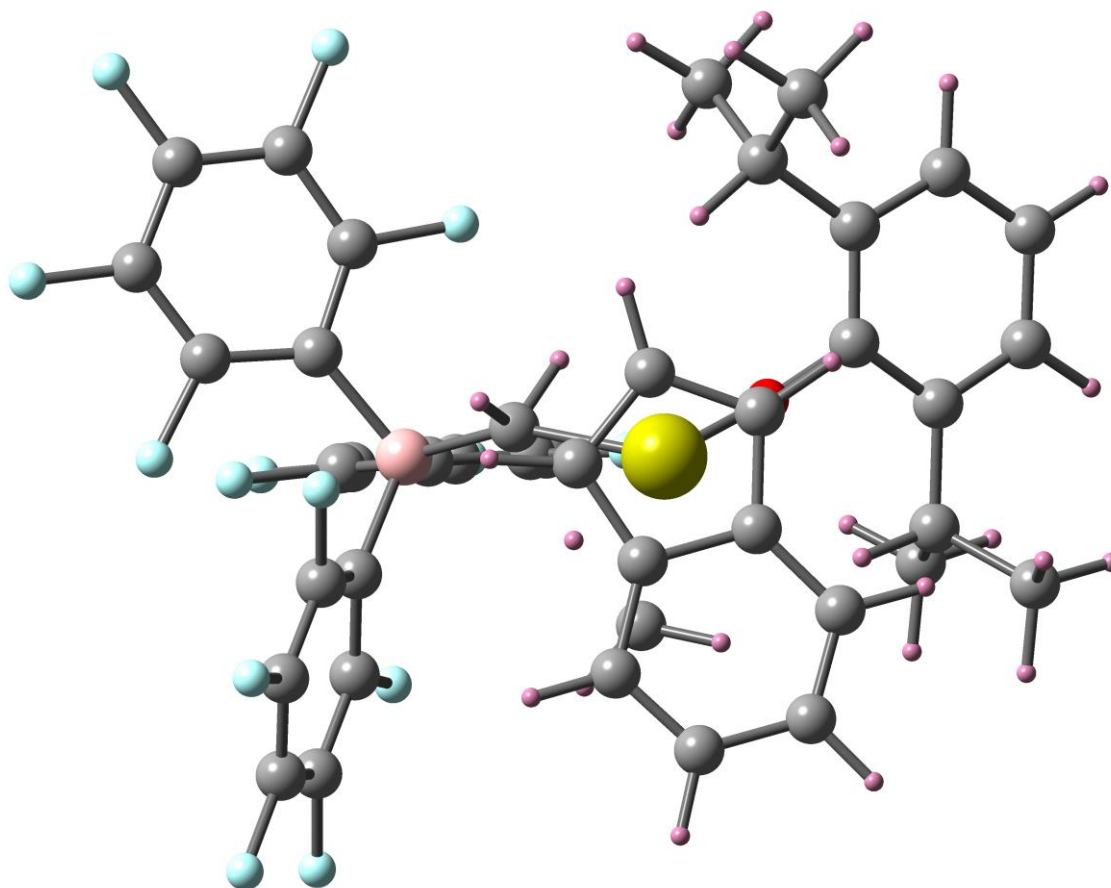
C	0.52991000	0.43507200	2.43196100
F	-1.35105900	0.47195700	3.97626800
C	1.87398800	0.63435900	2.05903700
F	4.03976600	1.32403600	2.92846700
F	-0.39551900	-0.09932300	1.51699600
B	2.53606300	0.38568100	0.54729500
C	3.29450100	1.84225400	0.15973700
C	3.57906300	-0.91971300	0.50532800
C	1.40622300	0.13009700	-0.69612500
C	4.68498300	2.08868500	0.05646200
C	2.51564700	2.99888200	-0.08251600
C	3.74789100	-1.88072000	1.52874400
C	4.36161700	-1.20135800	-0.64095300
H	0.56992000	0.84519100	-0.56387300
H	1.97087300	0.34404600	-1.61531900
H	1.08125900	-1.37257500	-0.42312400
C	5.24716600	3.32659600	-0.31912700
F	5.61889800	1.09452500	0.35961300
C	3.02318100	4.25458500	-0.46379600
F	1.12071700	2.94685200	0.08493600
C	4.63683800	-2.97503900	1.46002700
F	2.99254400	-1.82089900	2.70814600
C	5.25944700	-2.27431600	-0.76402600
F	4.27292300	-0.36274300	-1.76836600
C	4.41104700	4.42025300	-0.59563400
F	6.62637000	3.47815800	-0.41199100
F	2.16877700	5.32853100	-0.70592200
C	5.40854600	-3.17354100	0.30498600
F	4.74116900	-3.86971700	2.51934800
F	5.98763900	-2.46732100	-1.93676100
F	4.94499600	5.64427100	-0.97452400
F	6.27933000	-4.24984900	0.20739300
C	-5.30882400	2.88083500	-0.69518100
C	-5.55425000	3.39957800	-1.99295800
C	-5.73613600	3.64244600	0.42388600
C	-6.19859800	4.64208700	-2.16598600
H	-5.25171100	2.82699800	-2.87058200
C	-6.37363600	4.88976400	0.25410700
H	-5.55603300	3.26429100	1.43254500
C	-6.60807900	5.39544800	-1.04340800
H	-6.38169100	5.01944100	-3.17484700
H	-6.68340700	5.46311200	1.13095900
H	-7.10319700	6.35984800	-1.17792500
C	-5.93328900	-1.69355200	1.16359800
C	-6.60176700	-2.76638700	0.52103000
C	-6.20372500	-1.45608600	2.53617300
C	-7.50952300	-3.58124600	1.23029500
H	-6.42300100	-2.95846900	-0.53813100
C	-7.10529600	-2.27412700	3.25003800
H	-5.69901800	-0.63470400	3.04948700
C	-7.76296700	-3.34072500	2.59880100
H	-8.01922500	-4.39850700	0.71439800
H	-7.29219500	-2.07838500	4.30850000
H	-8.46409300	-3.97304700	3.14835000
C	-2.51507200	2.22029200	-1.59727000
C	-2.17161200	2.20109200	-2.97115900
C	-2.06970100	3.31264300	-0.81049100

C	-1.40564400	3.24188100	-3.54185800
H	-2.53769800	1.38942300	-3.60238900
C	-1.31357700	4.35660900	-1.37730500
H	-2.31581600	3.34393900	0.25162000
C	-0.97577300	4.32520800	-2.74636500
H	-1.14733500	3.21698600	-4.60294100
H	-0.97325100	5.18122200	-0.74944500
H	-0.38393100	5.13138900	-3.18459400
C	-3.23619800	-2.55363000	0.17264300
C	-3.32815200	-3.56319300	-0.81790700
C	-2.73932500	-2.90594400	1.45351000
C	-2.95116800	-4.89378500	-0.53318400
H	-3.72819200	-3.31441300	-1.80396700
C	-2.35692600	-4.23325300	1.73927500
H	-2.66043400	-2.14143700	2.22782000
C	-2.46494100	-5.23395600	0.74821400
H	-3.05348700	-5.66390500	-1.30181500
H	-1.98390100	-4.48559500	2.73442800
H	-2.18168000	-6.26439900	0.97396400
H	2.23446400	-0.19875900	-3.91194800
H	-0.33475500	0.44563000	-4.37539000
H	-1.87481600	-1.76088600	-4.02938600
C	2.54968400	-3.16170000	-3.29073100
H	3.56995400	-2.78105300	-3.29039700
C	2.28586400	-4.51398000	-3.07979600
H	3.11194800	-5.20735000	-2.90769200
C	0.94040100	-5.02696400	-3.09707600
H	0.78341500	-6.09555300	-2.93492200
C	-0.15181900	-4.19595100	-3.33837800
H	-1.16468000	-4.59847800	-3.36963300

Frequencies --	-993.3147	-10.0803	-6.3992
Frequencies --	6.4048	14.2263	19.0198
Frequencies --	21.3449	23.9213	26.8926
Frequencies --	27.4581	29.5243	33.7913
Frequencies --	38.1163	41.4164	41.8929
Frequencies --	44.0335	46.5276	48.8354
Frequencies --	52.6205	54.7410	61.7907
Frequencies --	67.4371	70.3791	73.0403
Frequencies --	79.2445	82.1432	101.9627
Frequencies --	104.8915	111.2204	113.7579
Frequencies --	117.1123	120.3327	122.7246
Frequencies --	124.6600	136.1348	138.5874
Frequencies --	140.3003	141.9217	146.4122
Frequencies --	156.1226	157.8900	161.1991
Frequencies --	166.7346	168.5206	176.9314
Frequencies --	193.7529	209.1250	209.7068
Frequencies --	210.0375	215.3223	217.6406
Frequencies --	222.2218	222.8348	228.1787
Frequencies --	236.9062	246.7349	250.4435
Frequencies --	255.2513	259.9797	264.3880
Frequencies --	265.0591	265.4843	274.3544
Frequencies --	275.0395	275.5658	281.4734
Frequencies --	285.3402	302.0499	303.2096
Frequencies --	309.6161	315.1937	324.4655
Frequencies --	326.1048	328.5954	329.8394
Frequencies --	335.6941	360.6211	369.7141
Frequencies --	372.8989	376.7630	377.9541
Frequencies --	382.2357	390.7483	395.7875

Frequencies --	403.8486	405.4710	407.0155
Frequencies --	407.4811	410.4927	410.9065
Frequencies --	430.8750	432.7352	433.6047
Frequencies --	436.6033	446.0949	451.0249
Frequencies --	457.2945	464.0695	482.6249
Frequencies --	486.3422	517.6831	525.1072
Frequencies --	525.7349	539.6613	539.7586
Frequencies --	543.0969	544.7206	547.0617
Frequencies --	548.2620	551.4473	565.8818
Frequencies --	580.2064	595.0307	597.2555
Frequencies --	611.7789	615.8730	617.6617
Frequencies --	620.0955	624.4522	624.6779
Frequencies --	633.0922	634.9354	635.3975
Frequencies --	637.0994	641.2345	642.2678
Frequencies --	653.8482	656.7326	678.6358
Frequencies --	688.8878	697.4196	707.4703
Frequencies --	709.4291	709.7503	713.8127
Frequencies --	714.1360	714.8613	723.0768
Frequencies --	734.2117	735.0362	735.9742
Frequencies --	742.4983	744.3561	745.1253
Frequencies --	748.4164	760.7136	765.3068
Frequencies --	767.7251	769.4712	773.2319
Frequencies --	781.7098	789.2161	795.1270
Frequencies --	805.1016	813.2462	843.6103
Frequencies --	858.2588	859.1116	859.2612
Frequencies --	861.9689	864.9345	868.7159
Frequencies --	871.7248	876.8027	879.6778
Frequencies --	884.7309	888.1772	903.9182
Frequencies --	912.0947	912.9056	915.0092
Frequencies --	928.6911	933.2254	935.1694
Frequencies --	939.8121	942.4596	967.3356
Frequencies --	980.2006	984.7757	985.6250
Frequencies --	988.3674	993.1749	996.0489
Frequencies --	1004.1014	1004.7599	1007.6466
Frequencies --	1008.8728	1009.8916	1011.2274
Frequencies --	1014.2982	1015.2445	1019.8428
Frequencies --	1020.0278	1026.0781	1029.7010
Frequencies --	1041.1759	1044.0068	1048.2988
Frequencies --	1049.0487	1052.3554	1052.4888
Frequencies --	1053.5114	1054.9825	1056.0797
Frequencies --	1056.8826	1066.3373	1088.8678
Frequencies --	1089.8004	1090.1242	1091.4580
Frequencies --	1092.3559	1128.0463	1129.5891
Frequencies --	1142.8035	1182.7209	1183.0458
Frequencies --	1183.7393	1184.8046	1185.2997
Frequencies --	1202.9652	1205.2157	1206.2880
Frequencies --	1207.1043	1210.0064	1211.2222
Frequencies --	1212.1984	1214.0224	1231.6905
Frequencies --	1242.0297	1255.8380	1263.3630
Frequencies --	1278.4378	1279.8904	1297.9773
Frequencies --	1305.9255	1316.2331	1321.0683
Frequencies --	1321.6059	1325.7960	1327.9203
Frequencies --	1330.9081	1331.2422	1334.3908
Frequencies --	1338.4800	1343.5103	1349.7687
Frequencies --	1360.7396	1366.3527	1367.4251
Frequencies --	1367.8853	1369.9598	1372.8328
Frequencies --	1376.6406	1378.3878	1411.6352
Frequencies --	1415.6118	1419.1529	1421.5723
Frequencies --	1426.4041	1441.4340	1443.2445
Frequencies --	1444.5739	1446.3661	1455.9474
Frequencies --	1463.1373	1466.8134	1468.1534
Frequencies --	1470.5132	1474.4054	1496.4198
Frequencies --	1496.8187	1502.3696	1504.1510

Frequencies --	1509.4558	1522.6114	1527.6606
Frequencies --	1553.6522	1590.6735	1593.9639
Frequencies --	1594.2962	1596.1178	1596.3636
Frequencies --	1598.1461	1598.1960	1599.6377
Frequencies --	1617.1850	1618.9284	1622.4473
Frequencies --	1623.3421	1623.5685	1624.5061
Frequencies --	1625.1605	1631.5030	1812.5825
Frequencies --	2981.0769	3038.7048	3114.2416
Frequencies --	3144.7142	3148.1176	3153.7884
Frequencies --	3154.4997	3155.3109	3160.1597
Frequencies --	3160.9023	3160.9563	3167.8016
Frequencies --	3170.2730	3170.4067	3173.1399
Frequencies --	3174.0857	3179.6197	3181.8624
Frequencies --	3182.6580	3183.9257	3185.8684
Frequencies --	3186.1972	3194.2230	3194.4955
Frequencies --	3196.3518	3196.8715	3199.9459
Frequencies --	3202.8195	3204.1350	3217.1236
Frequencies --	3244.2871	3254.9781	3284.0875

Catalyst 23:

vacuum	toluene-like solvent	D3 dispersion
-3235.1943619	-3235.2071812	-0.62628472

Imaginary frequency corresponding to vibration along the reaction coordinate: -1019 cm^{-1} .

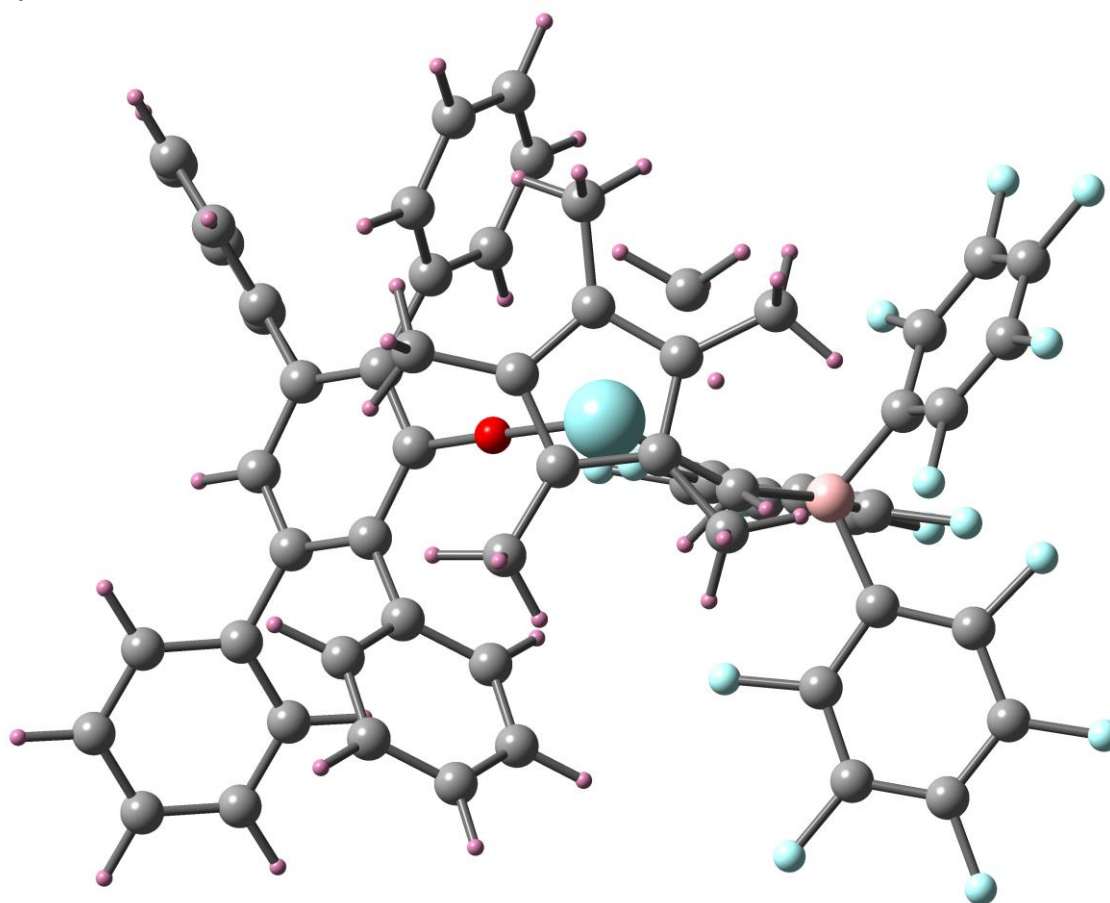
Ti	1.83221200	1.03922700	-0.78390200
C	1.24432800	1.95303100	1.24208700
H	1.19502400	1.29175100	2.11583800
H	2.25685200	2.38520500	1.20611900
H	0.54405600	2.78674400	1.35183100
O	3.00040400	-0.20046200	-0.29776000
C	4.03172600	-1.14179900	-0.18209400
C	4.17291100	-2.14929200	-1.18790600
C	4.89570000	-1.05791100	0.95458100
C	5.24489100	-3.06101900	-1.04033000
C	5.94356600	-2.00339600	1.04149900
C	6.12573500	-2.98964300	0.05439300
H	5.38652200	-3.84239100	-1.78745500
H	6.61971400	-1.97285900	1.89635700
H	6.94286300	-3.70801100	0.14450200
H	1.83281600	0.94106800	-3.78318400
C	2.03621400	1.70142900	-3.03240400
C	1.07860100	2.63718100	-2.51950900
C	3.30511600	1.91912100	-2.39085100

H	0.04121600	2.72094500	-2.82289000
C	1.77202700	3.51964300	-1.60980500
H	4.22596700	1.38120500	-2.59080600
C	3.16170900	3.06603300	-1.52079000
F	-1.61541600	-4.14639300	4.53000500
C	-1.58760100	-3.20137100	3.51477600
C	-2.78114500	-2.70679900	2.96083600
C	-0.36808400	-2.71219100	3.02415100
C	-2.72032600	-1.75030500	1.93167500
F	-4.00370800	-3.15908900	3.44202800
C	-0.36847500	-1.75366700	1.99099200
F	0.83243400	-3.17020200	3.56285200
C	-1.52442000	-1.22638100	1.38057400
F	-3.95395600	-1.27942000	1.46986600
F	0.91368200	-1.31952200	1.60083000
B	-1.58593600	-0.15234900	0.10489700
C	-2.50241100	-0.94027000	-1.06880800
C	-2.19751100	1.34196200	0.52846500
C	-0.08827100	0.17742100	-0.61747100
C	-3.81724200	-0.61365900	-1.48142600
C	-1.99131700	-2.08505900	-1.72501600
C	-2.42527400	1.80174700	1.84626600
C	-2.45498800	2.33435700	-0.44754900
H	0.46436600	-0.77524200	-0.72616900
H	-0.34501200	0.61357500	-1.59838400
H	0.51110100	1.17084400	0.44322100
C	-4.53603700	-1.31358000	-2.47272500
F	-4.51493200	0.44337100	-0.89240600
C	-2.66473000	-2.82005500	-2.71799300
F	-0.72056100	-2.58637900	-1.37643400
C	-2.90570100	3.08891300	2.17114100
F	-2.14953100	0.98797500	2.95282100
C	-2.92081400	3.63244100	-0.18131000
F	-2.24094300	2.04423700	-1.80905500
C	-3.95488700	-2.42428900	-3.10543100
F	-5.82091700	-0.91854800	-2.82582800
F	-2.06700300	-3.92784700	-3.31335700
C	-3.16240800	4.01569300	1.14907000
F	-3.10749300	3.45431200	3.49704500
F	-3.13188400	4.54165600	-1.21493400
F	-4.64453300	-3.12321300	-4.08566900
F	-3.62009300	5.29149100	1.44537000
C	3.21410600	-2.29217500	-2.38059100
H	2.43878800	-1.51751600	-2.29841000
C	4.70031700	-0.02147200	2.07081100
H	3.86739500	0.63182600	1.78535700
C	2.47222000	-3.66116000	-2.35648100
H	3.16824400	-4.50226800	-2.49417400
H	1.94244100	-3.80927400	-1.40463800
H	1.72668600	-3.70367900	-3.16550500
C	3.93755200	-2.07378100	-3.74195000
H	4.44255300	-1.09570000	-3.78182500
H	4.69835100	-2.84727600	-3.92492200
H	3.21177800	-2.12149500	-4.56989700
C	4.29385300	-0.70593400	3.41008000
H	3.39216200	-1.32236200	3.28299800
H	5.09604400	-1.35392700	3.79511000

H	4.08293100	0.05712600	4.17692000
C	5.95045200	0.88650300	2.25659700
H	6.82647800	0.31584700	2.59998000
H	6.22551000	1.38712800	1.31433600
H	5.74496700	1.66337300	3.01068800
C	1.35207300	4.67980900	-0.88473100
H	0.32776300	5.04535200	-0.97415400
C	2.28650800	5.35209900	-0.09626700
H	1.99045700	6.25249300	0.44594900
C	3.64581900	4.89186900	0.01244200
H	4.34430300	5.45253000	0.63713200
C	4.08811500	3.76382300	-0.68145100
H	5.12773600	3.43837700	-0.61398900

Frequencies --	-1018.7011	10.1194	17.3119
Frequencies --	21.6795	23.3802	26.1713
Frequencies --	28.8149	30.1146	32.1542
Frequencies --	37.9564	40.3367	42.1935
Frequencies --	48.2204	54.9339	57.2154
Frequencies --	59.7721	69.3758	71.9817
Frequencies --	78.0565	101.2689	107.2053
Frequencies --	112.1078	116.7572	118.5212
Frequencies --	123.6016	125.7837	126.5467
Frequencies --	137.5180	142.0969	145.7689
Frequencies --	148.2020	155.0400	157.4274
Frequencies --	159.1003	162.0533	164.8597
Frequencies --	172.0012	179.7513	202.5090
Frequencies --	213.6918	215.5661	218.1371
Frequencies --	219.1216	222.6303	224.6108
Frequencies --	232.2849	241.8755	248.2455
Frequencies --	251.6921	253.4295	264.3981
Frequencies --	264.5474	264.9839	272.8085
Frequencies --	274.6265	275.2500	276.3492
Frequencies --	282.7341	291.5735	300.1516
Frequencies --	302.7383	305.6352	309.8894
Frequencies --	312.1959	315.1873	326.6093
Frequencies --	328.0616	335.3190	352.1540
Frequencies --	362.1135	373.8042	376.9503
Frequencies --	377.7230	378.1505	381.3895
Frequencies --	392.5305	396.1811	424.3279
Frequencies --	430.9497	431.1941	432.7724
Frequencies --	433.6298	437.1965	440.5220
Frequencies --	451.0613	456.9112	463.6015
Frequencies --	484.3885	531.6297	535.9941
Frequencies --	538.3034	539.7113	543.0115
Frequencies --	544.4378	546.0649	552.7256
Frequencies --	565.1297	575.6414	595.7115
Frequencies --	596.7295	600.2495	611.8305
Frequencies --	616.8778	628.3756	634.9736
Frequencies --	635.5995	637.6299	641.8775
Frequencies --	657.2726	673.5347	707.8166
Frequencies --	717.0810	722.2017	723.5038
Frequencies --	726.5023	734.6370	736.2442
Frequencies --	746.3409	748.2627	761.0399
Frequencies --	761.6364	768.9901	770.7273
Frequencies --	791.8333	798.1782	812.3884
Frequencies --	816.6312	844.8671	862.3396
Frequencies --	867.8534	869.5040	877.1271
Frequencies --	878.6619	882.7229	886.7892
Frequencies --	900.3811	903.2887	912.7352
Frequencies --	919.4086	924.9567	932.7293

Frequencies --	933.7966	937.4714	941.0828
Frequencies --	963.3976	965.0521	976.9259
Frequencies --	992.1084	1001.8689	1007.1441
Frequencies --	1009.0212	1018.5183	1028.3528
Frequencies --	1039.8588	1049.7239	1052.5424
Frequencies --	1055.4275	1056.1849	1059.8760
Frequencies --	1067.9235	1073.5358	1087.6805
Frequencies --	1115.3136	1116.0475	1117.4228
Frequencies --	1140.1120	1165.5454	1182.8754
Frequencies --	1185.7460	1185.8568	1204.9945
Frequencies --	1211.0241	1213.1314	1215.3261
Frequencies --	1215.8880	1238.6433	1252.7273
Frequencies --	1256.7896	1274.9836	1277.3932
Frequencies --	1288.7292	1310.9896	1318.0210
Frequencies --	1319.0331	1320.6741	1325.1735
Frequencies --	1329.1458	1333.3545	1339.1743
Frequencies --	1344.2817	1346.8934	1350.9282
Frequencies --	1363.8826	1371.6066	1383.3131
Frequencies --	1400.8158	1404.0293	1412.1821
Frequencies --	1415.6444	1419.6358	1420.0607
Frequencies --	1421.9786	1423.0027	1424.4386
Frequencies --	1437.9487	1461.5646	1467.8271
Frequencies --	1468.7250	1469.0640	1471.7511
Frequencies --	1474.8685	1487.3295	1487.8922
Frequencies --	1488.0723	1488.7419	1499.2624
Frequencies --	1499.7780	1500.2947	1506.7206
Frequencies --	1510.7445	1532.7478	1552.0858
Frequencies --	1594.0746	1596.4663	1597.2329
Frequencies --	1598.0192	1604.8843	1617.9698
Frequencies --	1619.3718	1622.8017	1627.5084
Frequencies --	1810.0799	2980.9590	3005.9807
Frequencies --	3008.7301	3013.7589	3018.7135
Frequencies --	3028.0279	3061.8830	3087.7171
Frequencies --	3097.6427	3105.7181	3107.4292
Frequencies --	3110.4742	3116.8612	3125.4591
Frequencies --	3126.6003	3134.1596	3137.1561
Frequencies --	3138.5627	3166.5600	3167.2911
Frequencies --	3175.2551	3186.3721	3187.9908
Frequencies --	3194.0700	3199.8468	3200.2934
Frequencies --	3229.4856	3258.0479	3271.4879

Catalyst 24:

vacuum	toluene-like solvent	D3 dispersion
-3954.6148725	-3954.6302873	-0.87806709

Imaginary frequency corresponding to vibration along the reaction coordinate: -1063 cm^{-1} .

Zr	-0.07046400	-0.64507300	-1.87787200
C	0.74844200	-2.57857900	-0.63682000
H	0.74086500	-2.67030100	0.45742200
H	-0.18990300	-3.04624900	-0.97520300
H	1.58501600	-3.15999000	-1.03989800
O	-1.82743300	-0.33393600	-1.08591400
C	-3.07144100	-0.09269200	-0.50069800
C	-3.61446500	1.23089700	-0.54241500
C	-3.75263100	-1.18095100	0.12812000
C	-4.87160600	1.46384300	0.09544100
C	-5.01545900	-0.92593700	0.73998100
C	-5.54050900	0.38402400	0.71306900
H	-6.49469400	0.57241200	1.20310500
C	-0.20890400	0.06617600	-4.28947400
C	1.21656500	-0.19166600	-4.11989500
C	-0.90746400	-1.19909900	-4.20308400
C	1.38938300	-1.59995600	-3.90330300
C	0.07410100	-2.22544900	-3.92261000
F	0.40622100	0.30606700	6.15000600

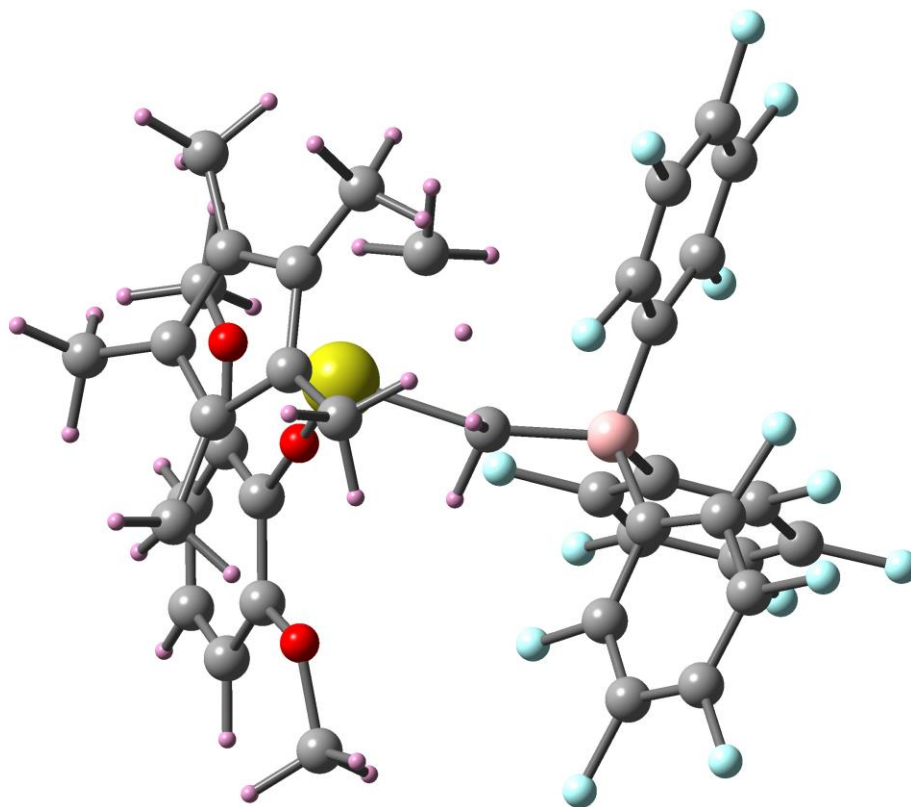
C	0.93558900	0.27591700	4.86743900
C	2.32085700	0.39219400	4.65745900
C	0.10065700	0.12347200	3.75087700
C	2.82710200	0.35240400	3.34574800
F	3.17267100	0.53241300	5.74680900
C	0.66541300	0.09647800	2.46014500
F	-1.27741700	-0.00671600	3.92345300
C	2.04054200	0.20413200	2.17620700
F	4.21860800	0.43625900	3.23247800
F	-0.27141600	-0.06643700	1.42048800
B	2.74757600	0.22845400	0.66099900
C	3.55058900	1.71611000	0.62386000
C	3.76987700	-1.07124200	0.41115000
C	1.67032500	0.21096300	-0.65134300
C	4.94945000	1.93902700	0.66705300
C	2.81314700	2.92346100	0.59920600
C	3.84358100	-2.23686200	1.20825500
C	4.62184700	-1.13216800	-0.71706800
H	0.93148100	1.02775400	-0.48365700
H	2.29179800	0.46244000	-1.52660100
H	1.24131500	-1.31692500	-0.58957100
C	5.55630500	3.21208500	0.62561000
F	5.84730700	0.87547200	0.78495900
C	3.36485300	4.21680300	0.55509200
F	1.40423700	2.88943600	0.65264300
C	4.70712100	-3.32496700	0.95966300
F	3.00180300	-2.40681300	2.31773400
C	5.49947900	-2.18749600	-1.01564500
F	4.62886300	-0.07114000	-1.64270600
C	4.76021600	4.36656900	0.55832000
F	6.94068300	3.33678600	0.65913500
F	2.54113800	5.34077300	0.51051600
C	5.55335800	-3.29984800	-0.15928600
F	4.71289300	-4.43132300	1.80271200
F	6.30061500	-2.14887300	-2.15411900
F	5.33832500	5.62745500	0.50997500
F	6.40443600	-4.36218200	-0.43079800
C	-5.52438800	2.81834800	0.18852800
C	-6.83639100	3.01358900	-0.31739700
C	-4.89404800	3.90279400	0.85266500
C	-7.49153700	4.25612200	-0.18180800
H	-7.34337200	2.19133800	-0.82740100
C	-5.54914600	5.14329500	0.99649000
H	-3.89569300	3.77334700	1.27177100
C	-6.84927900	5.32803800	0.47596400
H	-8.49851800	4.38489500	-0.58614700
H	-5.04635000	5.96120900	1.51794100
H	-7.35534200	6.29003000	0.58588500
C	-5.82590500	-1.98308200	1.44566100
C	-6.43931900	-3.04997600	0.74046800
C	-6.05413900	-1.88228900	2.84285000
C	-7.24976200	-3.99052900	1.41063400
H	-6.29498800	-3.13878500	-0.33734900
C	-6.85771200	-2.82611000	3.51743700
H	-5.59115200	-1.06868400	3.40538700
C	-7.46008800	-3.88500900	2.80331700
H	-7.71752000	-4.80077800	0.84601400

H	-7.01148100	-2.73357600	4.59521200
H	-8.08523400	-4.61473600	3.32320800
C	-2.91698700	2.36006100	-1.25421200
C	-3.51742900	2.96480900	-2.38993800
C	-1.70594400	2.91214400	-0.76351800
C	-2.93896800	4.09522500	-3.00357100
H	-4.45678700	2.56515100	-2.77624500
C	-1.12444600	4.04598200	-1.37335700
H	-1.24428200	2.48865900	0.12827900
C	-1.74137300	4.64403600	-2.49406100
H	-3.42980900	4.55402500	-3.86535900
H	-0.20905900	4.46901500	-0.95667900
H	-1.30201600	5.53242400	-2.95372500
C	-3.15108300	-2.56022100	0.21416700
C	-3.25258300	-3.48167600	-0.85814700
C	-2.54571600	-2.99690800	1.42070000
C	-2.77792800	-4.80550500	-0.72802100
H	-3.74113400	-3.17221500	-1.78470000
C	-2.06811700	-4.31765900	1.55445600
H	-2.46343900	-2.30486100	2.26005500
C	-2.18489900	-5.22910500	0.48174800
H	-2.88867900	-5.50741000	-1.55865400
H	-1.61483300	-4.63558100	2.49624100
H	-1.82744600	-6.25558000	0.59032300
C	-0.80168400	1.38015200	-4.75379100
H	-0.65245300	1.48247500	-5.84338000
H	-1.87783900	1.44379100	-4.56056000
H	-0.33128200	2.25194500	-4.28113900
C	2.30862500	0.83474800	-4.33840700
H	2.49416100	0.95304700	-5.42020600
H	2.03537600	1.82767200	-3.95273100
H	3.25874600	0.54600700	-3.87487500
C	-2.37514200	-1.42136000	-4.50503900
H	-3.00241300	-0.58202700	-4.17624700
H	-2.51787600	-1.53034000	-5.59436900
H	-2.76272800	-2.33366500	-4.03443400
C	2.70358100	-2.34745900	-3.87027700
H	2.90591700	-2.77395800	-4.86833800
H	3.54912100	-1.69828400	-3.62115800
H	2.69964300	-3.18885000	-3.16417200
C	-0.17454500	-3.71992100	-3.93167900
H	-0.05336100	-4.10791700	-4.95819500
H	0.53450000	-4.26663200	-3.29638700
H	-1.18861900	-3.97979000	-3.60331900

Frequencies --	-1062.7418	8.9278	12.1590
Frequencies --	15.7476	18.8665	22.4793
Frequencies --	26.9120	28.2658	30.2782
Frequencies --	33.4984	35.3365	37.4276
Frequencies --	40.9213	41.9342	43.0145
Frequencies --	44.5376	49.1903	50.8783
Frequencies --	52.0248	56.4916	59.9964
Frequencies --	65.4253	71.8902	73.9126
Frequencies --	79.9144	84.4486	89.8278
Frequencies --	101.9900	104.6992	111.0202
Frequencies --	114.1582	117.0423	119.7282
Frequencies --	120.2497	123.1761	125.8298
Frequencies --	128.5247	129.8441	135.1115

Frequencies --	137.7484	140.5144	141.5723
Frequencies --	143.0762	147.2518	153.0460
Frequencies --	155.9744	156.4461	158.5099
Frequencies --	160.8163	161.9927	168.0203
Frequencies --	175.0551	178.2911	187.3246
Frequencies --	194.6373	209.0953	211.1292
Frequencies --	213.2568	215.0508	217.4448
Frequencies --	223.3039	224.7520	231.9842
Frequencies --	247.1687	248.6752	256.1269
Frequencies --	257.9526	264.1827	264.4360
Frequencies --	264.9665	274.8352	275.6452
Frequencies --	278.3257	283.7063	286.6580
Frequencies --	293.8775	301.3981	301.9747
Frequencies --	302.5711	309.0310	312.3639
Frequencies --	320.3404	327.2359	329.0491
Frequencies --	331.8232	336.4034	346.7164
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Frequencies --	379.0736	381.3870	386.2647
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Frequencies --	449.8640	456.4994	463.2119
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Frequencies --	592.3621	595.4024	604.9589
Frequencies --	607.7817	614.2924	617.3452
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Frequencies --	634.5966	634.7881	635.4765
Frequencies --	637.3915	637.9404	640.4915
Frequencies --	653.1767	657.5861	667.5151
Frequencies --	688.4854	694.2581	695.3106
Frequencies --	709.8349	710.0237	711.9457
Frequencies --	716.2044	717.1949	719.7098
Frequencies --	722.3941	731.9399	742.6122
Frequencies --	743.8637	748.7037	759.2967
Frequencies --	768.7466	773.2899	776.7337
Frequencies --	779.0121	794.0872	799.1871
Frequencies --	801.0090	808.1969	840.8204
Frequencies --	858.9797	859.2798	860.0922
Frequencies --	861.7354	867.5190	870.2928
Frequencies --	876.0309	879.6238	901.7061
Frequencies --	907.9022	912.0967	916.5934
Frequencies --	930.4509	937.2258	939.8965
Frequencies --	945.4243	957.4821	967.8620
Frequencies --	970.2829	985.0911	986.5577
Frequencies --	990.2874	995.5402	997.4210
Frequencies --	1004.1691	1005.0084	1008.8363
Frequencies --	1012.1575	1013.4971	1016.6319
Frequencies --	1017.5400	1021.0773	1025.3209
Frequencies --	1027.1102	1039.0385	1039.8344
Frequencies --	1043.4983	1044.1245	1044.9749
Frequencies --	1045.6609	1048.2832	1049.5800
Frequencies --	1049.8155	1051.4587	1052.3274
Frequencies --	1055.3850	1055.9248	1056.3993
Frequencies --	1084.9082	1086.7708	1087.6308
Frequencies --	1089.1660	1089.7970	1091.2870
Frequencies --	1091.6447	1124.1814	1130.5230
Frequencies --	1131.3880	1171.6884	1173.7526
Frequencies --	1182.4593	1182.6765	1182.7396

Frequencies --	1184.9386	1203.6684	1205.3630
Frequencies --	1206.1527	1207.9202	1210.5108
Frequencies --	1211.9524	1213.3147	1231.3873
Frequencies --	1256.7945	1269.3290	1279.9539
Frequencies --	1301.5620	1306.7442	1317.2028
Frequencies --	1319.7065	1323.4438	1326.3016
Frequencies --	1327.0524	1331.0120	1332.4861
Frequencies --	1334.2505	1337.8605	1344.0552
Frequencies --	1350.1819	1366.6497	1367.7386
Frequencies --	1369.3064	1370.3339	1379.7973
Frequencies --	1382.7068	1410.2993	1410.9411
Frequencies --	1415.8562	1420.2160	1420.4542
Frequencies --	1420.8832	1425.9268	1427.4602
Frequencies --	1428.4718	1435.5293	1441.6788
Frequencies --	1442.9252	1443.8721	1444.9338
Frequencies --	1447.8002	1448.4709	1456.9432
Frequencies --	1465.5581	1467.7109	1468.6969
Frequencies --	1470.5964	1471.4036	1485.0706
Frequencies --	1491.3396	1491.5271	1496.6682
Frequencies --	1497.7943	1499.6484	1500.6626
Frequencies --	1502.6196	1505.6446	1508.3235
Frequencies --	1509.5431	1510.2381	1516.4496
Frequencies --	1521.6615	1525.9234	1531.3928
Frequencies --	1591.2805	1593.3159	1595.1378
Frequencies --	1595.3966	1597.0081	1597.0921
Frequencies --	1598.1521	1601.5261	1617.8375
Frequencies --	1620.4695	1622.0641	1622.3293
Frequencies --	1623.4404	1623.8019	1624.4799
Frequencies --	1829.0141	2927.4439	3010.8128
Frequencies --	3011.7894	3012.1943	3013.0310
Frequencies --	3015.5299	3026.7381	3083.9488
Frequencies --	3097.3550	3103.7989	3104.6510
Frequencies --	3107.4278	3113.3004	3127.9848
Frequencies --	3144.8488	3149.1551	3151.6902
Frequencies --	3152.0550	3152.4012	3153.8942
Frequencies --	3155.7019	3159.8191	3160.4891
Frequencies --	3161.4805	3166.2088	3169.4429
Frequencies --	3171.8877	3172.3198	3172.9501
Frequencies --	3173.0901	3176.4332	3182.6339
Frequencies --	3183.3333	3183.8136	3185.4198
Frequencies --	3191.0053	3193.1087	3193.8520
Frequencies --	3196.3827	3197.8199	3208.1674

Catalyst 30:

vacuum	toluene-like solvent	D3 dispersion
-3271.3036559	-3271.3153959	-0.59671304

Imaginary frequency corresponding to vibration along the reaction coordinate: -1075 cm^{-1} .

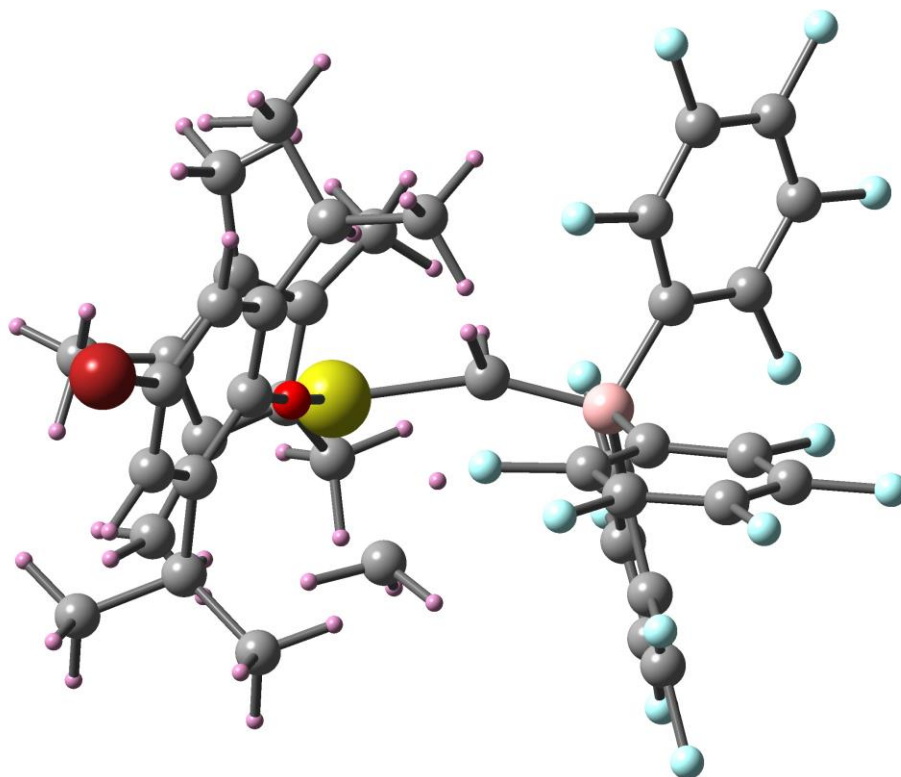
Ti	-1.93386500	1.30519300	0.36532700
C	-1.32663600	1.67295900	-1.83889700
H	-0.84161900	1.00124700	-2.56185800
H	-2.40402700	1.61239700	-2.04965400
H	-0.96271600	2.69296000	-1.99299300
O	-3.08123100	-0.01397900	0.07983100
C	-4.00694200	-1.01656400	-0.01523000
C	-3.99854900	-2.07667100	0.93974200
C	-4.94268500	-1.03056600	-1.08959200
C	-4.92309000	-3.13960500	0.81654100
C	-5.86201300	-2.09916600	-1.20340100
C	-5.84048900	-3.13912500	-0.25262500
H	-4.92726700	-3.95972200	1.53116100
H	-6.58055800	-2.13377500	-2.01926000
H	-6.54894200	-3.96400700	-0.34850600
C	-1.51661800	2.98608400	2.12718600
C	-1.56691000	3.73595700	0.90422200
C	-2.80566600	2.32857400	2.30563100
C	-2.88581200	3.54962000	0.31852400
C	-3.66413600	2.72272700	1.21205200
F	1.24390800	-5.44698900	-2.95780900

C	1.27688300	-4.20985000	-2.32797300
C	2.49939800	-3.62822700	-1.95157900
C	0.09119400	-3.50950000	-2.06162400
C	2.49963900	-2.37673500	-1.30955800
F	3.69138400	-4.29078500	-2.22403000
C	0.15237000	-2.25645100	-1.41912300
F	-1.13533600	-4.05448800	-2.43731500
C	1.33952600	-1.62666900	-0.99369900
F	3.76342200	-1.85361500	-1.01222100
F	-1.09021700	-1.62972200	-1.23985900
B	1.46215900	-0.18789200	-0.15365000
C	2.35774200	-0.59236700	1.22200000
C	2.15530200	1.02864400	-1.06655200
C	0.00974700	0.45805800	0.42382300
C	3.69641400	-0.22614200	1.50605000
C	1.79587800	-1.41830400	2.22495000
C	2.35545900	0.99926500	-2.46627300
C	2.52415900	2.26788700	-0.49200300
H	-0.57572800	-0.35935700	0.89832400
H	0.31951200	1.20941200	1.16889500
H	-0.60366100	1.09025200	-0.85587700
C	4.39050000	-0.58917800	2.67917100
F	4.44705800	0.52139700	0.59605900
C	2.44308700	-1.81104800	3.41117600
F	0.49494700	-1.94067300	2.06633900
C	2.91057600	2.05745200	-3.21772600
F	1.97239100	-0.11391400	-3.22835500
C	3.07580000	3.35494300	-1.18971300
F	2.34657600	2.47476400	0.88957100
C	3.75843800	-1.38333200	3.64925000
F	5.70214700	-0.17472600	2.88260200
F	1.79190100	-2.61681600	4.34457000
C	3.28247500	3.24817600	-2.57527400
F	3.07666000	1.93745100	-4.59343300
F	3.40581500	4.53494100	-0.52720900
F	4.42206000	-1.74745100	4.81299600
F	3.82054000	4.30622400	-3.29477900
C	-3.42895700	4.27778800	-0.88995800
H	-3.94621400	5.19981300	-0.57194400
H	-2.63756900	4.57838000	-1.58821900
H	-4.15839300	3.67300900	-1.44727300
C	-0.50573800	4.67912200	0.38615600
H	-0.42942000	4.67365800	-0.71000300
H	-0.75569000	5.71360600	0.68040300
H	0.48588800	4.45717000	0.79428800
C	-0.40126200	2.98663200	3.14875500
H	0.57008400	3.24687100	2.71337600
H	-0.61984700	3.73162300	3.93352800
H	-0.29278500	2.01579300	3.65359700
C	-3.21814600	1.53708900	3.52755400
H	-2.38724000	0.95123600	3.94454500
H	-3.56244600	2.22297600	4.32150900
H	-4.03682900	0.83870000	3.31399600
C	-5.13612600	2.41428000	1.06633600
H	-5.43547900	1.53314300	1.64762200
H	-5.73147200	3.26820300	1.43477000
H	-5.42431900	2.23763600	0.02158000

O	-3.03921700	-1.94895800	1.94490000
O	-4.85985800	0.05856400	-1.96738200
C	-2.79271500	-3.08903100	2.84076100
H	-2.55559700	-3.99836800	2.26596900
H	-1.92120400	-2.79385100	3.43552600
H	-3.65820400	-3.27097600	3.49943600
C	-5.67424300	0.03047300	-3.18940100
H	-5.38838900	0.93509100	-3.73994200
H	-5.44809400	-0.86035000	-3.79715300
H	-6.75150000	0.06383400	-2.95580600

Frequencies --	-1075.1603	6.6310	18.4921
Frequencies --	21.6846	25.9156	28.1977
Frequencies --	29.5651	30.4898	32.0149
Frequencies --	37.8624	39.8684	45.7961
Frequencies --	49.7199	51.1688	64.5539
Frequencies --	66.7690	88.4804	98.4158
Frequencies --	101.2052	103.9945	106.5134
Frequencies --	109.5889	111.0543	114.0426
Frequencies --	115.1166	118.2998	122.2121
Frequencies --	125.3369	134.7706	136.6959
Frequencies --	138.8343	141.7243	144.6066
Frequencies --	148.2170	154.6062	158.9287
Frequencies --	159.9720	160.8090	164.5362
Frequencies --	169.1160	172.4000	181.8716
Frequencies --	185.3640	188.1986	197.6638
Frequencies --	201.8350	212.6514	216.9134
Frequencies --	219.8601	223.1766	225.7918
Frequencies --	239.8163	260.6615	262.3098
Frequencies --	264.3899	265.1101	265.1449
Frequencies --	274.8896	276.1214	277.0541
Frequencies --	278.5412	287.1682	289.4362
Frequencies --	299.6478	301.3977	302.6701
Frequencies --	304.7817	306.7412	310.9685
Frequencies --	326.0203	327.8555	334.0829
Frequencies --	344.8132	347.2302	358.9571
Frequencies --	361.7539	370.8301	374.9911
Frequencies --	376.6184	377.5362	380.2866
Frequencies --	383.3633	390.8974	400.3635
Frequencies --	403.1379	431.5582	432.3560
Frequencies --	434.1936	450.2677	456.5631
Frequencies --	463.7874	481.6174	518.4438
Frequencies --	530.1760	533.7404	535.9376
Frequencies --	537.8372	540.8012	545.1587
Frequencies --	552.7346	555.4393	570.2356
Frequencies --	577.4580	582.0020	593.1672
Frequencies --	600.2593	600.9407	604.7968
Frequencies --	609.3323	614.6208	634.1551
Frequencies --	636.4472	638.4085	642.1552
Frequencies --	653.3472	672.2464	699.9835
Frequencies --	717.3884	720.5077	723.6346
Frequencies --	726.9064	733.6381	745.1672
Frequencies --	748.0224	759.0859	761.8142
Frequencies --	769.8577	801.2230	803.2065
Frequencies --	842.1750	842.6740	852.3590
Frequencies --	872.9035	881.0248	886.9484
Frequencies --	903.9414	912.7871	920.8250
Frequencies --	929.6096	950.8122	969.1692
Frequencies --	971.4820	986.7291	1015.0526
Frequencies --	1018.9057	1028.8342	1040.2288
Frequencies --	1042.4294	1044.9428	1046.3095
Frequencies --	1047.6838	1049.6852	1051.1265

Frequencies --	1054.5952	1057.1222	1083.0307
Frequencies --	1087.5437	1089.2474	1096.9105
Frequencies --	1100.0735	1125.8429	1126.9359
Frequencies --	1127.8800	1167.7597	1171.6224
Frequencies --	1174.7743	1176.8423	1206.8622
Frequencies --	1208.1072	1211.7683	1214.8304
Frequencies --	1237.1179	1255.2156	1268.0415
Frequencies --	1297.5798	1309.7864	1317.5293
Frequencies --	1319.4533	1326.0366	1337.6923
Frequencies --	1343.9214	1350.6890	1360.5013
Frequencies --	1376.9567	1408.3013	1410.7748
Frequencies --	1412.7070	1418.9458	1421.8925
Frequencies --	1422.4724	1426.0752	1426.8095
Frequencies --	1428.3364	1434.5499	1445.8858
Frequencies --	1449.9728	1452.7661	1456.3620
Frequencies --	1464.3857	1466.8159	1468.2208
Frequencies --	1469.5931	1471.1587	1474.4235
Frequencies --	1477.5636	1482.6959	1484.1023
Frequencies --	1486.2140	1487.5292	1488.1198
Frequencies --	1490.8321	1492.5838	1497.0169
Frequencies --	1499.2672	1500.2740	1505.8785
Frequencies --	1508.1944	1510.2668	1515.2618
Frequencies --	1526.1290	1590.9958	1594.5606
Frequencies --	1596.5624	1599.2113	1607.2835
Frequencies --	1616.7439	1619.9957	1621.9280
Frequencies --	1821.8062	2942.4819	3001.2350
Frequencies --	3004.1919	3007.9656	3009.2141
Frequencies --	3010.4218	3012.6523	3013.6765
Frequencies --	3036.2033	3089.9897	3097.7555
Frequencies --	3097.8447	3101.1815	3101.6925
Frequencies --	3103.2267	3104.3530	3106.0182
Frequencies --	3132.5422	3141.1193	3143.1194
Frequencies --	3149.7117	3156.0408	3157.5173
Frequencies --	3168.0611	3174.2078	3177.5227
Frequencies --	3192.3655	3215.8462	3223.7099

Catalyst 31:

vacuum	toluene-like solvent	D3 dispersion
-3290.6528385	-3290.6636299	-0.67960021

Imaginary frequency corresponding to vibration along the reaction coordinate: -1010 cm^{-1} .

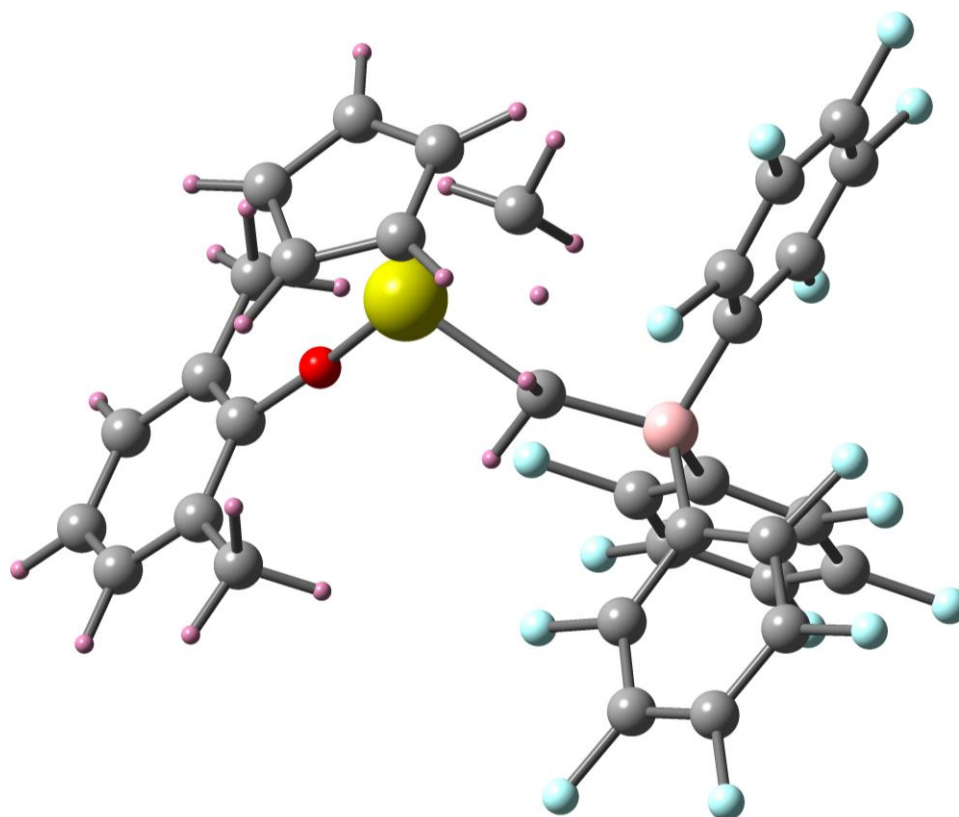
Ti	-0.77571600	1.84830400	0.49549600
C	-0.03239500	2.14201300	-1.70988500
H	0.08073800	1.35267600	-2.46570500
H	-1.01532200	2.59703700	-1.88000600
H	0.74101400	2.90267300	-1.84954000
O	-2.28781600	0.93172600	0.21708000
C	-3.54028500	0.31715200	0.11301900
C	-3.91332400	-0.68647300	1.06342900
C	-4.41063600	0.69486000	-0.96117500
C	-5.19678500	-1.27044900	0.94141800
C	-5.67835600	0.07488100	-1.04091600
C	-6.06350000	-0.88360800	-0.09071900
H	-5.50394400	-2.03624900	1.65026200
H	-6.35628300	0.33851000	-1.84955900
C	0.25628000	3.31626000	2.22807000
C	0.31806600	4.07877300	1.01670700
C	-1.14438100	3.02920300	2.50617300
C	-1.04476400	4.28520400	0.54382600
C	-1.94798100	3.68154700	1.49460200
F	0.34372300	-5.36702800	-3.11526600
C	0.73581300	-4.21631500	-2.44694000
C	2.07988700	-4.01605600	-2.08842200

C	-0.19875500	-3.22215000	-2.12182200
C	2.44675500	-2.84109800	-1.40717500
F	3.03108800	-4.97394600	-2.41858600
C	0.22827800	-2.06466800	-1.44176300
F	-1.53677200	-3.38201800	-2.47462500
C	1.55162000	-1.80799500	-1.03263600
F	3.81280600	-2.70577800	-1.13644300
F	-0.78725900	-1.12021100	-1.20216100
B	2.08940000	-0.48286700	-0.17019600
C	2.90756900	-1.14329300	1.15245700
C	3.04530800	0.52791800	-1.09689400
C	0.87137900	0.50373100	0.48652100
C	4.30856400	-1.16361000	1.36400500
C	2.19454600	-1.80526700	2.17983100
C	3.17552100	0.48248600	-2.50458800
C	3.76899400	1.59782300	-0.52083100
H	0.09581200	-0.15439500	0.93421100
H	1.38493700	1.09868100	1.25821800
H	0.44987600	1.34715100	-0.75579700
C	4.93619600	-1.73132900	2.49227800
F	5.18749300	-0.62647700	0.42086800
C	2.76893000	-2.39135100	3.32299800
F	0.79320500	-1.94048400	2.09195600
C	3.97833100	1.36151800	-3.26313900
F	2.46286300	-0.45366400	-3.26698500
C	4.57808900	2.50486800	-1.22454200
F	3.70952700	1.80637800	0.86971200
C	4.16186900	-2.34650900	3.48894800
F	6.31937100	-1.69492400	2.62499400
F	1.97162700	-3.00956200	4.28343500
C	4.69532400	2.38156100	-2.61909700
F	4.05113300	1.23692500	-4.64586800
F	5.25067800	3.52589100	-0.55786200
F	4.75978500	-2.90687900	4.60867800
F	5.48271800	3.26425300	-3.34404800
C	-2.97814400	-1.20526000	2.16710700
H	-2.06958400	-0.58842600	2.16755500
C	-3.99397900	1.68104800	-2.06274800
H	-3.12201700	2.23702500	-1.69742900
C	-2.53700100	-2.67016700	1.86936600
H	-3.39312700	-3.36071900	1.90906600
H	-2.08223300	-2.75361600	0.87313000
H	-1.79639800	-3.00077200	2.61258300
C	-3.60712700	-1.10255300	3.58668500
H	-3.95508500	-0.08224300	3.80807400
H	-4.46625200	-1.77961600	3.70434300
H	-2.86172300	-1.38521400	4.34683100
C	-3.54998200	0.90733000	-3.34186800
H	-4.39179900	0.34644800	-3.77579700
H	-3.18105800	1.60903300	-4.10742500
H	-2.75003900	0.18802200	-3.11604600
C	-5.08592300	2.73402900	-2.40296400
H	-5.96237000	2.28353300	-2.89136200
H	-5.43832000	3.26065600	-1.50245400
H	-4.67741200	3.48184900	-3.10168100
C	1.39614200	3.00160400	3.16999200
H	2.37303000	3.02438000	2.67592500

H	1.41888200	3.75229500	3.97914300
H	1.28569400	2.01970400	3.65267400
C	1.54861600	4.72970400	0.42953700
H	1.60917500	5.77577300	0.77843300
H	2.47445100	4.23367700	0.73854200
H	1.53054400	4.76744600	-0.66812200
C	-1.65581700	2.39270000	3.77950800
H	-2.70173500	2.07676500	3.69491100
H	-1.06266300	1.51894200	4.08546000
H	-1.60040800	3.12142900	4.60701200
C	-1.43894500	5.19154800	-0.60092300
H	-1.46471100	6.23917800	-0.25382400
H	-0.72764100	5.15016300	-1.43640900
H	-2.43748000	4.96061900	-0.99547100
C	-3.45196900	3.82268500	1.51788700
H	-3.95335700	2.93556500	1.92507500
H	-3.72929400	4.67839500	2.15812900
H	-3.87100400	4.01448700	0.52282400
Br	-7.84319000	-1.71368700	-0.22212700

Frequencies --	-1010.1888	10.2566	14.9443
Frequencies --	20.0905	25.9591	27.9980
Frequencies --	28.6298	31.8379	34.7729
Frequencies --	37.1286	40.6007	43.0914
Frequencies --	47.0057	54.5077	57.9844
Frequencies --	66.7316	69.0176	79.7240
Frequencies --	90.7290	93.1526	102.0733
Frequencies --	103.7439	111.0534	111.3795
Frequencies --	114.3258	117.9101	119.8882
Frequencies --	122.2106	123.7118	125.3817
Frequencies --	127.9465	135.4876	136.5508
Frequencies --	141.5397	142.6273	145.2893
Frequencies --	147.3265	149.5270	156.3618
Frequencies --	159.1958	161.6743	166.2263
Frequencies --	170.5132	174.5601	181.4645
Frequencies --	188.2289	199.5484	208.4886
Frequencies --	214.3294	217.2641	219.8428
Frequencies --	221.2011	223.5024	232.9938
Frequencies --	235.5190	237.7294	243.1290
Frequencies --	251.9248	253.4611	260.6431
Frequencies --	264.4269	264.6559	264.8544
Frequencies --	275.5134	276.6591	278.3139
Frequencies --	283.0952	289.2260	295.0978
Frequencies --	298.5116	302.0057	303.1064
Frequencies --	304.4005	304.6231	309.7709
Frequencies --	317.1246	322.8123	324.0227
Frequencies --	326.9382	331.3311	337.2896
Frequencies --	357.2864	368.0812	374.3968
Frequencies --	376.9216	378.5207	381.1524
Frequencies --	385.6424	388.6834	397.3242
Frequencies --	413.8233	422.8216	431.9464
Frequencies --	432.6859	434.2628	434.5504
Frequencies --	449.3758	457.0787	460.3364
Frequencies --	464.2704	477.7378	530.1705
Frequencies --	532.5994	534.4996	538.2557
Frequencies --	539.3493	545.1210	552.4892
Frequencies --	555.1604	565.0266	576.4809
Frequencies --	584.2830	593.4530	596.1759
Frequencies --	605.4990	609.1698	612.3847
Frequencies --	619.5390	623.8070	634.3806
Frequencies --	636.1990	638.2333	642.0504

Frequencies --	655.2621	672.2109	701.5930
Frequencies --	715.7401	721.8441	732.8835
Frequencies --	743.5252	746.5828	760.6997
Frequencies --	768.9108	769.4925	777.0693
Frequencies --	800.9584	804.2151	807.1617
Frequencies --	841.4362	868.9650	877.4078
Frequencies --	878.3753	881.2308	895.3218
Frequencies --	904.3365	904.5992	912.9496
Frequencies --	917.6023	924.8327	927.7750
Frequencies --	933.8136	945.0741	963.0568
Frequencies --	966.0081	968.4364	971.2228
Frequencies --	1009.3275	1019.4151	1027.6133
Frequencies --	1039.7975	1040.8402	1042.6778
Frequencies --	1044.6988	1046.5596	1048.3588
Frequencies --	1050.2901	1054.0581	1056.5626
Frequencies --	1070.4293	1084.9226	1086.1488
Frequencies --	1088.6864	1092.6431	1111.4187
Frequencies --	1114.8503	1124.3370	1125.7996
Frequencies --	1170.2901	1172.3056	1174.3116
Frequencies --	1186.4656	1187.6998	1209.9787
Frequencies --	1212.8677	1215.3931	1256.6305
Frequencies --	1263.4919	1266.1387	1286.9861
Frequencies --	1298.8592	1313.9321	1318.3586
Frequencies --	1319.5537	1321.1598	1325.8452
Frequencies --	1331.1039	1337.3052	1343.7923
Frequencies --	1349.4454	1352.6849	1369.9333
Frequencies --	1401.0131	1404.6328	1409.4200
Frequencies --	1411.2656	1413.7360	1418.6934
Frequencies --	1419.8895	1420.8629	1422.5250
Frequencies --	1423.6857	1424.4378	1425.7394
Frequencies --	1427.9576	1429.1099	1434.2043
Frequencies --	1435.5388	1449.6568	1453.4596
Frequencies --	1467.1842	1468.0639	1469.4798
Frequencies --	1471.9525	1475.3795	1483.1627
Frequencies --	1486.3849	1487.0573	1489.5490
Frequencies --	1489.9230	1491.1304	1495.9486
Frequencies --	1498.6648	1500.8614	1502.8873
Frequencies --	1503.2049	1506.0262	1507.7069
Frequencies --	1509.0248	1509.7397	1511.8652
Frequencies --	1517.2736	1524.7164	1529.0155
Frequencies --	1576.7393	1586.7697	1594.4977
Frequencies --	1596.4463	1598.6328	1617.8982
Frequencies --	1620.2342	1622.7126	1808.0397
Frequencies --	2952.5080	3009.9167	3010.5550
Frequencies --	3011.2772	3012.6845	3012.8857
Frequencies --	3013.7739	3014.8690	3015.2223
Frequencies --	3024.9667	3052.8921	3078.6863
Frequencies --	3090.4494	3095.3849	3098.5371
Frequencies --	3098.6052	3100.9053	3103.2938
Frequencies --	3107.4905	3109.6548	3114.8306
Frequencies --	3115.9959	3120.9978	3126.0609
Frequencies --	3130.8076	3136.7000	3140.5732
Frequencies --	3145.9235	3152.6789	3155.2647
Frequencies --	3157.8639	3164.3986	3171.5412
Frequencies --	3198.4011	3214.2148	3216.4392

Catalyst 33:

vacuum	toluene-like solvent	D3 dispersion
-2924.473904	-2924.4857874	-0.49703962

Imaginary frequency corresponding to vibration along the reaction coordinate: -1095 cm^{-1} .

Ti	-2.13115400	1.74012500	0.41519200
C	-1.41085300	2.03720400	-1.77590300
H	-1.04668300	1.28595700	-2.49088800
H	-2.46141100	2.22807800	-2.03497600
H	-0.82906300	2.95667500	-1.89118500
O	-3.53140300	0.67964500	0.19535200
C	-4.70754000	-0.07141500	0.21588900
C	-4.96329200	-0.91644500	1.33584900
C	-5.59669600	0.02951600	-0.89351000
C	-6.16592900	-1.66027200	1.32634800
C	-6.78238200	-0.73898200	-0.85022000
C	-7.07021000	-1.57466200	0.24820400
H	-6.38703700	-2.31681800	2.16971000
H	-7.47895700	-0.68493200	-1.68877200
H	-7.99067700	-2.16120600	0.26085800
H	-3.12960100	2.55948100	3.19792600
C	-2.70190600	3.03630300	2.32010300
C	-1.30352600	3.33334000	2.11375000
C	-3.43932900	3.57321300	1.20915100
H	-0.48967000	3.08074700	2.78681500
C	-1.17605400	4.00104600	0.86105400
H	-4.51680900	3.52735500	1.07871000

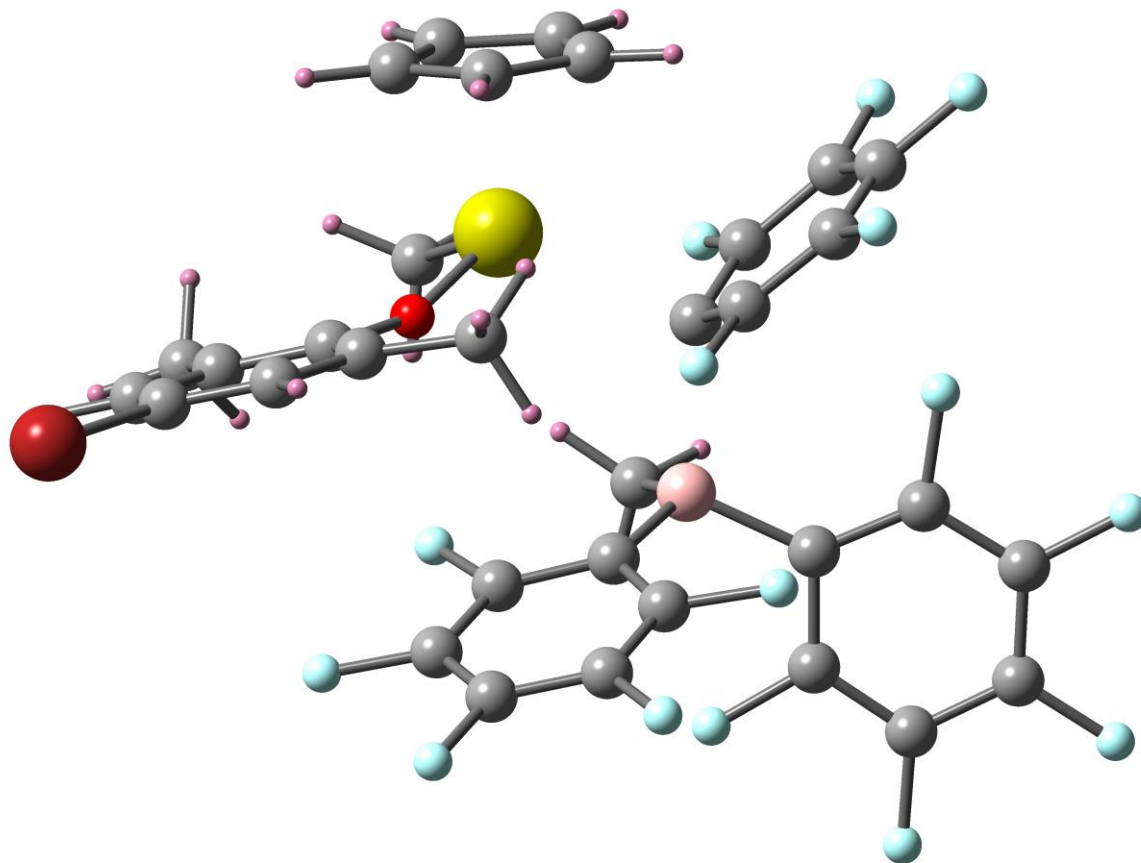
C	-2.49418400	4.13762700	0.28993200
H	-0.24821900	4.33974700	0.41115500
H	-2.73209000	4.62719300	-0.64970900
F	0.70351100	-4.57787900	-4.01253800
C	0.75687700	-3.53437600	-3.10035800
C	1.98574500	-3.11159800	-2.56442500
C	-0.41389400	-2.87550000	-2.69674600
C	2.00737000	-2.04989500	-1.64298300
F	3.16156800	-3.73983500	-2.95538200
C	-0.33183700	-1.81573400	-1.77041200
F	-1.64478300	-3.26915200	-3.21397800
C	0.86482500	-1.34187900	-1.19354900
F	3.27210300	-1.67465900	-1.17911400
F	-1.57198300	-1.22801600	-1.44938900
B	1.02315600	-0.14861000	-0.03596000
C	1.68507400	-0.95300900	1.28841400
C	1.92161500	1.16421200	-0.53738700
C	-0.43800500	0.51575800	0.47713100
C	3.01605300	-0.84491000	1.76166300
C	0.91945700	-1.89496400	2.01661100
C	2.29458300	1.45449600	-1.86946000
C	2.30840500	2.17761100	0.37145600
H	-1.15090800	-0.30064800	0.68189000
H	-0.18912500	1.09116000	1.39315400
H	-0.84352600	1.31387300	-0.77548700
C	3.52807700	-1.56176400	2.86333100
F	3.93817200	-0.00631700	1.13277700
C	1.38032200	-2.63521500	3.12098400
F	-0.40844000	-2.17568000	1.63002200
C	3.02875800	2.59407100	-2.26295400
F	1.91296300	0.61224000	-2.92305600
C	3.03393800	3.33308500	0.03678300
F	1.95686600	2.06215000	1.73099200
C	2.70361100	-2.46182700	3.55726800
F	4.84626100	-1.38891200	3.26726500
F	0.54312800	-3.53278100	3.77710100
C	3.41243100	3.54139300	-1.30095400
F	3.35834900	2.79659300	-3.59789100
F	3.37157200	4.27102800	1.00788300
F	3.18760100	-3.17240700	4.64579000
F	4.12679300	4.67316500	-1.66506500
C	-3.98634900	-1.04188000	2.49151800
H	-3.04282300	-1.51073800	2.17371300
H	-3.73873300	-0.06265000	2.93059500
H	-4.40900300	-1.66432500	3.29140500
C	-5.27978000	0.90245500	-2.09427600
H	-5.12345500	1.95490200	-1.80736900
H	-4.36662700	0.55623200	-2.60338400
H	-6.10011500	0.87519400	-2.82399200

Frequencies --	-1094.9368	13.4301	18.5642
Frequencies --	21.4827	28.1728	29.2242
Frequencies --	30.9053	35.4322	39.6189
Frequencies --	43.4234	45.3667	47.1683
Frequencies --	51.0986	74.4668	82.6052
Frequencies --	94.4022	102.4578	112.0207
Frequencies --	112.5445	122.5061	125.6920

Frequencies --	132.1604	136.8420	141.8430
Frequencies --	144.0049	147.2384	150.7655
Frequencies --	153.7205	156.8534	158.5993
Frequencies --	161.7950	164.9665	173.0044
Frequencies --	207.1413	210.0765	214.5094
Frequencies --	216.7771	219.9798	221.4749
Frequencies --	224.3997	225.8725	246.5573
Frequencies --	261.9205	264.3937	264.9516
Frequencies --	265.4401	267.9252	275.0482
Frequencies --	275.9546	282.0614	302.3234
Frequencies --	302.9652	308.5436	313.6673
Frequencies --	324.1449	326.2212	330.7876
Frequencies --	336.2487	345.9095	362.2397
Frequencies --	366.0512	376.5136	378.8352
Frequencies --	379.5489	381.6068	389.7675
Frequencies --	399.4250	431.0164	431.8691
Frequencies --	432.8530	450.5758	456.4220
Frequencies --	463.6039	481.3605	492.9342
Frequencies --	511.3331	535.4021	536.8912
Frequencies --	543.9073	545.9740	551.1795
Frequencies --	554.4649	564.2700	567.3621
Frequencies --	570.7831	573.6118	597.3084
Frequencies --	605.1460	635.4072	636.1147
Frequencies --	637.7677	642.3754	654.9439
Frequencies --	674.5047	707.4322	718.1875
Frequencies --	725.4696	734.5460	735.9167
Frequencies --	743.7945	748.1933	749.6025
Frequencies --	762.2522	773.1977	787.5876
Frequencies --	789.6579	802.7925	813.9772
Frequencies --	839.7462	842.1499	847.5391
Frequencies --	871.3991	873.6529	877.6201
Frequencies --	887.1454	901.3424	901.8324
Frequencies --	911.3953	911.9942	920.8350
Frequencies --	922.8369	936.4168	990.5973
Frequencies --	994.3959	1003.1426	1018.4447
Frequencies --	1023.1791	1028.5309	1034.8593
Frequencies --	1036.0489	1050.5571	1051.1072
Frequencies --	1052.2061	1056.1290	1056.4982
Frequencies --	1060.6580	1087.5484	1090.6766
Frequencies --	1092.3426	1109.0736	1126.9746
Frequencies --	1194.0345	1201.3199	1211.2964
Frequencies --	1214.3323	1216.4921	1268.4015
Frequencies --	1279.3670	1282.2118	1282.6940
Frequencies --	1290.4667	1318.1097	1320.1037
Frequencies --	1324.4162	1337.9249	1338.3291
Frequencies --	1344.4592	1349.4429	1363.6979
Frequencies --	1389.9969	1392.8583	1411.5551
Frequencies --	1419.9002	1420.4361	1422.5984
Frequencies --	1423.8457	1427.9227	1438.0068
Frequencies --	1454.3141	1465.2382	1467.8095
Frequencies --	1468.9348	1471.4209	1473.3734
Frequencies --	1487.2149	1490.9386	1493.8327
Frequencies --	1506.6922	1506.9555	1593.9054
Frequencies --	1595.9425	1597.3679	1605.6870
Frequencies --	1607.4351	1617.6051	1619.8591
Frequencies --	1622.1987	1820.0761	2960.0864
Frequencies --	3010.6198	3020.6590	3041.9346
Frequencies --	3086.4996	3095.5742	3106.9489
Frequencies --	3132.5733	3135.8426	3142.4800
Frequencies --	3166.3995	3177.3601	3190.2340
Frequencies --	3197.4113	3235.8035	3242.4453
Frequencies --	3255.9521	3258.2270	3277.5243

5. Transition States for Transfer of (C₆F₅) from Counterion to Cation ([return to table of contents](#))

Catalyst 1:



vacuum	toluene-like solvent	D3 dispersion
-2937.0260475	-2937.036449	-0.51564851

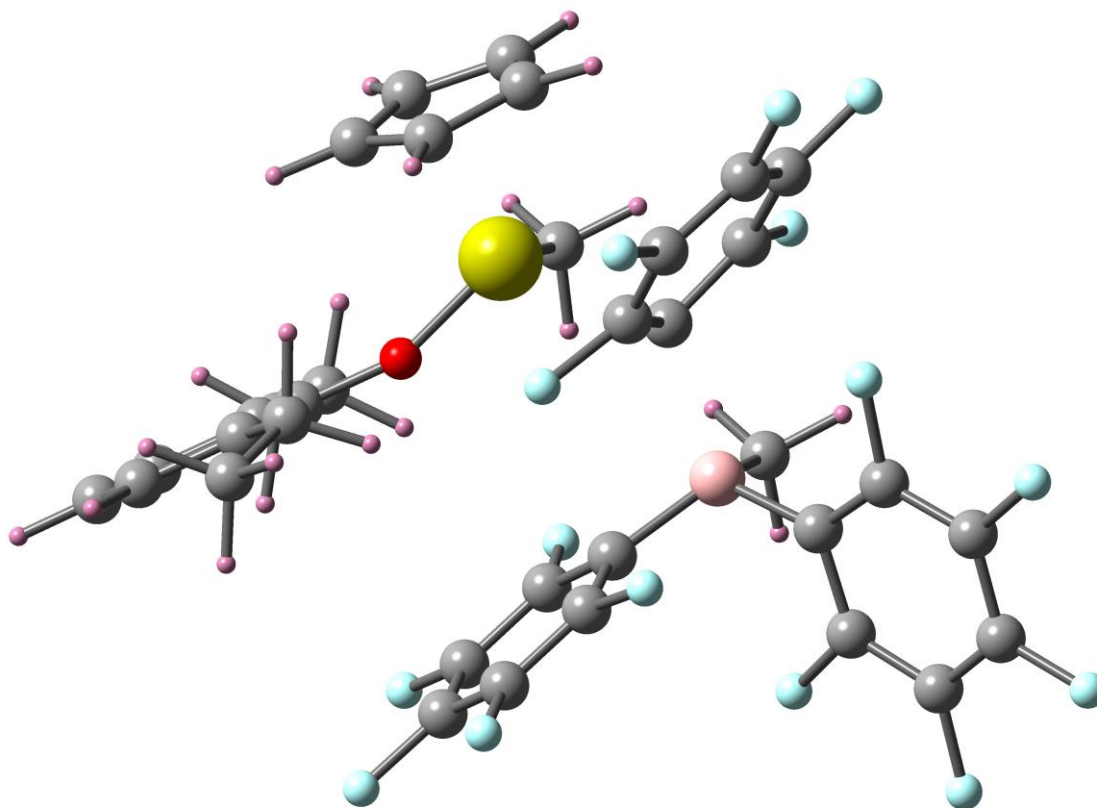
Imaginary frequency corresponding to vibration along the reaction coordinate: -199 cm^{-1} .

Ti	0.79028500	2.21430500	0.90507100
C	0.75143500	2.10262700	2.97811400
H	0.67565000	1.01726300	3.13885600
H	1.61794800	2.48666800	3.52913900
H	-0.16018100	2.61259200	3.32747100
O	2.07792300	1.03744500	0.54249700
C	3.33303800	0.51899400	0.20342800
C	3.64751700	0.25469900	-1.16486400
C	4.26342700	0.24491500	1.25419000
C	4.93178600	-0.25761400	-1.46574600
C	5.53222000	-0.27160700	0.90636600
C	5.85923200	-0.51048300	-0.44049600
H	5.18869100	-0.46417800	-2.50403000
H	6.25076500	-0.48973800	1.69529900
H	-0.23955300	4.23381100	-1.34807700

C	0.43272900	4.21339100	-0.49932000
C	0.11976800	4.61417700	0.84448400
C	1.81616700	3.84435500	-0.54551800
H	-0.83934200	4.97168800	1.20480900
C	1.30975200	4.48883800	1.62932700
H	2.36450900	3.52118700	-1.42317400
C	2.35901900	4.00200000	0.77394600
H	1.40533100	4.73706500	2.67971500
H	3.38591300	3.80455800	1.06628300
F	-7.18091000	-3.12883500	-0.24126400
C	-5.96559200	-2.50465500	-0.00531000
C	-5.71629200	-1.21121400	-0.48624300
C	-4.95454000	-3.15261700	0.72402800
C	-4.47216500	-0.59846400	-0.22982900
F	-6.69293400	-0.54243100	-1.21478700
C	-3.73318900	-2.49259700	0.94961700
F	-5.16921200	-4.43443400	1.21463300
C	-3.41414400	-1.18632100	0.48930200
F	-4.33600900	0.68696500	-0.77455900
F	-2.78821000	-3.22430300	1.68702300
B	-1.94363200	-0.58634000	1.00260500
C	-1.50207600	1.34329600	0.14797600
C	-2.36062800	2.38082800	0.61699200
C	-1.38934200	1.35129300	-1.27284700
C	-3.07393200	3.27690500	-0.19712600
F	-2.52197100	2.57930300	1.99555100
C	-2.09031400	2.20284600	-2.14411400
F	-0.49180000	0.47566100	-1.89190800
C	-2.94937800	3.17307800	-1.59493000
F	-3.87504900	4.27276500	0.34727200
F	-1.92834500	2.13184600	-3.52124100
F	-3.63505400	4.04008500	-2.42025200
C	2.66026400	0.44140400	-2.30249400
H	1.96275800	-0.40748800	-2.35671200
H	2.04686500	1.34107200	-2.19370500
H	3.18513000	0.49819900	-3.26580700
C	3.93659800	0.47344400	2.71840400
H	3.80171300	1.54249300	2.94225900
H	3.01297200	-0.04365700	3.00826100
H	4.74789800	0.10043300	3.35714200
C	-0.73432800	-1.56159900	0.47966100
C	0.37960600	-1.92783100	1.26957900
C	-0.78318900	-2.24991500	-0.76071200
C	1.35938900	-2.86423700	0.88883600
C	0.16948300	-3.19289000	-1.18890200
C	1.25435100	-3.50910000	-0.35342800
F	-1.82858500	-2.01111700	-1.65780900
F	0.05019500	-3.81370800	-2.42654300
F	2.20965000	-4.42911200	-0.75493800
F	2.43173600	-3.14789500	1.72836300
F	0.58481300	-1.34517900	2.52871100
C	-2.11018900	-0.29691800	2.58392500
H	-1.30653300	0.27216800	3.05107200
H	-3.05537600	0.22533900	2.78702200
H	-2.16008700	-1.26646900	3.10542100
Br	7.63342000	-1.21703500	-0.89393900

Frequencies --	-199.0619	10.7760	12.3254
Frequencies --	18.5417	26.2158	31.2325
Frequencies --	33.6777	35.8895	39.8789
Frequencies --	47.9418	49.9739	54.4847
Frequencies --	58.8780	62.9526	71.6113
Frequencies --	85.5378	88.0390	93.6179
Frequencies --	100.3881	109.9931	114.5517
Frequencies --	119.1958	120.7337	126.0016
Frequencies --	134.5669	136.4691	143.1160
Frequencies --	150.9991	156.7145	157.5032
Frequencies --	165.1800	173.9959	174.7729
Frequencies --	188.4902	195.0366	200.3604
Frequencies --	205.9132	218.6839	221.5458
Frequencies --	230.1899	234.1825	241.5210
Frequencies --	243.6162	250.7969	254.9239
Frequencies --	264.1906	265.4932	266.8470
Frequencies --	270.3158	271.4384	272.7289
Frequencies --	274.6629	277.2513	285.7934
Frequencies --	296.0358	301.6441	305.2137
Frequencies --	309.6386	318.8212	319.2960
Frequencies --	328.7309	330.3155	333.5853
Frequencies --	364.0411	373.2054	376.0429
Frequencies --	380.5670	402.6786	408.0855
Frequencies --	424.1563	426.0817	431.6973
Frequencies --	433.9180	436.8485	442.7092
Frequencies --	451.7227	454.9963	486.1741
Frequencies --	501.9490	505.3863	512.8458
Frequencies --	540.0501	545.0627	551.2137
Frequencies --	560.1624	561.1921	567.5687
Frequencies --	570.4534	573.3307	576.0000
Frequencies --	594.2887	629.3764	631.0534
Frequencies --	638.8027	642.3016	644.2907
Frequencies --	649.2514	677.4463	695.1268
Frequencies --	703.3435	716.4633	718.0544
Frequencies --	722.3332	728.3659	739.6311
Frequencies --	752.4673	783.2714	793.4739
Frequencies --	803.8983	807.9691	819.1307
Frequencies --	830.7732	842.2536	843.2475
Frequencies --	874.2314	886.1498	889.4831
Frequencies --	895.9084	899.5275	908.1028
Frequencies --	911.0177	918.4531	919.9114
Frequencies --	950.8940	987.9775	994.4410
Frequencies --	996.7215	1012.2288	1029.8366
Frequencies --	1037.2192	1042.8000	1044.6594
Frequencies --	1050.3273	1055.1242	1056.9145
Frequencies --	1059.5662	1061.7746	1082.7664
Frequencies --	1091.3390	1094.8253	1124.8801
Frequencies --	1132.7888	1181.2695	1186.9342
Frequencies --	1198.4178	1215.0351	1222.7287
Frequencies --	1251.7801	1266.1012	1283.6571
Frequencies --	1286.9982	1311.8366	1326.2773
Frequencies --	1332.7419	1340.7377	1351.2178
Frequencies --	1356.8739	1369.9313	1379.1491
Frequencies --	1395.6644	1401.3884	1413.6084
Frequencies --	1415.8846	1420.3242	1422.4748
Frequencies --	1426.2768	1429.2725	1431.8324
Frequencies --	1447.2579	1449.2641	1451.7491
Frequencies --	1455.9784	1470.6213	1473.7115
Frequencies --	1489.7202	1491.6744	1497.3988
Frequencies --	1502.2411	1503.4790	1508.5423
Frequencies --	1570.8352	1583.4564	1583.6489
Frequencies --	1589.2965	1595.2902	1597.4194

Frequencies --	1619.2024	1623.2178	3012.3550
Frequencies --	3031.4644	3035.2059	3042.2397
Frequencies --	3117.6156	3122.6308	3128.1894
Frequencies --	3140.7687	3150.1268	3160.5125
Frequencies --	3166.9953	3201.4358	3203.7638
Frequencies --	3213.5813	3249.4235	3255.4742
Frequencies --	3270.7647	3279.5911	3294.9892

Catalyst 2:

vacuum	toluene-like solvent	D3 dispersion
-3003.0411458	-3003.0512844	-0.54423054

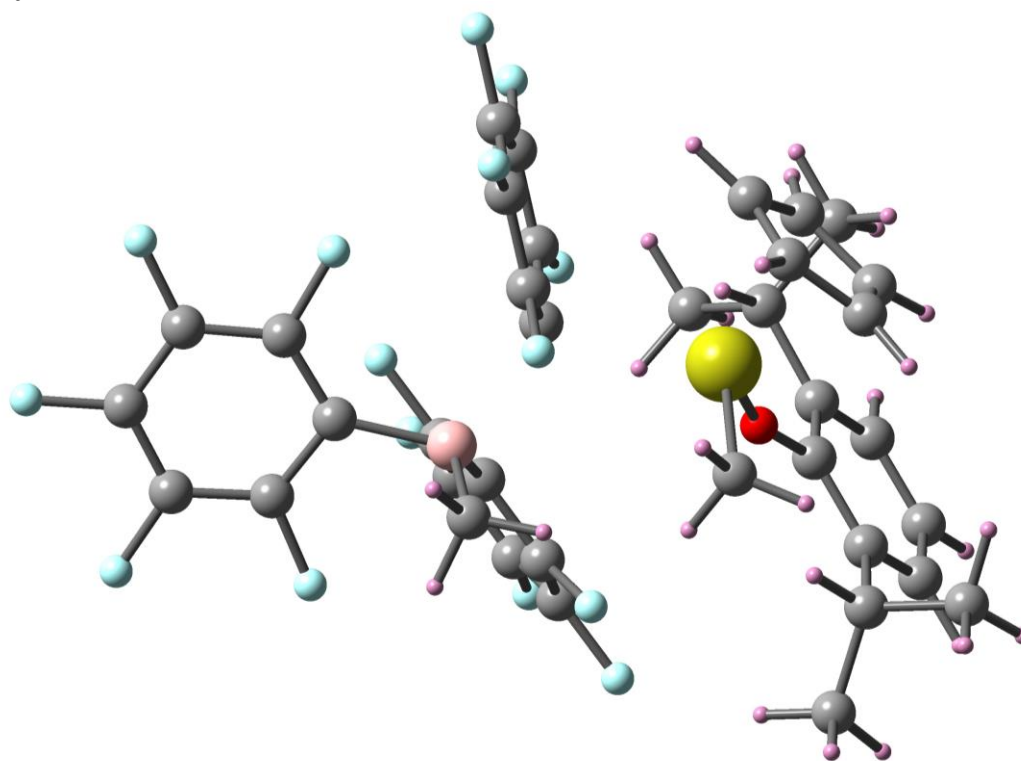
Imaginary frequency corresponding to vibration along the reaction coordinate: -202 cm^{-1} .

Ti	-1.66744500	1.86710000	-0.64591400
C	-1.77054100	1.88270700	-2.72068400
H	-1.62406300	0.82546000	-2.98546000
H	-2.68225600	2.25746500	-3.19911100
H	-0.91221500	2.48437600	-3.05994100
O	-2.70899700	0.47389000	-0.26601800
C	-3.83976100	-0.25755400	0.13844800
C	-3.99930400	-0.58512500	1.52247800
C	-4.77722400	-0.66195200	-0.86497400
C	-5.14856100	-1.32637900	1.88235100
C	-5.90514000	-1.39794800	-0.43677100
C	-6.09430600	-1.72512900	0.91931900
H	-5.30075500	-1.60432000	2.92348200
H	-6.63766700	-1.72913400	-1.17007400
C	-1.25910600	4.16221800	0.17911100
C	-1.99085100	4.31407600	-1.03773500
C	-2.08277700	3.43609000	1.11126100
C	-3.27353900	3.69033000	-0.86313000
C	-3.33817400	3.16693700	0.47077500

F	7.03782700	-2.30676800	-0.26947600
C	5.73605600	-1.84690300	-0.39773400
C	5.38445900	-0.55619300	0.02291400
C	4.73696200	-2.66275800	-0.95444200
C	4.05323900	-0.11277900	-0.12007300
F	6.34698500	0.27656900	0.58171900
C	3.42575100	-2.16758400	-1.07331900
F	5.05126600	-3.94715500	-1.38098700
C	3.00109000	-0.87399500	-0.66450100
F	3.82320000	1.18841300	0.34952600
F	2.50291500	-3.06136700	-1.64041500
B	1.41614500	-0.49161400	-1.02647900
C	0.84532000	1.43860000	-0.24905300
C	1.51053900	2.51411400	-0.91156600
C	0.89462700	1.58066800	1.16694300
C	2.21388000	3.54944900	-0.27171800
F	1.48450700	2.60197600	-2.30877500
C	1.57694100	2.58903900	1.86887500
F	0.18039300	0.67860500	1.96801200
C	2.25878600	3.57691600	1.13507700
F	2.84411800	4.55439400	-0.99414100
F	1.56695000	2.64725800	3.25637700
F	2.93444000	4.58658800	1.78922900
C	-2.96387500	-0.15731900	2.56281900
H	-3.02373600	0.93684000	2.69491400
C	-4.55220900	-0.31501100	-2.33613800
H	-3.55096100	-0.66657100	-2.62455400
C	0.41763500	-1.56920000	-0.30051100
C	-0.68731000	-2.17091200	-0.94637800
C	0.68735400	-2.12889600	0.97510300
C	-1.45741000	-3.21769800	-0.40511900
C	-0.05935300	-3.16483000	1.56604100
C	-1.14239700	-3.72243400	0.86591500
F	1.76088000	-1.65746100	1.73707500
F	0.26170600	-3.64288700	2.83131400
F	-1.89723900	-4.73978200	1.42925000
F	-2.52953200	-3.74850700	-1.11389900
F	-1.09713900	-1.73465400	-2.21296900
C	1.34939200	-0.30945800	-2.63109800
H	0.42355600	0.11624400	-3.02082700
H	2.18343400	0.30800700	-2.99126800
H	1.46265100	-1.30303000	-3.09392400
H	-6.97073700	-2.30077800	1.22344300
C	-3.06436700	-0.81435400	3.95807000
H	-3.99391500	-0.54607100	4.48356900
H	-3.00733400	-1.91217200	3.89806700
H	-2.22357000	-0.47233500	4.58127000
C	-5.57752400	-0.87167600	-3.34750000
H	-5.28924000	-0.56369600	-4.36487600
H	-5.60994300	-1.97196100	-3.33296600
H	-6.59562500	-0.49341900	-3.16350000
H	-0.27641900	4.56668400	0.37919900
H	-1.63660900	4.80177700	-1.94047900
H	-1.81953400	3.17856300	2.13224200
H	-4.06347800	3.63683500	-1.60517100
H	-4.18141400	2.64223700	0.90674600
H	-4.52422600	0.78254200	-2.43658900

H	-1.96220000	-0.35012700	2.16154500
Frequencies --	-201.5606	11.1817	20.9672
Frequencies --	26.8854	28.6098	33.4701
Frequencies --	35.2478	38.3413	39.4490
Frequencies --	42.8379	46.0397	54.1332
Frequencies --	57.3626	61.9299	69.1695
Frequencies --	74.6768	82.2943	91.0172
Frequencies --	96.3942	99.0520	110.6002
Frequencies --	113.9381	118.7590	120.2703
Frequencies --	125.2834	131.1310	135.4624
Frequencies --	142.9197	151.4111	156.7419
Frequencies --	162.3884	166.5986	185.1220
Frequencies --	186.5762	200.4607	202.9612
Frequencies --	212.8694	222.2047	224.1399
Frequencies --	226.4001	232.4790	240.0393
Frequencies --	242.5394	261.1842	264.5370
Frequencies --	265.3198	266.8911	270.2452
Frequencies --	271.2890	276.2987	277.0097
Frequencies --	279.9689	284.0418	297.3556
Frequencies --	298.6153	304.1899	305.0092
Frequencies --	309.5898	319.5842	320.0487
Frequencies --	323.8630	326.0288	332.2073
Frequencies --	333.9176	342.2018	372.2410
Frequencies --	373.5204	375.9387	381.8972
Frequencies --	400.6840	408.9594	423.8219
Frequencies --	426.7109	431.4878	433.6723
Frequencies --	442.8225	451.1806	455.0528
Frequencies --	486.5104	499.0979	508.5394
Frequencies --	532.3340	540.9545	545.0210
Frequencies --	547.3199	551.2898	565.1154
Frequencies --	573.1868	576.2652	577.4349
Frequencies --	595.0700	602.1896	627.0398
Frequencies --	629.0043	638.2016	642.1793
Frequencies --	643.8153	650.6366	676.5455
Frequencies --	683.8589	695.0257	713.4151
Frequencies --	715.8753	717.0676	721.3826
Frequencies --	732.2546	737.8336	751.0064
Frequencies --	773.4196	783.1466	792.3452
Frequencies --	798.9561	812.4742	819.8079
Frequencies --	830.9446	832.9179	843.0818
Frequencies --	846.5506	853.9366	883.8643
Frequencies --	895.7414	899.8706	902.7596
Frequencies --	908.1214	919.2202	920.4577
Frequencies --	924.1993	988.3812	994.3524
Frequencies --	994.5402	995.8604	996.1481
Frequencies --	1026.6113	1030.4111	1038.6919
Frequencies --	1042.2216	1043.8556	1057.2025
Frequencies --	1057.8456	1059.5869	1082.0520
Frequencies --	1090.0126	1091.6023	1097.4811
Frequencies --	1099.4627	1104.3029	1119.9192
Frequencies --	1133.5067	1170.0964	1181.0874
Frequencies --	1190.4939	1204.4926	1214.8379
Frequencies --	1222.3859	1250.2618	1257.0062
Frequencies --	1276.8441	1286.9210	1295.1396
Frequencies --	1298.8161	1310.8862	1325.4054
Frequencies --	1327.3686	1329.8895	1340.3658
Frequencies --	1344.7528	1356.2318	1370.9700
Frequencies --	1378.8375	1382.7834	1396.7676
Frequencies --	1400.9254	1414.4136	1414.8205
Frequencies --	1416.4617	1421.2860	1430.1777
Frequencies --	1431.8412	1446.4764	1447.3476
Frequencies --	1449.4121	1452.3627	1469.7854

Frequencies --	1471.0555	1473.1424	1485.3191
Frequencies --	1495.7951	1496.1486	1500.2351
Frequencies --	1503.6136	1504.4175	1507.1251
Frequencies --	1507.9990	1570.5209	1583.1709
Frequencies --	1595.7651	1597.0692	1597.8348
Frequencies --	1608.2552	1618.7454	1622.7207
Frequencies --	3012.4456	3013.1996	3015.1523
Frequencies --	3024.5359	3030.9653	3035.8454
Frequencies --	3090.6643	3110.0775	3114.8317
Frequencies --	3119.7285	3120.9546	3123.0466
Frequencies --	3138.0160	3138.4972	3165.5610
Frequencies --	3173.1254	3203.0503	3209.6151
Frequencies --	3218.3951	3248.4257	3253.0573
Frequencies --	3263.5569	3277.0311	3305.2587

Catalyst 3:

vacuum	toluene-like solvent	D3 dispersion
-3081.6156898	-3081.6255412	-0.58208600

Imaginary frequency corresponding to vibration along the reaction coordinate: -205 cm^{-1} .

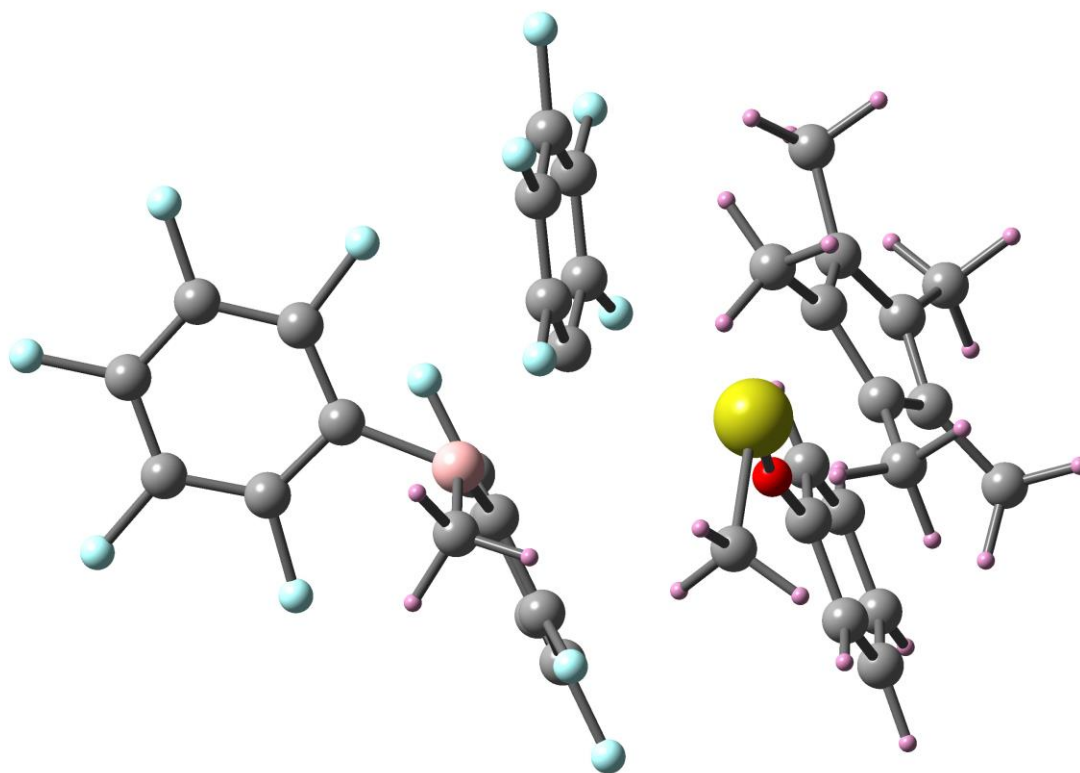
Ti	-1.64908800	1.76616600	-0.77102600
C	-1.72499000	1.58543800	-2.83811900
H	-1.39356100	0.54588200	-2.98501400
H	-2.69074400	1.73575300	-3.33324000
H	-0.98759000	2.28574300	-3.25914000
O	-2.67073200	0.39489500	-0.27446500
C	-3.77226900	-0.35662000	0.18412900
C	-3.97099900	-0.53448000	1.59370300
C	-4.65998500	-0.93024200	-0.78646900
C	-5.08161900	-1.31148600	2.00108600
C	-5.75226100	-1.68862100	-0.30533100
C	-5.96533300	-1.88424300	1.07032700
H	-5.25377800	-1.47017900	3.06565600
H	-6.44072900	-2.13745100	-1.02129800
C	-1.31637800	4.06672200	0.12202800
C	-1.71939200	4.24861800	-1.23645800
C	-2.36897000	3.38285600	0.81950300
C	-3.03160000	3.68735100	-1.38502400
C	-3.44003600	3.16012600	-0.11240000
F	7.36625500	-1.84509200	-0.28879300
C	6.03179100	-1.48872200	-0.41045500
C	5.58174900	-0.23065500	0.01503900
C	5.09681400	-2.37994400	-0.96287200
C	4.21924600	0.10675500	-0.12126100

F	6.47754500	0.67343100	0.57389300
C	3.75037200	-1.98844600	-1.07607800
F	5.50818400	-3.63624700	-1.39054300
C	3.22790300	-0.73153000	-0.66587400
F	3.88714500	1.37996100	0.36215800
F	2.89688500	-2.95429500	-1.63393300
B	1.61272700	-0.47862100	-1.01717900
C	0.88820000	1.42042100	-0.28088800
C	1.50234900	2.52955400	-0.93388500
C	0.90407200	1.56111700	1.13559600
C	2.14130900	3.59984100	-0.28478000
F	1.48361000	2.61225500	-2.33334300
C	1.52804900	2.60011200	1.84752100
F	0.21890700	0.62251400	1.92019000
C	2.16935300	3.62262400	1.12280700
F	2.72508000	4.64013600	-0.99694600
F	1.50087600	2.65555500	3.23511000
F	2.78629000	4.66275600	1.78815800
C	-3.06084800	0.07252200	2.67245900
H	-2.23751900	0.59589300	2.17598200
C	-4.49334700	-0.73794300	-2.30134900
H	-3.54254100	-0.22870100	-2.47154300
C	0.71309000	-1.61029300	-0.24786600
C	-0.35901300	-2.30674600	-0.85269400
C	1.06587700	-2.12873800	1.02498800
C	-1.00966000	-3.41822200	-0.28344200
C	0.44388700	-3.23070500	1.63888100
C	-0.60249500	-3.89089300	0.97381800
F	2.09906700	-1.54057100	1.76113900
F	0.84660400	-3.66873800	2.89473700
F	-1.23640700	-4.97585400	1.55909300
F	-2.05217200	-4.05248200	-0.95213000
F	-0.85007600	-1.91035900	-2.10406100
C	1.52089900	-0.34295600	-2.62421700
H	0.56147800	-0.00572000	-3.01595900
H	2.29793800	0.33414600	-3.00448200
H	1.71413000	-1.33392900	-3.06517200
H	-6.81214300	-2.48097000	1.41469700
C	-3.82814400	1.11116400	3.54601100
H	-4.29124600	1.90075900	2.93460200
H	-4.63047700	0.63409000	4.12818800
H	-3.13859700	1.58627900	4.26258100
C	-2.41127700	-1.01626500	3.57682300
H	-1.86511100	-1.75721800	2.97926200
H	-1.69574300	-0.55014900	4.27164900
H	-3.16032600	-1.55398800	4.17736000
C	-4.41771800	-2.08916300	-3.07100000
H	-4.24719800	-1.89871800	-4.14278000
H	-3.58782400	-2.70347000	-2.69924600
H	-5.34588200	-2.67256000	-2.98144900
C	-5.62341200	0.16818500	-2.87750900
H	-5.64625400	1.15249500	-2.38264100
H	-5.46778400	0.33010000	-3.95633900
H	-6.61545100	-0.29072700	-2.74839500
H	-0.39790200	4.42445800	0.56572000
H	-1.13357600	4.71650600	-2.02207800
H	-2.37348800	3.13312200	1.87396600

H	-3.61950500	3.68137700	-2.29580600
H	-4.38783100	2.67978000	0.10606400

Frequencies --	-205.1901	16.7548	21.0535
Frequencies --	26.1774	29.5297	33.3815
Frequencies --	34.1637	38.1361	40.1329
Frequencies --	45.7708	48.7324	53.4823
Frequencies --	58.5040	62.9995	66.2580
Frequencies --	78.6800	84.1732	86.7217
Frequencies --	91.3732	98.9431	100.6571
Frequencies --	108.2889	118.2349	118.8085
Frequencies --	123.8432	125.9410	128.8414
Frequencies --	134.6852	142.1741	150.6596
Frequencies --	154.0633	156.5554	164.5819
Frequencies --	173.9713	190.2230	199.7233
Frequencies --	201.8064	205.0856	206.8851
Frequencies --	213.2522	220.9821	232.0814
Frequencies --	235.2618	238.8973	240.0663
Frequencies --	246.0872	251.8350	257.9069
Frequencies --	263.9513	265.3394	266.6774
Frequencies --	268.6380	271.6572	275.4990
Frequencies --	275.7837	277.2620	289.9122
Frequencies --	295.6975	301.5955	303.5984
Frequencies --	305.5956	308.0720	313.7265
Frequencies --	318.0586	318.9258	321.5144
Frequencies --	326.6902	329.9088	332.3752
Frequencies --	373.4651	376.1996	377.1956
Frequencies --	380.5513	410.1679	423.0297
Frequencies --	424.4554	425.9695	432.1577
Frequencies --	433.1871	434.0502	437.3543
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Frequencies --	574.5336	592.3628	596.4299
Frequencies --	611.2684	621.3937	629.0757
Frequencies --	631.0942	638.0295	642.0106
Frequencies --	643.6672	649.6460	675.4917
Frequencies --	688.1502	694.9182	715.8309
Frequencies --	717.6438	721.1548	726.8185
Frequencies --	738.1543	750.0089	765.2896
Frequencies --	783.0749	796.5365	804.8646
Frequencies --	815.8896	819.8155	825.9559
Frequencies --	828.9023	842.5399	845.7575
Frequencies --	875.4919	886.4350	894.4110
Frequencies --	898.5369	901.0532	907.9241
Frequencies --	918.9826	921.8366	928.3175
Frequencies --	931.6239	933.1686	938.7052
Frequencies --	962.2102	964.4751	986.7113
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Frequencies --	1032.2967	1036.5610	1041.0676
Frequencies --	1042.1397	1055.0276	1057.4428
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Frequencies --	1327.3064	1329.5230	1332.7243
Frequencies --	1340.8965	1341.9377	1356.6241

Frequencies --	1368.9559	1378.4951	1383.0540
Frequencies --	1397.1734	1400.1510	1401.8494
Frequencies --	1404.1985	1414.6076	1419.8930
Frequencies --	1422.1445	1423.5645	1433.8603
Frequencies --	1438.2741	1447.5300	1448.0626
Frequencies --	1452.6811	1455.8192	1470.9219
Frequencies --	1473.4738	1474.1297	1488.7707
Frequencies --	1489.3387	1489.9220	1491.0368
Frequencies --	1496.8151	1501.2574	1501.7105
Frequencies --	1503.5412	1508.5581	1509.9796
Frequencies --	1569.6237	1581.9258	1594.2313
Frequencies --	1596.3665	1597.3022	1605.4732
Frequencies --	1619.8593	1622.9190	3004.5455
Frequencies --	3010.1859	3012.3005	3024.1021
Frequencies --	3024.6372	3038.1845	3103.4178
Frequencies --	3108.0779	3110.3832	3111.5889
Frequencies --	3115.6273	3117.6890	3120.7328
Frequencies --	3137.5083	3138.0653	3151.3716
Frequencies --	3154.1418	3165.5662	3168.5980
Frequencies --	3173.8989	3191.4364	3203.5664
Frequencies --	3213.2518	3248.5513	3258.2232
Frequencies --	3276.1382	3284.6222	3309.5132

Catalyst 4:

vacuum	toluene-like solvent	D3 dispersion
-3042.3473585	-3042.3576523	-0.55856653

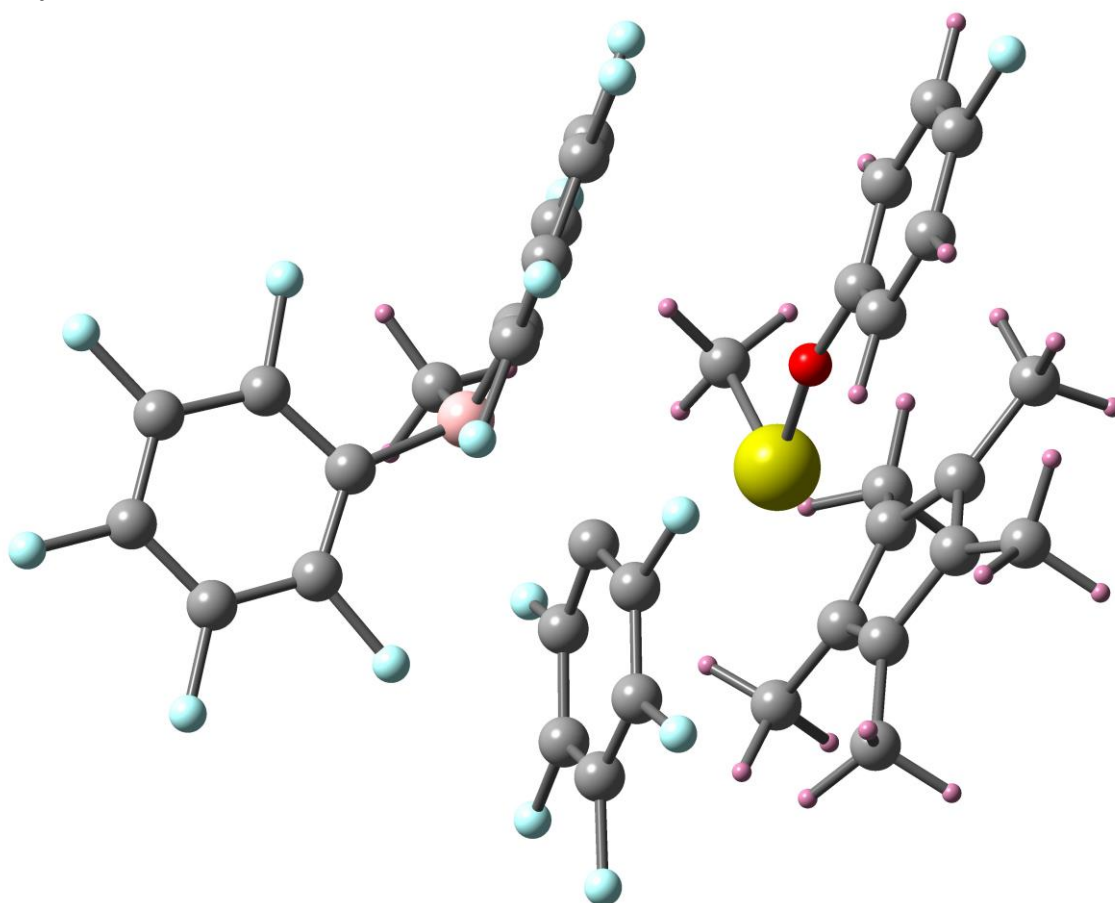
Imaginary frequency corresponding to vibration along the reaction coordinate: -225 cm^{-1} .

Ti	2.38064000	-0.59862500	-0.66243300
C	2.32226500	-0.13612300	-2.68329300
H	1.53366600	0.62791200	-2.72509600
H	3.23610900	0.27592000	-3.12863000
H	2.01550400	-1.03456800	-3.24363300
O	2.42979100	1.06607000	-0.05672700
C	2.76054100	2.32303600	0.42995200
C	2.54201400	2.63542200	1.79392900
C	3.28330100	3.29288900	-0.45999100
C	2.85841100	3.92617900	2.26356700
C	3.59608300	4.57830600	0.02446900
C	3.38806000	4.89908500	1.38528000
H	2.68004900	4.17314400	3.31219900
H	3.98673200	5.33065500	-0.66364100
C	3.51859700	-2.45156300	0.56390000
C	3.52559900	-2.84071000	-0.82890200
C	4.26746900	-1.22103000	0.69269300
C	4.30807700	-1.86964300	-1.55645400
C	4.75792000	-0.86023400	-0.61914400
F	-7.39807200	-1.01320500	-0.26943800
C	-6.03540300	-0.78527900	-0.39324500
C	-5.10446900	-1.65877600	0.18703000

C	-5.55418700	0.32796800	-1.10199100
C	-3.72446000	-1.40468600	0.04490900
F	-5.54657800	-2.76541300	0.90346900
C	-4.16645600	0.53078500	-1.21296000
F	-6.45007200	1.21647000	-1.68475400
C	-3.17018000	-0.31525500	-0.65381100
F	-2.89595300	-2.33143400	0.69129800
F	-3.79072600	1.67674000	-1.93236900
B	-1.59325500	0.09614600	-1.03186600
C	-0.13069300	-1.21881700	-0.07379800
C	-0.22591400	-2.55682200	-0.54387200
C	-0.08901200	-1.14990800	1.34686200
C	-0.37708700	-3.69282800	0.26894600
F	-0.16229000	-2.81191000	-1.92496400
C	-0.25062000	-2.24139000	2.21621700
F	0.16209900	0.08172900	1.97219700
C	-0.41182900	-3.52558100	1.66463800
F	-0.46610400	-4.97359900	-0.26851800
F	-0.20409700	-2.09245900	3.59815500
F	-0.53859100	-4.62521600	2.49201300
C	-1.27972600	1.58516200	-0.42895300
C	-0.65233000	2.62001600	-1.16099400
C	-1.78451200	2.01800700	0.82417100
C	-0.53234200	3.95064500	-0.71690700
C	-1.67462900	3.32939900	1.32047900
C	-1.04504700	4.31160700	0.53839700
F	-2.44765400	1.11520100	1.66225300
F	-2.18157800	3.66406500	2.57125300
F	-0.91639800	5.61071300	1.00657700
F	0.09754200	4.90760900	-1.50596400
F	-0.09818200	2.37061800	-2.42348700
C	-1.40958900	-0.20286600	-2.60715200
H	-0.38505400	-0.16162400	-2.97706300
H	-1.82404400	-1.18651400	-2.86744400
H	-1.98363600	0.54890600	-3.17155900
C	3.08997300	-3.30603400	1.73455000
H	3.98119800	-3.81717200	2.13910700
H	2.66049700	-2.72463700	2.56041000
H	2.37870200	-4.08928700	1.45513000
C	3.00903100	-4.13424900	-1.41921800
H	3.85851000	-4.79994900	-1.65081200
H	2.34992100	-4.67868900	-0.73488400
H	2.45769600	-3.98120400	-2.35773000
C	4.63837300	-0.56281600	2.00169800
H	4.90770900	0.49249800	1.87888000
H	3.83016000	-0.61553500	2.74453600
H	5.51305500	-1.07554500	2.43945800
C	4.79007600	-2.04519200	-2.97571900
H	5.63354900	-2.75786900	-2.98611600
H	4.01495500	-2.45285900	-3.63856300
H	5.15324500	-1.10887800	-3.41692100
C	5.72157700	0.26018800	-0.93451600
H	5.66702100	1.07769100	-0.20615600
H	6.75641700	-0.12439800	-0.91858300
H	5.55217200	0.68993300	-1.93141100
H	3.62239100	5.89914800	1.75408100
H	2.11449500	1.88707700	2.45902900

H	3.41944700	3.04378000	-1.51200300
Frequencies --	-224.9637	11.2449	17.8277
Frequencies --	19.5667	29.1770	33.1210
Frequencies --	34.4478	38.1151	45.5432
Frequencies --	47.6428	51.0929	54.5260
Frequencies --	56.4106	60.6424	63.3895
Frequencies --	79.6752	91.8682	95.1397
Frequencies --	103.8125	110.7463	112.6687
Frequencies --	115.7865	117.4829	120.0175
Frequencies --	122.4089	127.6511	135.4030
Frequencies --	136.6603	144.9579	148.2688
Frequencies --	149.9659	151.6949	157.3741
Frequencies --	158.8692	164.8594	168.5876
Frequencies --	185.0294	195.3620	202.4553
Frequencies --	204.4040	207.5656	215.1810
Frequencies --	223.0355	234.8326	237.7622
Frequencies --	251.2555	263.9220	265.2544
Frequencies --	267.0475	268.6535	270.6202
Frequencies --	275.4091	277.7852	277.9023
Frequencies --	286.8929	287.6922	292.8001
Frequencies --	294.5147	299.0206	301.4300
Frequencies --	306.0564	307.0413	317.1578
Frequencies --	317.2462	319.4248	328.2891
Frequencies --	329.7279	334.2104	368.9262
Frequencies --	371.9365	375.4119	381.3731
Frequencies --	389.4691	403.3330	407.9933
Frequencies --	408.5198	423.3004	425.2582
Frequencies --	431.5930	434.1132	442.4201
Frequencies --	450.6334	454.9283	455.4231
Frequencies --	485.7054	505.9552	514.1932
Frequencies --	529.1356	535.1924	540.1524
Frequencies --	542.7193	551.4169	551.4953
Frequencies --	571.9503	584.7430	592.5976
Frequencies --	593.1914	601.2269	612.5341
Frequencies --	618.6595	628.6434	638.2400
Frequencies --	642.6850	645.2247	648.8561
Frequencies --	655.6618	673.1316	688.7227
Frequencies --	691.8925	700.4834	714.3610
Frequencies --	717.0052	720.0524	738.1807
Frequencies --	750.8877	761.2380	782.3435
Frequencies --	798.5288	805.5859	831.2207
Frequencies --	836.6357	889.9897	899.0609
Frequencies --	907.6351	921.0807	921.3475
Frequencies --	925.2501	965.4896	968.6650
Frequencies --	976.1939	986.3389	992.1995
Frequencies --	996.0696	998.6546	1008.0774
Frequencies --	1030.1944	1036.3320	1039.0277
Frequencies --	1040.5477	1041.1886	1043.3615
Frequencies --	1047.6895	1048.7923	1057.5266
Frequencies --	1059.2159	1084.3998	1085.5468
Frequencies --	1087.2269	1090.4700	1123.2044
Frequencies --	1171.1291	1174.9599	1175.9933
Frequencies --	1184.0829	1189.3304	1192.8808
Frequencies --	1213.8650	1221.8063	1235.3640
Frequencies --	1246.6413	1310.3572	1325.8315
Frequencies --	1326.8663	1334.8648	1341.9032
Frequencies --	1356.8892	1373.8602	1374.7866
Frequencies --	1379.8578	1409.4319	1414.3003
Frequencies --	1414.9921	1422.1878	1423.3002
Frequencies --	1426.8614	1427.0469	1431.6984
Frequencies --	1433.5445	1436.9815	1447.9182
Frequencies --	1450.2032	1453.1312	1455.4964

Frequencies --	1457.2136	1462.5066	1471.0083
Frequencies --	1472.9478	1483.2244	1483.6026
Frequencies --	1490.5519	1492.6691	1496.5742
Frequencies --	1497.9506	1499.8525	1505.9003
Frequencies --	1507.2077	1507.7746	1508.5051
Frequencies --	1514.2942	1518.9424	1574.0200
Frequencies --	1585.6926	1596.6076	1596.7340
Frequencies --	1597.5057	1607.5648	1619.8250
Frequencies --	1622.3132	3008.2107	3008.6159
Frequencies --	3010.6953	3012.3788	3014.3976
Frequencies --	3016.4670	3038.1487	3099.1728
Frequencies --	3100.2464	3101.1635	3104.3907
Frequencies --	3110.5503	3120.3190	3136.8186
Frequencies --	3145.8601	3150.2138	3155.5984
Frequencies --	3158.0085	3161.9196	3168.3425
Frequencies --	3172.3194	3177.1135	3195.0953
Frequencies --	3208.2184	3211.8346	3221.5810

Catalyst 5:

vacuum	toluene-like solvent	D3 dispersion
-3141.5719347	-3141.5830509	-0.55910048

Imaginary frequency corresponding to vibration along the reaction coordinate: -228 cm^{-1} .

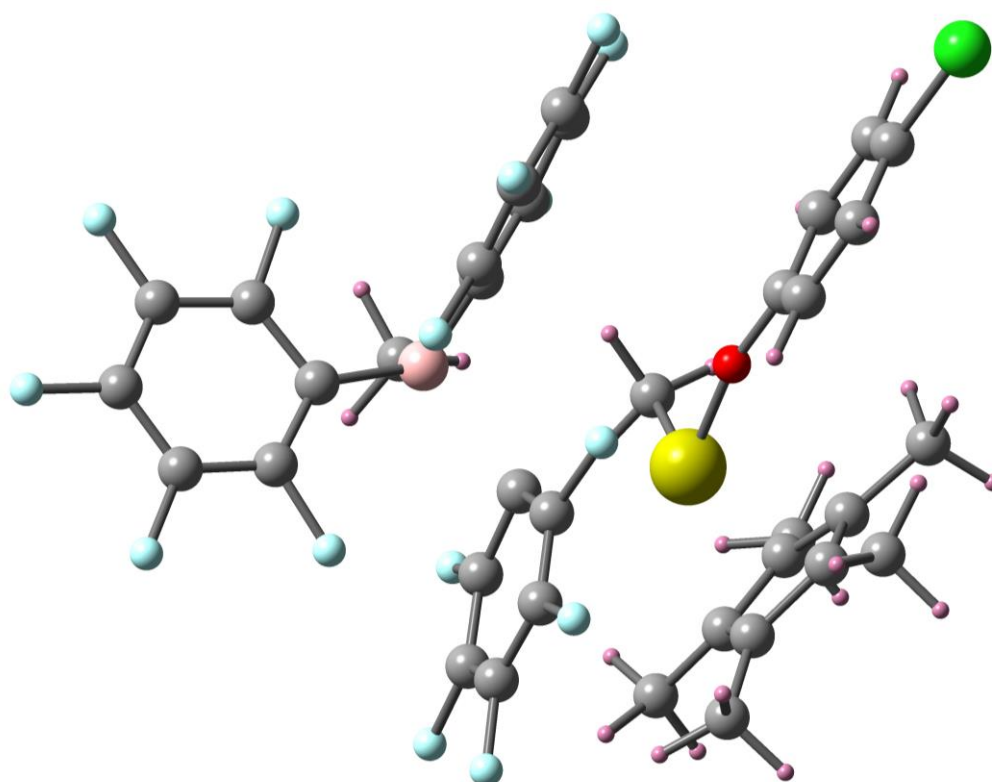
Ti	2.14731800	-1.09846700	-0.72093400
C	2.13629600	-0.70293700	-2.75684100
H	1.46975000	0.16779600	-2.82397600
H	3.10028900	-0.44575200	-3.21324900
H	1.69885600	-1.56251700	-3.29029600
O	2.47004600	0.55993500	-0.17244500
C	3.01331700	1.75342500	0.27406300
C	2.87257700	2.13265800	1.63247600
C	3.68030500	2.59996500	-0.64677300
C	3.41526100	3.35371300	2.07561900
C	4.22550400	3.82058600	-0.20680600
C	4.08715300	4.16959200	1.14808600
H	3.31472100	3.67323800	3.11245500
H	4.73295000	4.49436600	-0.89633900
C	3.01105500	-3.03033300	0.58103700
C	2.89928900	-3.49814900	-0.78356000
C	3.96555700	-1.94441500	0.60881100
C	3.80627000	-2.72073100	-1.59426600
C	4.45756100	-1.75090800	-0.73711700

F	-7.56406400	0.06467800	-0.16356100
C	-6.18532400	0.06717500	-0.31386400
C	-5.39310700	-0.91198000	0.30261200
C	-5.54803800	1.05267500	-1.08607300
C	-3.99334900	-0.88793100	0.13194200
F	-5.99005800	-1.89499600	1.08387700
C	-4.14805900	1.02637400	-1.22310300
F	-6.30318200	2.04166700	-1.70483100
C	-3.28782700	0.06214800	-0.63077600
F	-3.30883600	-1.89834300	0.82027700
F	-3.60863800	2.05980000	-2.00618200
B	-1.67328700	0.20068300	-1.04358800
C	-0.41939300	-1.28550800	-0.04482200
C	-0.74178100	-2.61134600	-0.44347100
C	-0.33264900	-1.15628200	1.36945100
C	-1.05198200	-3.66760000	0.42964100
F	-0.75827000	-2.93858900	-1.81063600
C	-0.64511400	-2.16357600	2.29693800
F	0.12711900	0.04769000	1.92769800
C	-1.02333600	-3.43040200	1.81535600
F	-1.36043100	-4.94088400	-0.03945900
F	-0.53932200	-1.95742400	3.66810300
F	-1.30293700	-4.45406200	2.70027900
C	-1.11574100	1.64403700	-0.51071500
C	-0.33691300	2.52980300	-1.29090000
C	-1.52435100	2.20576000	0.72645600
C	0.01051600	3.83804200	-0.90390500
C	-1.19353300	3.50077600	1.16445600
C	-0.41962000	4.33156600	0.33725000
F	-2.31002500	1.45800800	1.60987500
F	-1.62143800	3.96626800	2.40241800
F	-0.07145900	5.60920000	0.74792900
F	0.78475200	4.64096900	-1.73564200
F	0.15038300	2.14111000	-2.54569400
C	-1.56500500	-0.19327900	-2.60494300
H	-0.55323400	-0.34203700	-2.98239200
H	-2.14054400	-1.10487100	-2.81645900
H	-2.01440900	0.61712400	-3.20022200
C	2.48949500	-3.72681900	1.81712400
H	3.30272300	-4.34036500	2.24290600
H	2.17504600	-3.03248600	2.60685900
H	1.66054200	-4.40895400	1.60506900
C	2.15143900	-4.71851200	-1.27393900
H	2.87122200	-5.52022500	-1.51268500
H	1.45936300	-5.11850500	-0.52577400
H	1.57383600	-4.52441600	-2.18870800
C	4.49789000	-1.29045000	1.86250900
H	4.93671000	-0.30473900	1.66948200
H	3.72450000	-1.16702000	2.63321300
H	5.29135800	-1.92184600	2.29968100
C	4.19101200	-3.05378400	-3.01500500
H	4.94838800	-3.85739000	-3.00684800
H	3.34020500	-3.41712000	-3.60658000
H	4.63076600	-2.20068400	-3.54613200
C	5.58487100	-0.83353600	-1.15016500
H	5.68128500	0.03726800	-0.49067900
H	6.54276900	-1.38112900	-1.10837600

H	5.47015900	-0.46494800	-2.17881800
H	2.33170400	1.48743400	2.32149400
H	3.75256300	2.31131000	-1.69442800
F	4.63663700	5.38279200	1.59090100

Frequencies --	-227.6342	11.9149	14.5368
Frequencies --	17.4376	25.7440	30.0528
Frequencies --	31.7471	35.3565	40.2307
Frequencies --	45.0224	50.4649	54.2877
Frequencies --	56.0803	58.8754	63.2661
Frequencies --	79.3270	91.3165	94.2549
Frequencies --	100.5204	108.8404	110.4406
Frequencies --	115.3694	120.1907	122.7419
Frequencies --	126.0333	128.4572	136.6241
Frequencies --	138.1911	142.1729	145.8761
Frequencies --	148.7621	151.0483	157.2304
Frequencies --	158.5243	164.1872	168.6033
Frequencies --	175.8047	188.9643	200.0158
Frequencies --	202.9203	206.7791	214.1875
Frequencies --	221.5732	236.1739	239.8662
Frequencies --	251.4247	261.8323	263.9531
Frequencies --	265.1766	267.5190	268.3254
Frequencies --	271.5667	275.7087	276.9110
Frequencies --	277.7651	282.1170	289.6027
Frequencies --	294.9065	295.6658	302.0325
Frequencies --	304.5233	306.1641	306.4675
Frequencies --	312.2095	317.2351	320.2713
Frequencies --	328.6467	333.1613	352.6065
Frequencies --	363.7001	370.8531	375.0488
Frequencies --	381.6408	387.3188	403.8894
Frequencies --	409.7785	411.3357	416.0613
Frequencies --	422.7621	425.1561	431.6855
Frequencies --	433.9592	441.3688	450.8729
Frequencies --	454.6652	464.9653	485.0145
Frequencies --	506.3181	516.1256	530.2052
Frequencies --	534.6586	539.9229	542.9174
Frequencies --	551.4392	552.8562	570.3048
Frequencies --	571.9789	586.2037	590.7408
Frequencies --	592.6883	605.4535	611.1180
Frequencies --	628.7684	632.9556	637.2710
Frequencies --	642.0540	644.6784	650.0555
Frequencies --	673.2721	690.0620	693.0097
Frequencies --	702.4416	715.1196	717.1095
Frequencies --	719.8294	737.6631	750.3073
Frequencies --	782.0173	792.2522	798.8102
Frequencies --	807.3869	810.5155	827.6894
Frequencies --	835.4158	890.0896	897.8637
Frequencies --	907.5027	916.8935	922.0318
Frequencies --	949.3123	961.8240	963.4506
Frequencies --	972.8931	985.4062	990.5896
Frequencies --	996.6797	1013.8037	1036.1222
Frequencies --	1039.2080	1040.8839	1041.1357
Frequencies --	1043.7824	1046.9778	1049.7659
Frequencies --	1057.3801	1059.0099	1085.1341
Frequencies --	1085.4486	1086.9521	1113.8476
Frequencies --	1123.2893	1169.4410	1171.7333
Frequencies --	1175.3355	1175.9235	1187.2049
Frequencies --	1202.6609	1214.0444	1221.9998
Frequencies --	1244.8457	1250.5252	1306.3006
Frequencies --	1310.8204	1327.0557	1336.4032
Frequencies --	1342.3470	1356.4473	1359.5768
Frequencies --	1366.9873	1379.1121	1411.4723

Frequencies --	1414.0328	1414.1990	1421.9012
Frequencies --	1423.1447	1423.9448	1426.8348
Frequencies --	1430.1007	1432.2832	1433.4735
Frequencies --	1438.4711	1448.1824	1450.4744
Frequencies --	1453.7112	1457.4792	1463.8636
Frequencies --	1471.2564	1472.9565	1482.5812
Frequencies --	1492.0823	1493.3053	1494.5372
Frequencies --	1494.7083	1497.9287	1501.5701
Frequencies --	1502.2055	1505.7638	1507.5458
Frequencies --	1509.1235	1517.1794	1520.5938
Frequencies --	1574.2055	1585.6928	1596.4963
Frequencies --	1597.4814	1598.0264	1615.7673
Frequencies --	1620.1375	1622.1574	3010.1601
Frequencies --	3010.8062	3011.0425	3013.2058
Frequencies --	3016.1062	3017.1600	3038.4266
Frequencies --	3100.8938	3102.0361	3102.4350
Frequencies --	3105.2104	3109.2533	3121.1977
Frequencies --	3138.4273	3147.3780	3151.4700
Frequencies --	3155.9467	3159.3966	3162.8621
Frequencies --	3172.7928	3203.0830	3207.7598
Frequencies --	3208.6027	3220.9885	3233.0261

Catalyst 6:

vacuum	toluene-like solvent	D3 dispersion
-3056.7016427	-3056.7124197	-0.56622308

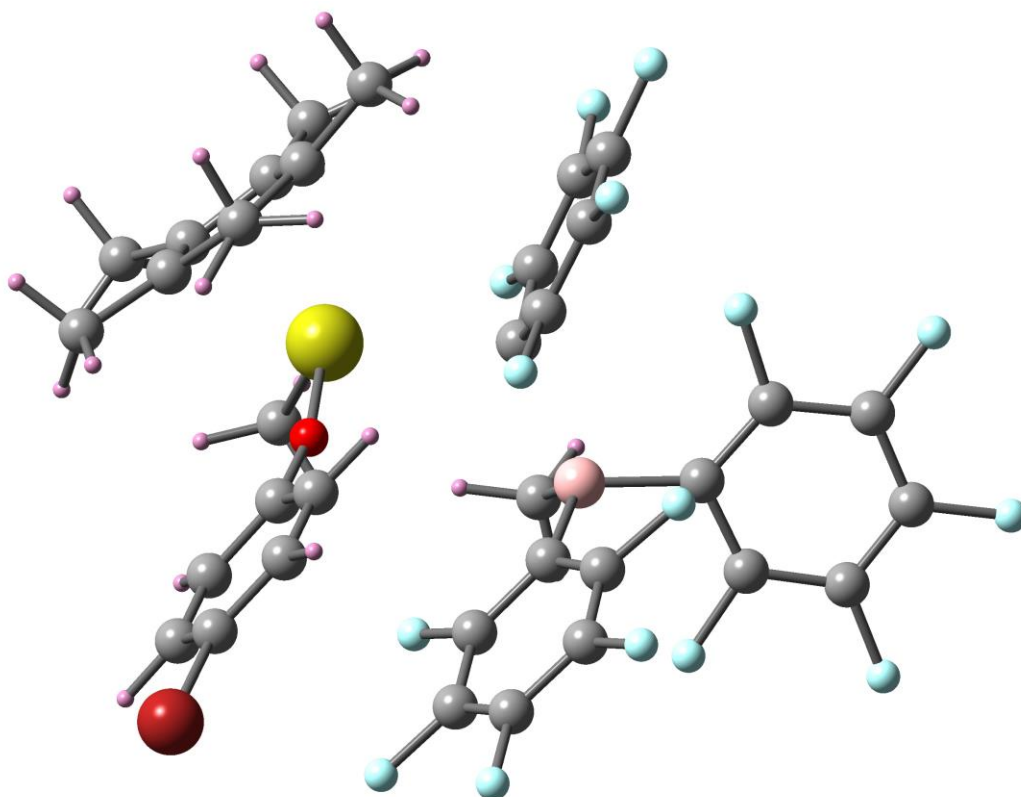
Imaginary frequency corresponding to vibration along the reaction coordinate: -228 cm^{-1} .

Ti	1.74760100	-1.62929600	-0.75294100
C	1.74662600	-1.30122500	-2.79759200
H	1.25312700	-0.32182800	-2.86449100
H	2.72181500	-1.24007400	-3.29568700
H	1.13258200	-2.07530100	-3.28640600
O	2.41937800	-0.05660600	-0.26898200
C	3.19554100	1.01569600	0.13566900
C	3.18064200	1.43165900	1.48968900
C	3.97739400	1.70755500	-0.82181800
C	3.96438900	2.53170700	1.88818700
C	4.76135000	2.80596800	-0.42081300
C	4.75238800	3.20551400	0.93177500
H	3.95134300	2.86366300	2.92597100
H	5.35573200	3.34959900	-1.15463000
C	2.15235700	-3.75583000	0.51238600
C	2.03683000	-4.13241500	-0.87795100
C	3.27288400	-2.85115000	0.64513700
C	3.11660200	-3.50050200	-1.60003500
C	3.87547100	-2.69771300	-0.66112000
F	-7.50800200	1.49597700	-0.01857800
C	-6.16200600	1.21624100	-0.20212500
C	-5.56368800	0.11602300	0.42867600
C	-5.36411300	2.02964200	-1.02378300

C	-4.19346200	-0.14738800	0.22336400
F	-6.32149200	-0.70376300	1.25743500
C	-4.00278500	1.71780600	-1.19393500
F	-5.92419800	3.13155600	-1.65887500
C	-3.33575300	0.61709700	-0.59027500
F	-3.70466600	-1.25403100	0.93047000
F	-3.29221000	2.59841600	-2.02550000
B	-1.74092200	0.41187300	-1.05135500
C	-0.78472100	-1.26511400	-0.03090000
C	-1.37755300	-2.51077600	-0.37554400
C	-0.63070700	-1.11503200	1.37584000
C	-1.86819100	-3.45562500	0.54101700
F	-1.50094900	-2.86919300	-1.72906200
C	-1.10973500	-2.01233200	2.34463100
F	0.07494200	-0.01134100	1.88169000
C	-1.75252900	-3.18831400	1.91654100
F	-2.43504100	-4.65649900	0.12350200
F	-0.92311900	-1.79235500	3.70524400
F	-2.20571500	-4.10766800	2.84265300
C	-0.88565900	1.72976800	-0.59130000
C	0.02977600	2.41077900	-1.42698200
C	-1.13015200	2.40628500	0.63162400
C	0.64806700	3.63327200	-1.10303700
C	-0.52870200	3.62096800	1.00772900
C	0.36984600	4.24696600	0.12783900
F	-2.02256400	1.86723200	1.56418500
F	-0.81130500	4.20655100	2.23640700
F	0.98420800	5.43962600	0.47678600
F	1.54083200	4.23180600	-1.98663700
F	0.38541200	1.88818700	-2.67771800
C	-1.76930300	-0.04198000	-2.60029200
H	-0.82077900	-0.39540700	-3.00501800
H	-2.51863000	-0.82897000	-2.76175800
H	-2.07460100	0.82323000	-3.20950100
C	1.45734000	-4.41968400	1.67833000
H	2.11520300	-5.21892600	2.06299700
H	1.26986200	-3.73909000	2.51794800
H	0.51393400	-4.89887800	1.39949200
C	1.09215700	-5.15818300	-1.46359600
H	1.61628100	-6.12256900	-1.58369900
H	0.21850500	-5.34078200	-0.82869600
H	0.72207700	-4.86876700	-2.45703800
C	3.82128400	-2.33790300	1.95676800
H	4.44538800	-1.44586700	1.82980500
H	3.02688100	-2.09049700	2.67532800
H	4.45082800	-3.11366800	2.42683100
C	3.53487000	-3.85264200	-3.00656100
H	4.10310000	-4.79926700	-2.98773700
H	2.67866900	-4.00345800	-3.67711400
H	4.18682600	-3.09364100	-3.45676300
C	5.17444500	-1.98946300	-0.96774700
H	5.39964100	-1.19543400	-0.24641900
H	6.00837700	-2.71199800	-0.92993600
H	5.18136600	-1.54149600	-1.97096100
H	2.55197400	0.91487500	2.21191000
H	3.95792200	1.40024100	-1.86661000
C1	5.77779600	4.61728100	1.45463000

Frequencies --	-228.4720	12.2669	16.6598
Frequencies --	18.1886	22.8003	29.6019
Frequencies --	32.3432	35.3161	39.5712
Frequencies --	45.0674	48.1604	53.3373
Frequencies --	55.6884	56.3282	62.3235
Frequencies --	74.7910	85.1613	90.4634
Frequencies --	93.8016	97.9988	99.1486
Frequencies --	108.0065	110.8850	114.1552
Frequencies --	116.1284	122.0906	125.7586
Frequencies --	127.9419	133.5266	136.5828
Frequencies --	142.0555	144.0055	149.2758
Frequencies --	157.2682	163.8679	165.3522
Frequencies --	172.3122	179.9317	187.5179
Frequencies --	190.2476	200.6906	203.4717
Frequencies --	219.2655	224.4727	228.5741
Frequencies --	235.9179	245.1164	263.7895
Frequencies --	264.6601	265.8110	266.9604
Frequencies --	269.5669	272.8192	274.1007
Frequencies --	275.8944	278.1447	279.4222
Frequencies --	285.8973	289.6852	293.3713
Frequencies --	296.8726	301.9956	302.8843
Frequencies --	304.1643	308.0080	315.8146
Frequencies --	319.5244	328.9544	331.7882
Frequencies --	333.6999	364.9481	371.5002
Frequencies --	374.9790	380.8230	385.5470
Frequencies --	399.7256	409.4581	410.5054
Frequencies --	422.7217	424.7479	431.3763
Frequencies --	434.0684	441.9094	450.5864
Frequencies --	454.8765	457.3576	468.6313
Frequencies --	485.0551	491.5896	504.3027
Frequencies --	528.6525	535.1868	539.5004
Frequencies --	542.8625	551.4024	552.3209
Frequencies --	572.2480	585.2708	588.5855
Frequencies --	591.7586	602.8641	607.7054
Frequencies --	628.6417	628.7690	637.7707
Frequencies --	641.4602	644.5851	645.1084
Frequencies --	647.4416	673.8677	676.7807
Frequencies --	692.2466	708.7856	714.2455
Frequencies --	716.7616	719.9326	737.8768
Frequencies --	750.4050	782.0159	784.9636
Frequencies --	788.7731	799.7425	806.8990
Frequencies --	828.3674	890.2329	898.2793
Frequencies --	907.7023	917.8303	919.4854
Frequencies --	938.7497	953.4261	963.8520
Frequencies --	970.9643	986.1615	990.9469
Frequencies --	996.7426	1012.8467	1036.0615
Frequencies --	1036.9885	1039.8054	1041.2636
Frequencies --	1043.8881	1045.7762	1047.4286
Frequencies --	1057.2465	1059.0856	1075.8830
Frequencies --	1084.7172	1086.3111	1087.5129
Frequencies --	1117.2245	1124.4379	1171.7791
Frequencies --	1175.1971	1175.8847	1184.8003
Frequencies --	1190.9229	1214.0228	1222.0425
Frequencies --	1242.1994	1247.7940	1310.1919
Frequencies --	1310.7022	1326.3818	1335.1014
Frequencies --	1341.8716	1352.7986	1356.8445
Frequencies --	1369.6271	1379.4816	1411.8242
Frequencies --	1414.3760	1414.7889	1415.0285
Frequencies --	1421.4531	1422.9206	1426.1830
Frequencies --	1427.8114	1430.3789	1432.0454
Frequencies --	1435.6545	1447.7856	1450.4008
Frequencies --	1454.7744	1455.9255	1461.6011

Frequencies --	1471.0292	1473.1353	1481.0217
Frequencies --	1484.6372	1489.4872	1492.0248
Frequencies --	1492.5312	1497.0997	1498.9130
Frequencies --	1502.5513	1505.0253	1505.5041
Frequencies --	1506.8026	1514.8474	1517.1636
Frequencies --	1574.0282	1580.5371	1585.5361
Frequencies --	1596.2330	1597.1860	1602.8070
Frequencies --	1620.0868	1622.3365	3008.9289
Frequencies --	3009.6616	3011.3623	3012.0820
Frequencies --	3013.2907	3016.2234	3039.2867
Frequencies --	3096.9984	3101.3036	3102.8866
Frequencies --	3104.4601	3112.2422	3121.7151
Frequencies --	3138.1565	3146.6954	3149.4227
Frequencies --	3156.1839	3160.3028	3161.7782
Frequencies --	3173.2675	3199.2037	3203.4948
Frequencies --	3206.8454	3218.0024	3230.2420

Catalyst 7:

vacuum	toluene-like solvent	D3 dispersion
-3054.9057635	-3054.916401	-0.56778672

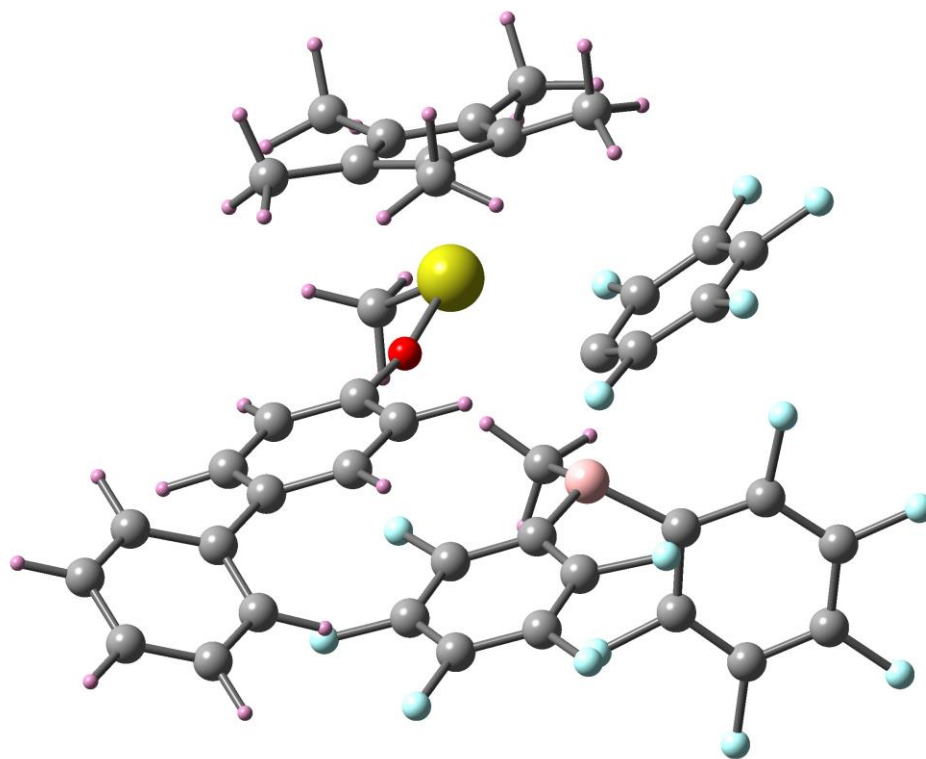
Imaginary frequency corresponding to vibration along the reaction coordinate: -220 cm^{-1} .

Ti	-0.82072300	2.22434100	-0.77811400
C	-0.84684900	1.97377200	-2.83494300
H	-0.70739500	0.88830300	-2.93334000
H	-1.76086900	2.26200800	-3.36784300
H	0.01364500	2.51209900	-3.26590200
O	-1.97192000	0.93022800	-0.38167000
C	-3.06627100	0.14767500	-0.05790600
C	-3.24925100	-0.30657700	1.27087200
C	-3.98498000	-0.21944300	-1.07123300
C	-4.35952700	-1.11321500	1.58827800
C	-5.09544000	-1.02487100	-0.75400100
C	-5.27974300	-1.46060500	0.57581900
H	-4.49455700	-1.46846100	2.60983900
H	-5.79554100	-1.31416900	-1.53755900
C	-0.58228200	4.33022600	0.56153200
C	-0.30400000	4.69282400	-0.80928200
C	-1.93484300	3.82175600	0.62954200
C	-1.50092000	4.45628100	-1.58257500
C	-2.50773600	3.90705000	-0.69601600
F	6.93725600	-3.67733700	0.09283500
C	5.75541200	-2.98214700	-0.11594300
C	5.51447700	-1.76218500	0.53205800

C	4.76926000	-3.48447200	-0.98116000
C	4.30517200	-1.07485200	0.29981700
F	6.46443900	-1.24091200	1.40327500
C	3.58252400	-2.75451500	-1.17673400
F	4.97403500	-4.69407800	-1.63411200
C	3.27737100	-1.51169300	-0.55744400
F	4.16703200	0.11498100	1.02711700
F	2.65856200	-3.34882100	-2.05135500
B	1.84472600	-0.80171800	-1.05171200
C	1.43833000	1.06804400	-0.01364200
C	2.40459500	2.06845200	-0.31146500
C	1.20108100	0.95220400	1.38520900
C	3.14217000	2.79167800	0.64057900
F	2.67367300	2.39590600	-1.65140900
C	1.91262300	1.63133300	2.38794900
F	0.16131100	0.12816800	1.84565000
C	2.90793800	2.54899200	2.00549900
F	4.07168500	3.75843300	0.26804400
F	1.62503100	1.45837300	3.73754700
F	3.60293600	3.25890200	2.96527100
C	0.60366800	-1.79138500	-0.65068100
C	-0.44706200	-2.13934600	-1.53094500
C	0.58082200	-2.52930600	0.56078900
C	-1.42555000	-3.11427400	-1.25859200
C	-0.38211700	-3.50154300	0.88665300
C	-1.39708300	-3.80343000	-0.03650900
F	1.56291800	-2.31083800	1.53289000
F	-0.34169800	-4.16430800	2.10805600
F	-2.36323600	-4.75167900	0.26215300
F	-2.42579300	-3.39248700	-2.18476100
F	-0.57681600	-1.51170700	-2.77719300
C	2.06712700	-0.35665100	-2.58779700
H	1.28932700	0.27827900	-3.01250800
H	3.02883000	0.16071200	-2.70794100
H	2.11114100	-1.26529100	-3.20845500
C	0.24054900	4.70986300	1.77084300
H	-0.14781600	5.66537200	2.16571000
H	0.17173900	3.98349900	2.59001800
H	1.29701300	4.87473000	1.53758900
C	0.93484800	5.38427700	-1.33354000
H	0.73811800	6.46431600	-1.45064300
H	1.79396800	5.28213500	-0.66177100
H	1.24042800	5.00546100	-2.31906400
C	-2.66415000	3.46988100	1.90598700
H	-2.02305900	2.93835200	2.62382000
H	-3.00966900	4.39247100	2.40429600
H	-3.54884900	2.84826300	1.72542700
C	-1.73582100	4.96450900	-2.98396500
H	-1.97670300	6.04128000	-2.94175800
H	-0.85305700	4.85543300	-3.62762100
H	-2.57764700	4.46418100	-3.47875200
C	-3.95176500	3.65583400	-1.06247700
H	-4.44065500	2.94972100	-0.38146700
H	-4.51695100	4.60294500	-1.01278700
H	-4.06343200	3.26624200	-2.08348500
H	-2.52333300	-0.04733800	2.03918400
H	-3.82319700	0.10802800	-2.09754400

Br	-6.83060900	-2.57672800	1.02170000
Frequencies --	-219.6126	12.5360	15.1006
Frequencies --	16.9388	20.1377	30.5524
Frequencies --	33.5704	36.0661	40.0694
Frequencies --	45.4829	47.4569	51.7297
Frequencies --	54.5754	56.9030	63.6624
Frequencies --	73.0155	90.8712	92.7902
Frequencies --	94.6243	96.6639	100.1467
Frequencies --	111.1314	113.6529	117.0482
Frequencies --	121.3383	124.1271	126.8069
Frequencies --	130.4067	134.6059	136.4612
Frequencies --	143.4107	144.9019	150.0386
Frequencies --	157.1734	163.8993	165.1636
Frequencies --	171.8970	174.7125	179.7268
Frequencies --	192.4643	201.7190	203.7498
Frequencies --	215.6460	222.9071	232.4247
Frequencies --	236.1054	241.2924	247.4781
Frequencies --	263.7952	264.4330	265.7888
Frequencies --	267.6956	268.2419	273.2260
Frequencies --	274.9075	276.8666	278.2140
Frequencies --	283.1487	288.2582	294.7019
Frequencies --	297.7702	301.6056	302.2895
Frequencies --	305.2338	308.3489	317.3104
Frequencies --	319.5437	329.9726	334.2690
Frequencies --	341.7532	371.6697	373.6475
Frequencies --	375.2966	381.5956	385.1461
Frequencies --	399.5332	408.5377	412.2059
Frequencies --	422.7422	424.9764	431.7799
Frequencies --	433.1830	434.4061	442.5132
Frequencies --	450.9303	455.3462	458.0721
Frequencies --	485.6513	507.2598	512.1845
Frequencies --	529.3373	534.9265	540.5298
Frequencies --	542.7546	551.8328	553.4463
Frequencies --	573.4800	585.2551	592.8732
Frequencies --	594.4851	604.4337	617.1305
Frequencies --	628.3554	629.0769	638.2183
Frequencies --	641.8530	645.3392	648.1988
Frequencies --	674.2452	679.8545	692.8952
Frequencies --	697.2334	710.9434	714.4460
Frequencies --	716.8081	720.1774	737.4964
Frequencies --	750.9208	782.3527	800.6679
Frequencies --	806.8859	822.3743	830.6910
Frequencies --	835.0818	890.3569	898.9308
Frequencies --	907.6242	918.8999	923.1553
Frequencies --	957.7772	965.1167	970.8465
Frequencies --	972.2584	987.0541	992.2456
Frequencies --	996.5568	1016.2878	1036.3795
Frequencies --	1038.2838	1040.6096	1041.1851
Frequencies --	1043.8407	1046.3913	1048.0998
Frequencies --	1057.1992	1058.9303	1064.9060
Frequencies --	1084.8709	1086.0301	1087.7403
Frequencies --	1116.0697	1123.9824	1171.9831
Frequencies --	1175.4580	1176.1288	1190.0948
Frequencies --	1193.3865	1213.8498	1222.1383
Frequencies --	1243.2468	1248.4505	1308.5089
Frequencies --	1310.7892	1326.4376	1334.2157
Frequencies --	1341.9068	1348.8969	1356.7093
Frequencies --	1371.8343	1380.3921	1407.8953
Frequencies --	1411.4443	1414.5624	1415.8347
Frequencies --	1421.6293	1423.6752	1426.7972
Frequencies --	1428.7201	1430.9446	1431.9197
Frequencies --	1436.4299	1448.5153	1450.5628

Frequencies --	1456.0670	1456.4460	1462.3435
Frequencies --	1470.6170	1473.1179	1479.8938
Frequencies --	1481.0290	1490.8778	1491.8590
Frequencies --	1493.5148	1497.3813	1500.5531
Frequencies --	1502.3931	1504.8226	1505.1533
Frequencies --	1507.0160	1515.4003	1518.4550
Frequencies --	1574.1390	1576.4956	1585.8925
Frequencies --	1596.4255	1596.7277	1597.2536
Frequencies --	1619.3761	1622.7095	3008.8792
Frequencies --	3009.4047	3011.9259	3012.2522
Frequencies --	3013.5748	3015.1666	3039.1465
Frequencies --	3095.8279	3102.0974	3102.9583
Frequencies --	3105.2717	3110.0596	3121.5177
Frequencies --	3137.8675	3147.5992	3149.6357
Frequencies --	3155.9016	3160.3506	3160.6978
Frequencies --	3170.7997	3195.7765	3199.7157
Frequencies --	3204.0985	3214.1551	3226.0303

Catalyst 8:

vacuum	toluene-like solvent	D3 dispersion
-3273.2985885	-3273.3102219	-0.63421510

Imaginary frequency corresponding to vibration along the reaction coordinate: -224 cm^{-1} .

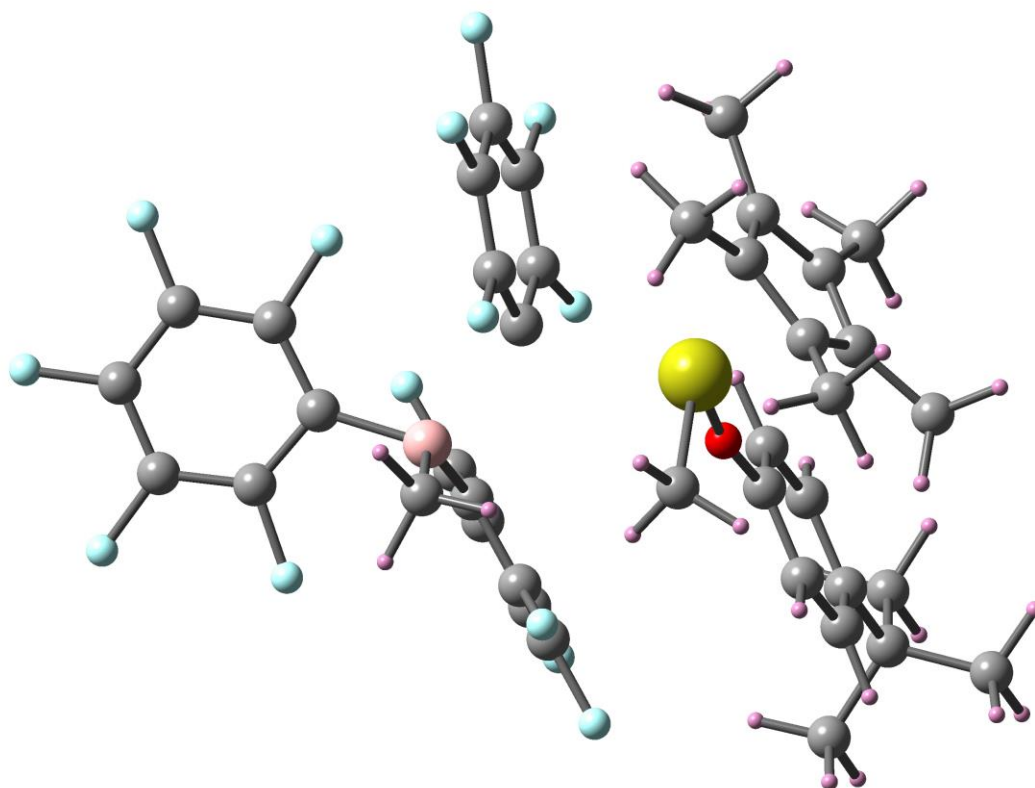
Ti	-0.21542400	2.44727700	-0.74967900
C	-0.23485300	2.27237200	-2.81705900
H	-0.27536400	1.18280500	-2.95490700
H	-1.08540200	2.72416800	-3.34239800
H	0.70528200	2.67662200	-3.22669300
O	-1.58712400	1.37277000	-0.42808600
C	-2.80944900	0.77943400	-0.15343700
C	-3.07114700	0.24655900	1.13156700
C	-3.78297200	0.67363500	-1.17593700
C	-4.30096300	-0.38680200	1.38205400
C	-5.00952900	0.04259600	-0.90659400
C	-5.29876900	-0.50433900	0.37450400
H	-4.49302000	-0.78086700	2.38092200
H	-5.73244400	-0.06545300	-1.71610600
C	0.30315000	4.40931900	0.70734800
C	0.74904700	4.77438700	-0.61859200
C	-1.12253000	4.17043300	0.65508500
C	-0.40733400	4.80215400	-1.48328100
C	-1.56455700	4.41945600	-0.69942000
F	6.30985000	-4.83040000	0.04837700
C	5.28492300	-3.91797400	-0.15441400
C	5.27296300	-2.68846600	0.51986900

C	4.23259200	-4.20418700	-1.03983900
C	4.21945000	-1.77814200	0.29503600
F	6.29420500	-2.37752800	1.41079500
C	3.20909100	-3.25731100	-1.22721500
F	4.21118800	-5.41641500	-1.71943400
C	3.13722500	-1.99406800	-0.57927900
F	4.30261000	-0.59832700	1.04602300
F	2.20261500	-3.64292400	-2.12764900
B	1.86967200	-1.01673300	-1.06572500
C	1.78739200	0.87713400	0.03329400
C	2.92784300	1.68883200	-0.21360700
C	1.50620900	0.75643500	1.42264700
C	3.76547000	2.23289300	0.77450100
F	3.28164000	2.00271800	-1.53736800
C	2.31164800	1.25396900	2.46005200
F	0.32096000	0.12639600	1.83588100
C	3.46416200	1.98858400	2.12602300
F	4.86467200	3.02335700	0.45108500
F	1.97312800	1.08521800	3.79852100
F	4.25853800	2.52400500	3.12202000
C	0.46130600	-1.76869300	-0.70583500
C	-0.62097300	-1.89641000	-1.60746600
C	0.28388900	-2.51580400	0.48704000
C	-1.76591500	-2.68122600	-1.37130500
C	-0.84824200	-3.29735000	0.77874000
C	-1.88514300	-3.38654100	-0.16421100
F	1.27374800	-2.50358300	1.47573000
F	-0.95502700	-3.97815100	1.98692100
F	-3.01843200	-4.14113900	0.10455700
F	-2.78301400	-2.75479100	-2.31693300
F	-0.60968200	-1.22873500	-2.83859600
C	2.19671200	-0.56708900	-2.58019500
H	1.55936100	0.21865100	-2.98595200
H	3.24031000	-0.23567000	-2.67045200
H	2.07840100	-1.44526200	-3.23446300
C	1.09104100	4.54846000	1.98929600
H	0.86701100	5.53547600	2.43084900
H	0.82440200	3.79942100	2.74555200
H	2.17347800	4.51348800	1.83307700
C	2.12754000	5.25083200	-1.02131000
H	2.10877600	6.34143700	-1.18969000
H	2.88366800	5.05490200	-0.25355400
H	2.47820700	4.78931100	-1.95553100
C	-2.00558700	3.90969700	1.85373700
H	-2.94658600	3.41727500	1.58201000
H	-1.51071500	3.28521400	2.61064300
H	-2.26413200	4.86587800	2.34171600
C	-0.42892200	5.39629900	-2.87023800
H	-0.48431200	6.49650200	-2.79195600
H	0.47588900	5.15826600	-3.44514500
H	-1.29637200	5.06955600	-3.45696500
C	-2.99801500	4.46982300	-1.17462600
H	-3.66287200	3.83937200	-0.57278000
H	-3.37469100	5.50524500	-1.10200600
H	-3.10430900	4.16190000	-2.22398400
H	-2.31602900	0.31933200	1.91212400
H	-3.56436900	1.05364100	-2.17355900

C	-6.59594000	-1.19467000	0.64648000
C	-6.64327700	-2.37515500	1.43815400
C	-7.81813400	-0.69754900	0.11610600
C	-7.86498600	-3.03151500	1.69079100
H	-5.71812700	-2.80405700	1.82687300
C	-9.04104200	-1.35132200	0.37029500
H	-7.81765200	0.22014400	-0.47538500
C	-9.07088200	-2.52247400	1.15957300
H	-7.87296200	-3.94464300	2.29043500
H	-9.96795600	-0.94429000	-0.04072600
H	-10.01743000	-3.03153900	1.35498100

Frequencies --	-223.9969	11.8255	13.1201
Frequencies --	16.1785	21.7740	27.5120
Frequencies --	31.5479	33.5658	35.1524
Frequencies --	40.9250	41.4340	48.6493
Frequencies --	53.2484	54.5497	60.9382
Frequencies --	68.1621	70.7782	77.2432
Frequencies --	88.5249	90.3576	95.0956
Frequencies --	102.0133	105.3847	111.3214
Frequencies --	113.6520	114.2023	118.9638
Frequencies --	121.3450	125.2920	128.0433
Frequencies --	131.1615	137.2548	145.7116
Frequencies --	146.3560	149.7410	157.3389
Frequencies --	163.9659	165.1901	167.6870
Frequencies --	173.8874	187.1873	188.2510
Frequencies --	199.7531	202.9015	211.1775
Frequencies --	218.7036	223.5677	236.6830
Frequencies --	238.1414	249.0752	264.0207
Frequencies --	265.4271	267.1481	267.4527
Frequencies --	270.9930	275.1722	277.5583
Frequencies --	279.7999	280.3092	285.2980
Frequencies --	291.3066	291.7913	296.6860
Frequencies --	301.2790	302.4512	304.3329
Frequencies --	307.1278	316.9749	319.0076
Frequencies --	329.0217	333.0323	334.9058
Frequencies --	352.2428	370.6155	375.6414
Frequencies --	381.9714	383.5375	394.8698
Frequencies --	406.1402	409.0611	415.3231
Frequencies --	422.8784	423.6757	425.1577
Frequencies --	431.5723	434.1615	434.4270
Frequencies --	442.6898	450.8947	455.0714
Frequencies --	463.3376	485.6664	502.7081
Frequencies --	515.1305	529.5282	535.5152
Frequencies --	539.5570	542.8930	551.2813
Frequencies --	552.4833	557.3277	572.7030
Frequencies --	584.6956	590.9715	591.5963
Frequencies --	600.9259	606.2317	621.7897
Frequencies --	629.2212	637.2843	637.8162
Frequencies --	639.8597	641.9915	644.4668
Frequencies --	649.1177	673.3852	687.1235
Frequencies --	692.6271	706.8699	715.1331
Frequencies --	717.3468	720.3951	722.8887
Frequencies --	737.9069	748.7971	750.6983
Frequencies --	773.6894	782.3620	799.4997
Frequencies --	806.9280	828.2427	837.1484
Frequencies --	852.7787	858.7602	890.1245
Frequencies --	898.8919	907.7908	920.0101
Frequencies --	926.2595	932.3684	964.1712
Frequencies --	966.4192	970.5428	978.9442
Frequencies --	985.7075	986.0876	990.6317

Frequencies --	996.7271	999.7778	1005.8841
Frequencies --	1022.8817	1035.8370	1038.8579
Frequencies --	1040.3987	1041.1978	1045.1293
Frequencies --	1046.5523	1048.1851	1049.6766
Frequencies --	1057.6900	1059.1926	1059.7579
Frequencies --	1084.5180	1086.2842	1086.4344
Frequencies --	1094.8433	1123.6332	1130.5070
Frequencies --	1171.8799	1174.9407	1175.6159
Frequencies --	1183.4476	1184.1107	1199.3812
Frequencies --	1210.2990	1213.7957	1221.7439
Frequencies --	1243.1324	1247.6379	1301.0760
Frequencies --	1310.7812	1315.4364	1326.5740
Frequencies --	1327.5188	1335.9163	1342.6515
Frequencies --	1356.4560	1357.0751	1369.9438
Frequencies --	1374.4682	1379.1728	1411.6843
Frequencies --	1414.0117	1414.8341	1422.0029
Frequencies --	1423.4741	1424.7201	1426.1794
Frequencies --	1428.2249	1430.2427	1432.3151
Frequencies --	1435.5507	1447.9282	1450.2088
Frequencies --	1451.0763	1451.3846	1455.8836
Frequencies --	1462.0781	1470.5802	1472.9742
Frequencies --	1480.9490	1488.5800	1491.6019
Frequencies --	1492.8208	1495.3555	1497.7864
Frequencies --	1501.3753	1502.8955	1505.3658
Frequencies --	1505.6864	1507.9267	1515.2592
Frequencies --	1516.6772	1519.7791	1569.9169
Frequencies --	1574.2442	1586.0085	1597.0112
Frequencies --	1598.2407	1598.6229	1618.1963
Frequencies --	1619.7125	1622.4263	1624.4538
Frequencies --	3008.6593	3009.4840	3010.5201
Frequencies --	3011.8678	3015.0865	3016.0315
Frequencies --	3037.9080	3100.4449	3101.4523
Frequencies --	3101.5147	3103.6983	3110.3865
Frequencies --	3120.3734	3137.3743	3147.0796
Frequencies --	3149.8719	3154.7045	3154.9161
Frequencies --	3157.0804	3161.9634	3162.7307
Frequencies --	3172.1466	3174.1694	3180.2836
Frequencies --	3183.7338	3185.2893	3195.8448
Frequencies --	3206.3646	3211.0048	3223.0959

Catalyst 9:

vacuum	toluene-like solvent	D3 dispersion
-3199.5049347	-3199.5141791	-0.63045252

Imaginary frequency corresponding to vibration along the reaction coordinate: -223 cm^{-1} .

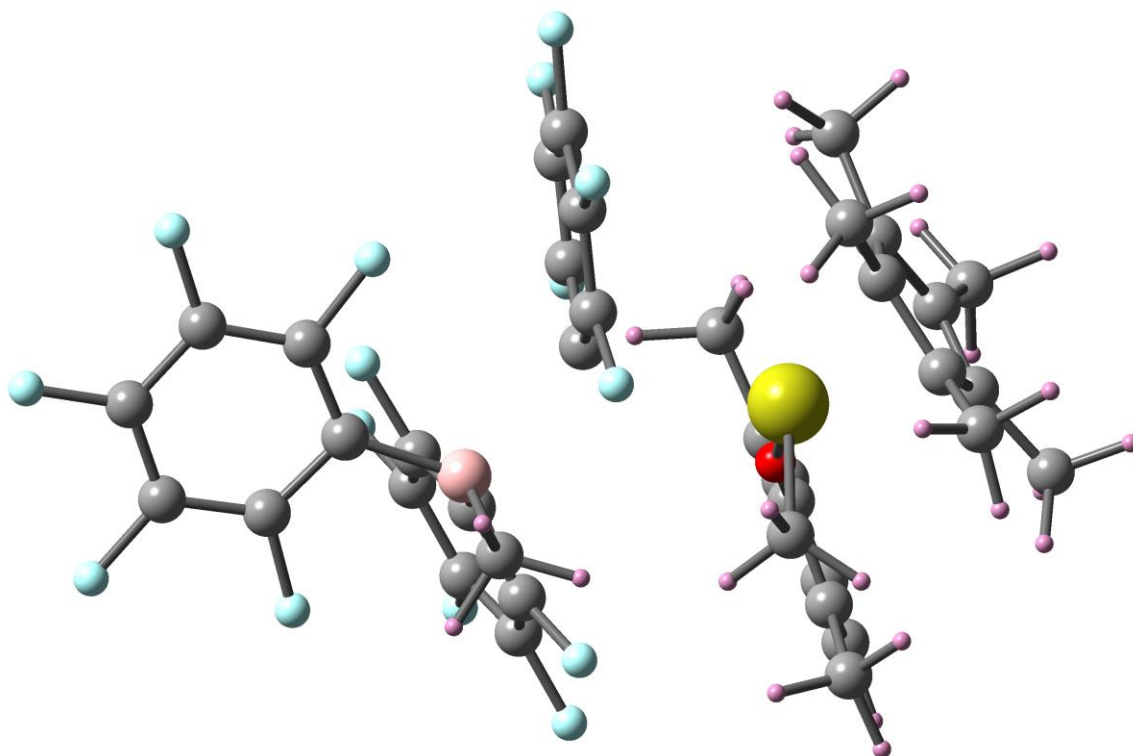
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C	-0.89866900	1.97757000	-2.82113900
H	-0.77296600	0.89041800	-2.91990500
H	-1.81194600	2.27529400	-3.35025300
H	-0.03412100	2.50560900	-3.25707400
O	-2.00634500	0.95327800	-0.35354000
C	-3.09622000	0.16029900	-0.02222600
C	-3.27494600	-0.29736300	1.30150500
C	-4.01597500	-0.22015000	-1.02821400
C	-4.37037400	-1.12980200	1.60918400
C	-5.10093300	-1.04922800	-0.69837700
C	-5.31187200	-1.53047200	0.62509900
H	-4.46945100	-1.47287300	2.63727400
H	-5.78340500	-1.33615200	-1.49849000
C	-0.60295600	4.34962700	0.56768300
C	-0.33214400	4.70980100	-0.80498800
C	-1.95685600	3.84610000	0.64505700
C	-1.53398100	4.47484000	-1.57056000
C	-2.53729300	3.93018000	-0.67714200
F	6.90179200	-3.69556900	0.05785500
C	5.71961800	-2.99858600	-0.14438900
C	5.48782800	-1.77396300	0.49820900

C	4.72444600	-3.50380400	-0.99746000
C	4.27819000	-1.08462000	0.27322000
F	6.44759100	-1.25005000	1.35714200
C	3.53785000	-2.77193700	-1.18640700
F	4.92040500	-4.71798400	-1.64509100
C	3.24162400	-1.52483400	-0.57173500
F	4.15007800	0.11000300	0.99348500
F	2.60433100	-3.36819200	-2.04968900
B	1.80739800	-0.81523400	-1.05752900
C	1.40971600	1.07874200	-0.01540500
C	2.37647600	2.07256900	-0.32911700
C	1.19091800	0.96616000	1.38594200
C	3.12903300	2.79630200	0.61083800
F	2.63002200	2.39443000	-1.67416800
C	1.91775000	1.64603400	2.37746500
F	0.15553000	0.14557400	1.86189500
C	2.91076600	2.55934600	1.97941400
F	4.05832100	3.75820800	0.22354500
F	1.64825900	1.47738500	3.73183500
F	3.62086600	3.27007200	2.92836900
C	0.56515700	-1.79400500	-0.63852100
C	-0.49231500	-2.14551100	-1.50969900
C	0.54740700	-2.52000800	0.58019100
C	-1.47209300	-3.11485300	-1.22224500
C	-0.41934500	-3.48264100	0.92258300
C	-1.43978700	-3.78892200	0.00759400
F	1.53918800	-2.29983100	1.54176400
F	-0.37707500	-4.13250400	2.15124700
F	-2.41094800	-4.72961800	0.32305600
F	-2.47610800	-3.40423100	-2.14086800
F	-0.62496900	-1.53114000	-2.76136300
C	2.01473900	-0.36896000	-2.59381400
H	1.22960800	0.26263500	-3.00988000
H	2.97323700	0.15214900	-2.72265500
H	2.05637800	-1.27766600	-3.21497200
C	0.23048400	4.72417200	1.77155700
H	-0.15689300	5.67519000	2.17799200
H	0.17288600	3.99109400	2.58570100
H	1.28406400	4.89404500	1.52844700
C	0.90588700	5.39602400	-1.33838900
H	0.71351900	6.47694800	-1.45520700
H	1.76917300	5.29039100	-0.67237800
H	1.20309400	5.01470200	-2.32556300
C	-2.67990000	3.49683900	1.92585400
H	-3.55530100	2.86022200	1.75272400
H	-2.03002900	2.98074700	2.64699900
H	-3.03730800	4.41957500	2.41597800
C	-1.77397100	4.97845600	-2.97290000
H	-1.99339900	6.06004500	-2.93625500
H	-0.90044500	4.84748700	-3.62524200
H	-2.63052000	4.49074400	-3.45488300
C	-3.98376500	3.67837700	-1.03408200
H	-4.46540200	2.96817300	-0.35209700
H	-4.55055200	4.62426300	-0.97783000
H	-4.10155400	3.29040300	-2.05499900
H	-2.55459800	-0.02410100	2.07102900
H	-3.86642400	0.11546900	-2.05429300

C	-6.50869000	-2.47422600	0.92940300
C	-6.34724600	-3.79072000	0.09835600
H	-7.18266300	-4.47666900	0.31068900
H	-6.34002400	-3.59657100	-0.98393700
H	-5.40780500	-4.30454800	0.35198500
C	-6.59386900	-2.86320200	2.43453300
H	-6.72489200	-1.98151200	3.08136300
H	-7.46073000	-3.52201900	2.59481000
H	-5.69987200	-3.41130900	2.76867000
C	-7.84916700	-1.76988900	0.53781900
H	-7.99167300	-0.84372700	1.11679300
H	-7.88357200	-1.50996200	-0.53002400
H	-8.70145800	-2.43622300	0.74499700

Frequencies --	-222.9409	13.8786	16.4921
Frequencies --	17.5608	24.3742	28.4481
Frequencies --	30.6435	35.9593	37.9025
Frequencies --	44.5009	47.3333	50.3960
Frequencies --	54.6676	56.2637	61.4715
Frequencies --	65.3422	73.3074	87.0741
Frequencies --	90.2965	92.2023	94.7313
Frequencies --	99.6880	111.1057	112.5502
Frequencies --	115.9459	118.9896	123.1045
Frequencies --	126.8103	129.1120	133.1424
Frequencies --	136.4553	142.0362	145.3051
Frequencies --	149.8819	157.3688	163.5262
Frequencies --	165.6151	169.6587	172.2073
Frequencies --	176.6294	182.7272	196.3266
Frequencies --	202.2238	207.8042	217.6869
Frequencies --	223.6922	225.2667	231.1918
Frequencies --	235.6037	245.3650	257.2369
Frequencies --	264.1625	265.0101	266.4954
Frequencies --	267.8132	272.2981	272.9492
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Frequencies --	284.1273	288.4119	294.7811
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Frequencies --	303.9993	304.8470	308.4323
Frequencies --	317.1327	318.3969	319.9530
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Frequencies --	374.9544	381.7004	384.3778
Frequencies --	394.5286	408.2815	412.8205
Frequencies --	419.1034	422.8054	424.7750
Frequencies --	431.5672	432.9318	434.1729
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Frequencies --	455.6557	478.8280	485.3037
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Frequencies --	540.3540	542.5867	551.6479
Frequencies --	553.6530	555.3624	558.6519
Frequencies --	572.6808	585.5454	592.5683
Frequencies --	595.0750	604.9828	620.3749
Frequencies --	628.3167	637.8000	639.4390
Frequencies --	641.9680	645.0356	648.1260
Frequencies --	673.0138	692.1134	694.3599
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Frequencies --	898.5708	907.6014	918.2670
Frequencies --	925.8975	931.4348	935.3249

Frequencies --	958.2986	965.2909	970.2626
Frequencies --	971.1926	984.2519	986.5808
Frequencies --	992.0658	996.6289	1022.6348
Frequencies --	1035.4333	1038.6928	1038.8842
Frequencies --	1040.8683	1042.0727	1043.6442
Frequencies --	1044.6028	1047.0475	1048.9245
Frequencies --	1057.4492	1059.2701	1084.9997
Frequencies --	1085.9227	1087.9085	1121.5911
Frequencies --	1124.0475	1132.0577	1172.1211
Frequencies --	1174.4527	1176.3066	1191.0830
Frequencies --	1202.3807	1213.9128	1216.6137
Frequencies --	1221.3700	1223.2120	1244.6259
Frequencies --	1248.5137	1276.0150	1310.9541
Frequencies --	1326.6347	1327.6504	1335.4026
Frequencies --	1341.9419	1351.4083	1356.9990
Frequencies --	1371.5028	1379.7991	1397.6367
Frequencies --	1400.9061	1411.5582	1414.5770
Frequencies --	1415.6571	1421.7683	1422.4960
Frequencies --	1424.0366	1426.5229	1427.3379
Frequencies --	1428.8492	1431.1083	1432.2286
Frequencies --	1436.5655	1448.0449	1450.7473
Frequencies --	1456.2652	1458.2024	1462.9452
Frequencies --	1470.0014	1472.9671	1481.0666
Frequencies --	1483.5203	1488.4807	1491.0366
Frequencies --	1491.7009	1492.1365	1493.0392
Frequencies --	1497.4196	1499.5107	1500.5791
Frequencies --	1502.1984	1504.4584	1505.1146
Frequencies --	1507.3967	1508.6741	1514.4881
Frequencies --	1515.5810	1518.7062	1521.9733
Frequencies --	1574.7300	1577.9905	1585.9037
Frequencies --	1596.9799	1598.3789	1617.5344
Frequencies --	1619.0357	1622.5931	3007.5666
Frequencies --	3007.7287	3008.3186	3010.9068
Frequencies --	3011.2323	3011.2725	3012.6239
Frequencies --	3014.8095	3016.9046	3037.7970
Frequencies --	3095.4402	3101.2953	3102.4513
Frequencies --	3104.2652	3108.4198	3109.3246
Frequencies --	3113.4088	3116.4853	3120.7143
Frequencies --	3121.5163	3126.4305	3130.3902
Frequencies --	3137.1297	3147.0263	3149.4506
Frequencies --	3155.6121	3159.2818	3159.8211
Frequencies --	3169.8261	3181.5308	3201.5320
Frequencies --	3204.1073	3204.5717	3221.5297

Catalyst 10:

vacuum	toluene-like solvent	D3 dispersion
-3120.9240937	-3120.933983	-0.59515968

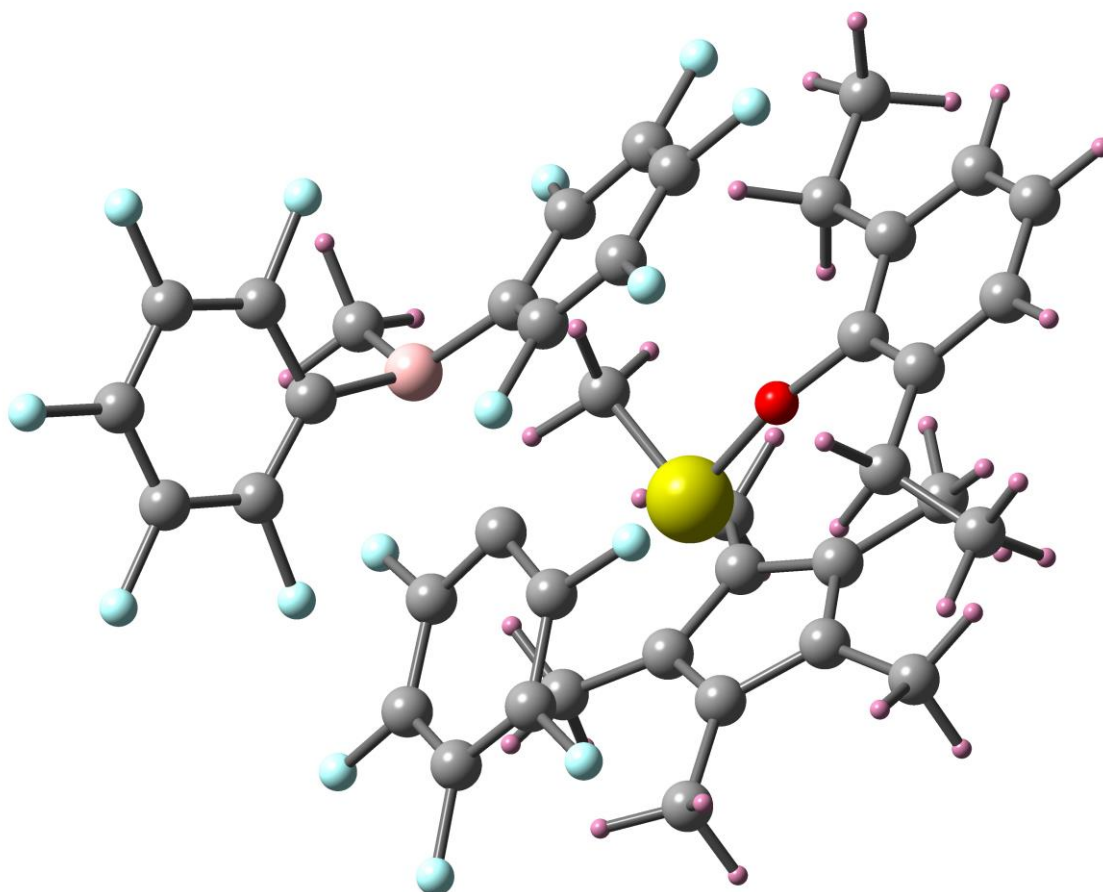
Imaginary frequency corresponding to vibration along the reaction coordinate: -240 cm^{-1} .

Ti	2.29154100	-0.92115900	-0.58603900
C	2.08121300	-0.70040100	-2.63045900
H	1.45174300	0.19670200	-2.70286200
H	2.98245800	-0.55956900	-3.23757500
H	1.52916200	-1.58371000	-2.98891400
O	2.61325500	0.77141100	-0.11961600
C	3.18509500	1.98544000	0.28652300
C	3.15713100	2.35578800	1.66661100
C	3.76284900	2.83490800	-0.71006200
C	3.76105000	3.58284200	2.03227600
C	4.35003300	4.04813200	-0.28298000
C	4.35886500	4.42310300	1.07482800
H	3.74738400	3.88079700	3.08260400
H	4.78920800	4.71043100	-1.03104800
C	2.97524800	-3.32744200	-0.43987600
C	3.79185800	-2.71737200	-1.45908400
C	3.26517900	-2.66866300	0.82001500
C	4.58455500	-1.67867000	-0.83568100
C	4.27715300	-1.66582500	0.57640700
F	-7.71802600	-0.08769100	-0.28328300
C	-6.33802600	-0.03463700	-0.41350100
C	-5.52779400	-1.05426400	0.10733200

C	-5.71956300	1.04213300	-1.07070100
C	-4.12696200	-0.97862000	-0.03900600
F	-6.10901200	-2.12960900	0.76952300
C	-4.31806400	1.06525600	-1.18872400
F	-6.49396500	2.07006200	-1.59540900
C	-3.44136800	0.06699100	-0.68576000
F	-3.42229700	-2.04029300	0.53990100
F	-3.79162700	2.18336000	-1.85665900
B	-1.83402400	0.28707100	-1.05782700
C	-0.50113700	-1.30723200	-0.11528900
C	-0.76337200	-2.59340900	-0.65084500
C	-0.48697400	-1.30975900	1.30130100
C	-1.08208800	-3.73528200	0.10407500
F	-0.70683700	-2.79992100	-2.04307700
C	-0.79061100	-2.41071300	2.12083900
F	-0.11473400	-0.13804500	1.98584600
C	-1.10365600	-3.63704900	1.50726200
F	-1.34292000	-4.96406900	-0.49703400
F	-0.74683800	-2.33028900	3.51008200
F	-1.38141000	-4.75202100	2.27931700
C	2.46831700	1.53282400	2.73993500
H	1.40592500	1.80765500	2.81756800
H	2.49805800	0.45807600	2.54202700
H	2.92656400	1.71765100	3.72213000
C	3.72936600	2.50454800	-2.19130800
H	4.16862900	1.52374900	-2.41014600
H	2.69799900	2.49161300	-2.56931800
H	4.28465100	3.25940800	-2.76426400
C	-1.29043500	1.66904800	-0.38649900
C	-0.48094400	2.60791700	-1.06735500
C	-1.73173600	2.12947700	0.88111500
C	-0.13649200	3.87685000	-0.56435900
C	-1.40080800	3.37956200	1.43514800
C	-0.59702500	4.26875800	0.70204900
F	-2.55110200	1.32173400	1.67441400
F	-1.85998700	3.74536000	2.69556400
F	-0.25479600	5.50598700	1.22621900
F	0.65851000	4.74284700	-1.30821900
F	0.03786100	2.31773100	-2.33640900
C	-1.65883100	0.00330100	-2.63067800
H	-0.62891600	-0.04305600	-2.98563200
H	-2.16304800	-0.92892900	-2.91929300
H	-2.15187400	0.82112600	-3.18245700
C	2.18690000	-4.60240100	-0.64201000
H	2.89228600	-5.43662200	-0.80021000
H	1.57602100	-4.86439400	0.22733100
H	1.53068700	-4.57044400	-1.52178200
C	3.96223100	-3.24386800	-2.86282700
H	4.70714300	-4.05917400	-2.85968900
H	3.03076000	-3.65741400	-3.27161300
H	4.32445600	-2.47834600	-3.56040600
C	2.78848000	-3.09423300	2.19158000
H	2.54075100	-2.24536100	2.84415300
H	1.91075900	-3.74688400	2.14662600
H	3.58780200	-3.66298500	2.69699800
C	5.70186000	-0.90409300	-1.49363200
H	6.63650500	-1.49017400	-1.44136400

H	5.50884700	-0.70465900	-2.55591100
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C	5.05669000	-0.91462800	1.62996100
H	4.52919600	-0.87021000	2.58956600
H	6.01311700	-1.43632700	1.80995600
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Frequencies --	636.5218	642.1954	644.0103
Frequencies --	647.2036	668.5983	685.3507
Frequencies --	688.9484	711.1727	717.1975
Frequencies --	719.8270	736.6660	739.2673
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Frequencies --	993.0069	1000.5080	1003.5962
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Frequencies --	1058.6947	1062.0571	1064.9288
Frequencies --	1086.7174	1087.8053	1093.0031
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Frequencies --	1186.8487	1194.1684	1216.0421
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Frequencies --	1341.6619	1343.8804	1354.7582
Frequencies --	1358.6379	1370.7066	1375.6279
Frequencies --	1412.3276	1414.3741	1416.2815
Frequencies --	1420.3166	1421.6434	1423.0449
Frequencies --	1425.5843	1426.6636	1428.8770
Frequencies --	1430.0837	1430.8707	1434.6719
Frequencies --	1437.8015	1446.9233	1449.1298
Frequencies --	1450.2288	1459.2140	1463.8378
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Frequencies --	1505.4517	1508.2222	1508.6131
Frequencies --	1509.8676	1513.3009	1516.1685
Frequencies --	1522.7994	1576.9838	1584.6182
Frequencies --	1596.5824	1597.6273	1601.9022
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Frequencies --	3009.1620	3010.9253	3013.7778
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Frequencies --	3031.1033	3040.4670	3042.3818
Frequencies --	3101.5655	3102.0083	3104.3652
Frequencies --	3108.0713	3112.1174	3117.9697
Frequencies --	3121.5325	3137.1146	3143.2711
Frequencies --	3145.7730	3146.3124	3149.9953
Frequencies --	3160.4673	3164.2520	3164.9961
Frequencies --	3169.3718	3172.8176	3175.1431
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Catalyst 11:

vacuum	toluene-like solvent	D3 dispersion
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Imaginary frequency corresponding to vibration along the reaction coordinate: -240 cm^{-1} .

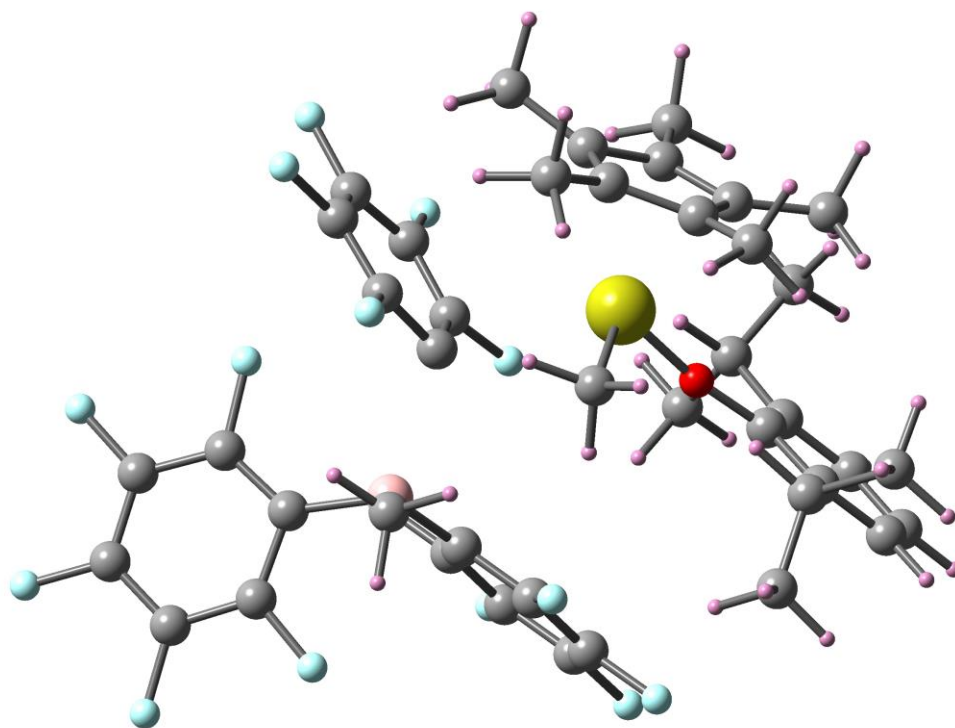
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H	2.77717300	-0.66844100	-3.20631700
H	1.33901600	-1.72736200	-3.02123700
O	2.56742900	0.47988100	-0.06387100
C	3.20992200	1.65427600	0.36299700
C	3.15515600	2.03100700	1.74258000
C	3.87960200	2.45417500	-0.62218800
C	3.81515600	3.22704400	2.11600600
C	4.52334400	3.63049700	-0.17979300
C	4.49845100	4.01552500	1.17455300
H	3.78258900	3.54873500	3.15617700
H	5.03636200	4.26293800	-0.90139900
C	2.65321100	-3.39524100	0.43614600
C	2.72797600	-3.59024800	-0.99099900
C	3.62938800	-2.39322600	0.80782400
C	3.77020500	-2.72925400	-1.50399100
C	4.32687500	-1.98407500	-0.39106800

F	-7.85939700	0.42638500	-0.27813400
C	-6.48053700	0.38034800	-0.42228100
C	-5.74764800	-0.72611100	0.03191400
C	-5.78674800	1.43969700	-1.03096300
C	-4.34618600	-0.75027600	-0.12636600
F	-6.40599400	-1.79024200	0.63759400
C	-4.38854000	1.36258000	-1.16203500
F	-6.48446600	2.54812100	-1.49582400
C	-3.58713200	0.27791100	-0.71644500
F	-3.72178900	-1.90028000	0.37095900
F	-3.78184800	2.46483300	-1.78736600
B	-1.97355500	0.38753300	-1.09716200
C	-0.74263300	-1.31795400	-0.14733900
C	-1.04896500	-2.58050700	-0.71284900
C	-0.77312400	-1.34010300	1.26829800
C	-1.44004900	-3.71843300	0.01445400
F	-0.97944800	-2.76069800	-2.10806900
C	-1.16539100	-2.43427300	2.05923000
F	-0.36731000	-0.19766700	1.98256200
C	-1.51935600	-3.63391400	1.41604200
F	-1.72364100	-4.93120000	-0.61283600
F	-1.17409400	-2.37442300	3.45110400
F	-1.88130500	-4.74304000	2.16062500
C	2.35365400	1.24590800	2.78010600
H	2.19778800	0.22155000	2.43141400
C	3.86330300	2.06174600	-2.09938600
H	2.81675400	2.04025600	-2.43734700
C	-1.31425100	1.71548700	-0.42371800
C	-0.41567700	2.57487200	-1.09828300
C	-1.71920700	2.21562100	0.84136500
C	0.04566900	3.80435400	-0.59127500
C	-1.27324900	3.42780800	1.39883200
C	-0.38286800	4.23667000	0.67301400
F	-2.62130200	1.49351500	1.62698300
F	-1.70299100	3.83474800	2.65708500
F	0.07479800	5.43356400	1.20282400
F	0.92525000	4.59042600	-1.32885000
F	0.08004300	2.23991300	-2.36569700
C	-1.82827000	0.08880300	-2.66946500
H	-0.80769400	-0.03326300	-3.03399900
H	-2.40207200	-0.80382800	-2.95376200
H	-2.26539400	0.94139100	-3.21738900
H	4.99559500	4.93484800	1.48991900
C	2.94464500	1.20336800	4.21180200
H	3.98185300	0.83251400	4.21863600
H	2.93644300	2.18990800	4.69785600
H	2.33596400	0.53273400	4.83878500
C	4.66631400	2.95798200	-3.06762400
H	4.59174900	2.55023200	-4.08824600
H	4.27229300	3.98524900	-3.09703100
H	5.73510200	3.00581300	-2.80436300
H	4.22714600	1.02849800	-2.19580800
H	1.34396800	1.68573000	2.83874300
C	1.92042400	-4.27071800	1.42649100
H	2.63224000	-5.00925200	1.83537600
H	1.52035700	-3.71439600	2.28355200
H	1.10394300	-4.83881200	0.97051800

C	1.98830200	-4.62791300	-1.80452200
H	2.64859900	-5.49293100	-1.99125700
H	1.09419700	-5.00575000	-1.29747400
H	1.67427400	-4.24634500	-2.78572600
C	4.03445300	-2.06102000	2.22509400
H	3.18394700	-2.05312500	2.91999300
H	4.74018300	-2.82781400	2.59121600
H	4.54112800	-1.09211200	2.30032900
C	4.35437100	-2.81320400	-2.89335300
H	5.08118200	-3.64360400	-2.93180500
H	3.59338900	-3.01369400	-3.65821700
H	4.89121700	-1.90035400	-3.18216600
C	5.57281600	-1.12894500	-0.42806800
H	5.53147200	-0.29208200	0.27990800
H	6.44858900	-1.74440900	-0.15746400
H	5.76657700	-0.71384800	-1.42485400

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Frequencies --	15.5358	24.5968	27.8604
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Frequencies --	50.1467	58.4770	62.0436
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Frequencies --	110.0827	113.5372	116.5204
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Frequencies --	3023.3234	3025.1868	3042.0892
Frequencies --	3051.7086	3095.6356	3101.4504
Frequencies --	3103.9734	3105.7998	3109.4453
Frequencies --	3110.1453	3112.5743	3114.3515
Frequencies --	3114.4384	3116.5576	3125.4491
Frequencies --	3146.1542	3150.7036	3152.7612
Frequencies --	3153.9753	3157.5756	3164.6712
Frequencies --	3171.5433	3173.4498	3180.6269
Frequencies --	3201.9159	3203.0803	3214.9389

Catalyst 12:

vacuum	toluene-like solvent	D3 dispersion
-3278.0682546	-3278.0780308	-0.66483448

Imaginary frequency corresponding to vibration along the reaction coordinate: -237 cm^{-1} .

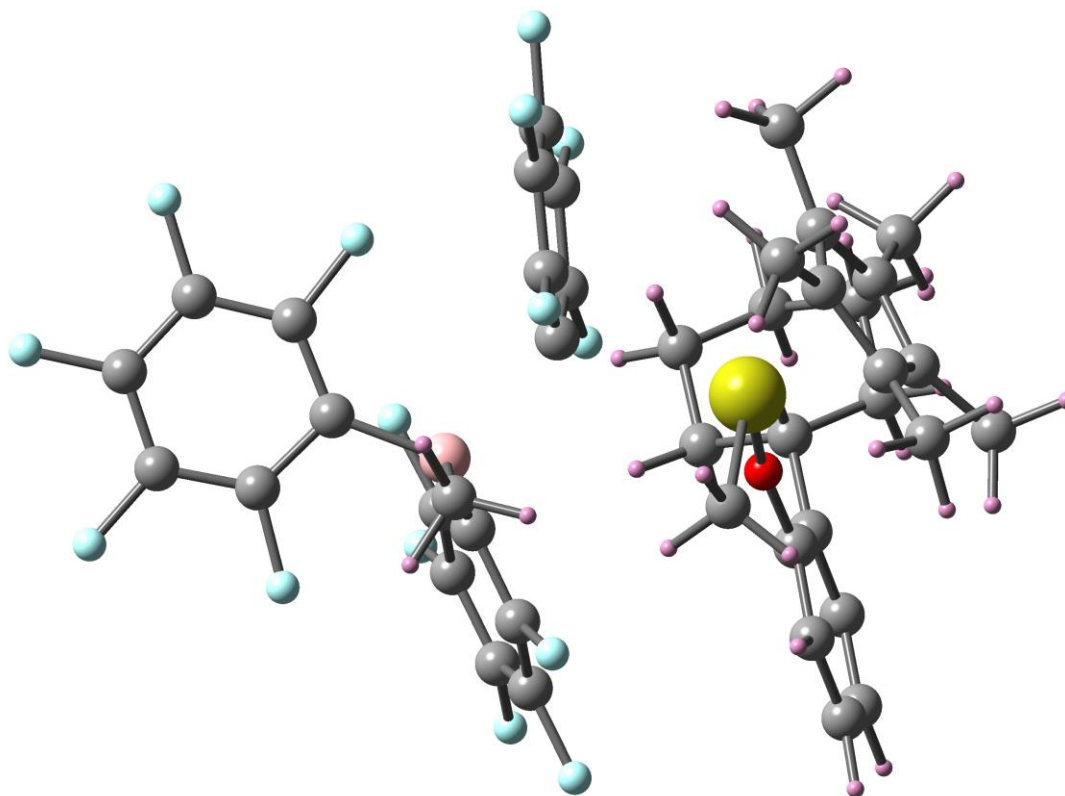
Ti	-2.08781900	1.26343100	-0.57180200
C	-1.75413900	0.90792600	-2.57964100
H	-1.30848200	-0.09686700	-2.57209200
H	-2.57694900	0.93975500	-3.30044300
H	-0.99421900	1.65716300	-2.85665500
O	-2.69818000	-0.33262800	-0.04958900
C	-3.37772700	-1.50406200	0.33841300
C	-3.35273700	-1.91311500	1.71456000
C	-4.06333900	-2.27340200	-0.66263400
C	-3.99039100	-3.13244000	2.04649500
C	-4.67790200	-3.48056900	-0.25589000
C	-4.63934900	-3.91725400	1.07888800
H	-3.97332700	-3.47285800	3.08178300
H	-5.19089400	-4.08926400	-1.00038800
C	-2.35501400	3.72778500	-0.06238600
C	-2.78045300	3.56747900	-1.42635300
C	-3.19371300	2.89405700	0.77702000
C	-3.90925800	2.66228600	-1.43746300
C	-4.17763700	2.25676600	-0.07090200
F	8.06160500	-0.32609300	-0.53545900
C	6.67690600	-0.31005800	-0.61663200
C	5.93414100	0.71247500	-0.00758000

C	5.98718100	-1.32134900	-1.30632900
C	4.52687600	0.70815600	-0.10379400
F	6.58860500	1.71709700	0.69577800
C	4.58294700	-1.27401500	-1.37395300
F	6.69422500	-2.35461900	-1.90973200
C	3.77416400	-0.26363000	-0.78973500
F	3.89032400	1.75200900	0.57515400
F	3.97704600	-2.33509600	-2.06745900
B	2.15072600	-0.40175800	-1.10374800
C	0.90048800	1.31987300	-0.09572000
C	1.28840300	2.58526400	-0.59124600
C	0.85619200	1.27700800	1.31447000
C	1.71053800	3.66524000	0.20172600
F	1.26458100	2.83476400	-1.98208600
C	1.24226900	2.32186800	2.17412900
F	0.37533300	0.11355200	1.95214100
C	1.69731300	3.52405900	1.60156500
F	2.09569500	4.88394200	-0.35667700
F	1.16046600	2.20940200	3.56186400
F	2.07077800	4.58421000	2.41140800
C	-2.68929500	-1.10931200	2.84518500
H	-2.22999600	-0.21192100	2.41384500
C	-4.17711600	-1.85560500	-2.13781100
H	-3.69964800	-0.87789500	-2.25274100
C	1.54086400	-1.72692300	-0.38850700
C	0.63277200	-2.60931100	-1.01883000
C	2.00637900	-2.20394700	0.86412600
C	0.22645900	-3.84754900	-0.48574000
C	1.62642400	-3.42891200	1.44119300
C	0.72861400	-4.26519100	0.75664400
F	2.89214400	-1.43334600	1.62089600
F	2.11655500	-3.81552400	2.68297800
F	0.33017300	-5.47298700	1.30850500
F	-0.66715000	-4.65990600	-1.17679000
F	0.07556000	-2.28883000	-2.26297900
C	1.89942000	-0.09006000	-2.65617100
H	0.85224200	0.01273700	-2.94079700
H	2.43295800	0.81872600	-2.96540900
H	2.31226400	-0.92533200	-3.24656200
C	-1.43161000	4.80713000	0.44907100
H	-2.03272100	5.71497600	0.63661700
H	-0.95559100	4.54587900	1.40016800
H	-0.65350200	5.08494300	-0.26907300
C	-2.24115900	4.32870400	-2.61442100
H	-2.80809300	5.26675300	-2.74904400
H	-1.18506900	4.60067700	-2.49017800
H	-2.33042300	3.76022200	-3.54878400
C	-3.18380100	2.91040200	2.28967900
H	-3.75749700	2.08344300	2.71866300
H	-2.16919100	2.87012000	2.71231900
H	-3.64102100	3.84780500	2.65204800
C	-4.80698200	2.39426500	-2.62242500
H	-5.65654500	3.09948200	-2.60356500
H	-4.28947700	2.54098800	-3.57843400
H	-5.22797100	1.38203800	-2.61635000
C	-5.40303200	1.51085900	0.40211700
H	-5.20596200	0.88558500	1.27989200

H	-6.18555500	2.23712600	0.68387200
H	-5.82534300	0.86411500	-0.37534200
H	-5.11274300	-4.85885700	1.36325500
C	-3.73597100	-0.64939000	3.90573800
H	-4.57554700	-0.10207800	3.45103800
H	-4.16108400	-1.50660200	4.44883500
H	-3.25650000	0.00746000	4.64912000
C	-1.55077200	-1.90781900	3.54348800
H	-0.79927800	-2.24380000	2.82024800
H	-1.04161600	-1.26988300	4.28191500
H	-1.93728500	-2.79244200	4.07163300
C	-3.43451600	-2.84361100	-3.08543800
H	-3.48684400	-2.47960800	-4.12452100
H	-2.37799600	-2.94669600	-2.81208600
H	-3.88778300	-3.84634100	-3.05959200
C	-5.66387800	-1.70424600	-2.58117900
H	-6.22281500	-1.02380100	-1.92059700
H	-5.71197700	-1.30709000	-3.60818600
H	-6.18949700	-2.67048100	-2.57956200

Frequencies --	-237.3892	13.4420	15.7520
Frequencies --	23.6599	25.9910	29.3885
Frequencies --	30.5419	31.3161	34.4141
Frequencies --	37.5813	41.8278	44.6330
Frequencies --	49.8450	53.5113	61.2790
Frequencies --	71.3549	73.1674	82.0484
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Frequencies --	119.6968	123.1199	124.6339
Frequencies --	126.7788	129.7035	132.2361
Frequencies --	138.9665	150.1689	155.6387
Frequencies --	158.3713	162.4798	162.8305
Frequencies --	169.4319	175.3376	176.2189
Frequencies --	186.5438	187.5743	202.3060
Frequencies --	205.1365	217.3848	218.9372
Frequencies --	225.9277	227.8359	232.6837
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Frequencies --	249.9716	255.8810	260.0559
Frequencies --	264.1450	265.1145	265.8564
Frequencies --	267.5529	270.4845	274.4671
Frequencies --	275.4249	279.9659	281.5852
Frequencies --	285.4376	289.0213	297.7117
Frequencies --	298.2547	300.0134	302.1412
Frequencies --	304.2689	310.1025	312.4437
Frequencies --	316.2462	317.4137	320.8434
Frequencies --	326.3112	328.4442	333.7369
Frequencies --	361.4256	366.2556	375.2093
Frequencies --	381.7472	382.1120	398.9198
Frequencies --	410.6932	421.3352	425.3336
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Frequencies --	537.5049	539.8713	541.4690
Frequencies --	545.3485	550.8760	552.2099
Frequencies --	562.6986	579.4475	589.0371
Frequencies --	592.6494	594.5094	604.0271
Frequencies --	607.3159	620.7239	628.7936
Frequencies --	628.8595	637.2642	642.6945
Frequencies --	643.1340	643.9099	663.4572

Frequencies --	684.6206	687.4809	708.6665
Frequencies --	717.6109	719.0614	727.3635
Frequencies --	740.1979	753.7783	761.2829
Frequencies --	784.9357	796.7874	800.5772
Frequencies --	805.5761	815.3397	841.1244
Frequencies --	876.0941	881.1011	896.3333
Frequencies --	907.7476	916.7426	921.2954
Frequencies --	922.5307	930.5584	933.3602
Frequencies --	938.1512	960.2912	964.0830
Frequencies --	967.1949	969.6326	976.3380
Frequencies --	991.0785	994.4945	1003.5036
Frequencies --	1023.4003	1038.3780	1039.8539
Frequencies --	1043.2279	1045.1474	1046.4280
Frequencies --	1050.0589	1056.3637	1059.2418
Frequencies --	1065.1771	1072.5750	1088.0144
Frequencies --	1088.2913	1099.0125	1109.8856
Frequencies --	1111.6321	1114.6074	1125.3661
Frequencies --	1166.5976	1167.0451	1169.9672
Frequencies --	1172.6242	1175.4113	1181.6469
Frequencies --	1186.9313	1205.1785	1217.0436
Frequencies --	1227.2242	1240.5711	1247.8293
Frequencies --	1274.7020	1301.5211	1314.2426
Frequencies --	1321.9930	1326.9792	1330.1007
Frequencies --	1331.8518	1343.9059	1351.6077
Frequencies --	1359.3153	1370.4779	1374.7542
Frequencies --	1380.7087	1401.4117	1403.9686
Frequencies --	1412.4491	1413.3309	1416.1359
Frequencies --	1421.1181	1423.2278	1423.6376
Frequencies --	1424.5027	1425.5085	1428.0371
Frequencies --	1429.8978	1432.3537	1433.6462
Frequencies --	1435.9192	1442.6075	1450.1924
Frequencies --	1452.3841	1456.2629	1464.6752
Frequencies --	1470.7234	1472.6717	1472.8707
Frequencies --	1482.3974	1488.9123	1489.8513
Frequencies --	1490.3627	1490.9339	1492.2815
Frequencies --	1493.9151	1496.8095	1499.8057
Frequencies --	1502.0160	1502.7606	1503.1953
Frequencies --	1504.0417	1506.9532	1508.2621
Frequencies --	1510.5129	1512.1681	1514.1225
Frequencies --	1517.8098	1522.1325	1577.5340
Frequencies --	1582.9002	1594.3188	1596.7802
Frequencies --	1597.2612	1605.4356	1619.4045
Frequencies --	1622.3720	3010.1399	3010.3757
Frequencies --	3011.2836	3011.5169	3012.3370
Frequencies --	3012.7987	3013.6862	3016.5901
Frequencies --	3020.1373	3028.9482	3030.3692
Frequencies --	3095.3730	3097.5624	3105.4796
Frequencies --	3106.8240	3107.7797	3111.3910
Frequencies --	3112.7623	3115.2686	3117.8741
Frequencies --	3119.1811	3119.2723	3124.2315
Frequencies --	3131.2146	3135.3208	3143.0479
Frequencies --	3149.9149	3158.5210	3165.3254
Frequencies --	3166.1794	3167.7879	3168.3310
Frequencies --	3175.2428	3178.0991	3178.5094
Frequencies --	3188.0371	3201.1761	3210.8690

Catalyst 13:**distal conformation**

vacuum	toluene-like solvent	D3 dispersion
-3276.8807033	-3276.8904312	-0.66362404

Imaginary frequency corresponding to vibration along the reaction coordinate: -240 cm^{-1} .

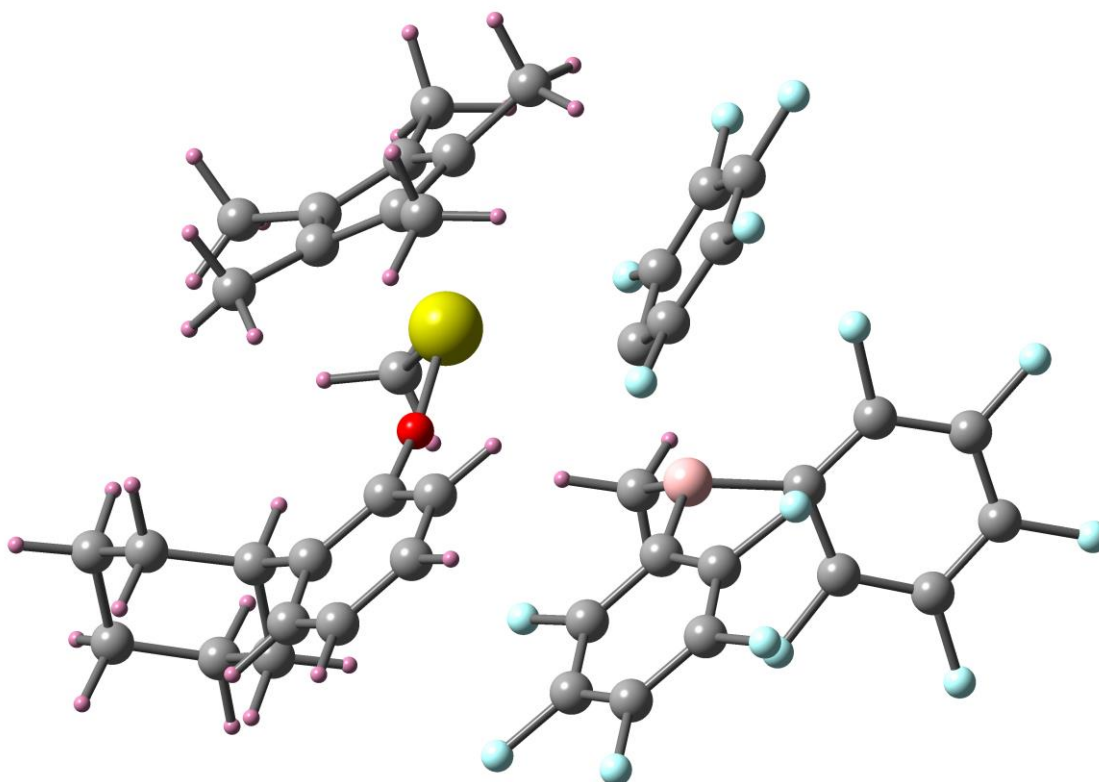
Ti	1.86779300	-1.32567200	-1.05574600
C	1.46789400	-1.04276600	-3.06685800
H	0.77230900	-0.19357500	-3.03667000
H	2.31404300	-0.78778900	-3.71530200
H	0.96111400	-1.93732500	-3.46217600
O	2.37195600	0.34771600	-0.71047600
C	3.00227400	1.59486400	-0.80018100
C	3.41115600	2.33326200	0.35285800
C	3.19518700	2.10475800	-2.11152200
C	4.02927400	3.58923200	0.10567100
C	3.81094700	3.35005900	-2.31117700
C	4.23582000	4.09689100	-1.19050000
H	4.34832900	4.18993900	0.95763900
H	3.94208600	3.73646900	-3.32354300
C	2.60598700	-3.54286600	-0.08378500
C	2.52215600	-3.75170100	-1.50697800
C	3.56738500	-2.48958300	0.16403300
C	3.46609200	-2.86041500	-2.14391200
C	4.11128400	-2.07353600	-1.11118300
F	-7.82515500	0.05738000	0.60236100

C	-6.48404000	0.03390700	0.24912300
C	-5.59596300	-0.86391000	0.85917400
C	-5.98291000	0.91095100	-0.72726000
C	-4.23730000	-0.86978700	0.48092000
F	-6.05800400	-1.73703700	1.83755500
C	-4.61872200	0.85941400	-1.06697000
F	-6.83529400	1.81770200	-1.34602600
C	-3.66840500	-0.02791500	-0.49370200
F	-3.44271900	-1.78604300	1.18084400
F	-4.21205400	1.78257700	-2.04413900
B	-2.14043200	0.04947500	-1.15731900
C	-0.70708700	-1.36342300	-0.14042500
C	-1.08241700	-2.71751900	-0.34157700
C	-0.42505700	-1.07939000	1.22166300
C	-1.27381100	-3.66365500	0.67907900
F	-1.29197300	-3.19744600	-1.64783100
C	-0.58452400	-1.97917300	2.29062400
F	0.07178900	0.18680900	1.57105000
C	-1.03626100	-3.28206900	2.01137500
F	-1.65016600	-4.97622700	0.40144600
F	-0.28410500	-1.62514400	3.60360200
F	-1.18768800	-4.19959600	3.03488000
C	-1.50830800	1.53162500	-0.89212800
C	-0.85308600	2.30061400	-1.88299300
C	-1.73772000	2.25153800	0.30887800
C	-0.45971300	3.64290300	-1.72077300
C	-1.35533200	3.58775600	0.52344000
C	-0.71044200	4.29567200	-0.50424500
F	-2.38581200	1.63505800	1.38367800
F	-1.59989500	4.21299900	1.74133000
F	-0.31538400	5.61104000	-0.31333100
F	0.17523300	4.32549400	-2.75240200
F	-0.56017700	1.75225100	-3.13829200
C	-2.23483500	-0.55082000	-2.64813400
H	-1.27840000	-0.73013700	-3.14037200
H	-2.80401600	-1.49001100	-2.65671700
H	-2.78789600	0.16724900	-3.27522800
C	2.04761700	-4.45441100	0.98391300
H	2.79475900	-5.24071200	1.19267900
H	1.86037800	-3.94058800	1.93461300
H	1.13043000	-4.96676100	0.67739000
C	1.72409100	-4.82602600	-2.21069200
H	2.36553700	-5.70357700	-2.40551200
H	0.86841300	-5.17168800	-1.61921100
H	1.33679600	-4.48885900	-3.18200400
C	4.07618000	-2.08674500	1.52867000
H	4.60405700	-1.12828900	1.51209900
H	3.27077800	-2.01333200	2.27312900
H	4.78791100	-2.84513500	1.89875300
C	3.90561700	-2.94736500	-3.58551200
H	4.72302500	-3.68529400	-3.66779700
H	3.09985100	-3.27707600	-4.25350500
H	4.29279700	-1.99377900	-3.96712700
C	5.29455400	-1.15640900	-1.31706700
H	5.35899100	-0.37626200	-0.54958000
H	6.22982100	-1.74159500	-1.27034800
H	5.27245300	-0.65535500	-2.29362700

H	2.84377100	1.52581200	-2.96242100
H	4.71034800	5.07066200	-1.32479300
C	3.18478400	1.86898600	1.79598200
C	4.51194700	1.79047100	2.61734300
C	2.16185200	2.78640700	2.54228300
H	2.74660600	0.86199200	1.76892400
C	4.26447800	1.31371400	4.07176800
H	4.98912500	2.78429300	2.64827900
H	5.22952100	1.11881100	2.11596000
C	1.91169300	2.30745500	3.99368600
H	2.53987400	3.82308400	2.56076500
H	1.21268900	2.80374400	1.98962800
C	3.22857400	2.20528800	4.80025700
H	5.21994500	1.31170200	4.62456200
H	3.90161900	0.26988500	4.06442700
H	1.21424600	3.00226600	4.49108100
H	1.41245400	1.32339100	3.97113400
H	3.02613600	1.80122300	5.80670000
H	3.65233800	3.21624900	4.94345200

Frequencies --	-240.0613	12.1998	14.7806
Frequencies --	16.2177	25.8826	28.5638
Frequencies --	33.0700	34.1555	38.9018
Frequencies --	42.8722	47.3145	50.4664
Frequencies --	54.4006	59.1397	61.3212
Frequencies --	68.1026	75.4061	80.3210
Frequencies --	87.1220	90.8761	95.3392
Frequencies --	97.6519	111.3589	113.7528
Frequencies --	116.8626	119.1987	121.4129
Frequencies --	127.2596	135.3331	139.9340
Frequencies --	144.2326	149.0924	149.9831
Frequencies --	152.8547	157.2329	158.2520
Frequencies --	159.8810	164.6721	170.4975
Frequencies --	175.9859	181.7022	192.9378
Frequencies --	204.9583	205.1640	220.0928
Frequencies --	224.6494	227.6965	229.0436
Frequencies --	235.5118	245.9104	249.1066
Frequencies --	264.1521	265.7260	265.9992
Frequencies --	267.5679	269.4096	271.8252
Frequencies --	275.9898	276.2916	282.0278
Frequencies --	284.9825	287.6951	289.1447
Frequencies --	298.2598	299.3571	302.5475
Frequencies --	303.0312	303.7464	307.3134
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Frequencies --	328.6240	332.9305	336.0860
Frequencies --	351.8524	368.0936	373.4594
Frequencies --	375.0106	381.1511	384.4151
Frequencies --	403.6379	409.7859	421.5297
Frequencies --	424.3257	431.4834	433.1566
Frequencies --	433.3641	439.1359	440.2229
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Frequencies --	496.2865	501.4833	504.5345
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Frequencies --	551.8943	552.1534	567.4055
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Frequencies --	602.7641	608.4134	617.4000
Frequencies --	628.6718	637.1965	642.0902
Frequencies --	644.5889	646.4428	658.0638
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Frequencies --	711.6632	717.3310	719.2322

Frequencies --	738.5242	743.5444	751.3230
Frequencies --	767.8951	769.6117	782.8766
Frequencies --	790.2303	799.8990	806.7411
Frequencies --	820.1168	833.2018	866.7631
Frequencies --	872.1439	887.8413	888.8968
Frequencies --	896.9832	902.4851	907.6930
Frequencies --	916.5948	923.9742	930.2728
Frequencies --	964.3487	967.0574	967.9511
Frequencies --	984.4146	992.0393	995.2441
Frequencies --	998.3679	999.7210	1031.9809
Frequencies --	1039.1451	1040.5948	1042.8240
Frequencies --	1044.8660	1046.6768	1047.2360
Frequencies --	1053.9459	1055.6388	1057.1950
Frequencies --	1058.2615	1060.9706	1086.4620
Frequencies --	1087.5071	1087.7711	1090.3976
Frequencies --	1093.4307	1115.8380	1124.4116
Frequencies --	1151.7823	1170.9127	1172.8261
Frequencies --	1175.5361	1183.3192	1187.2719
Frequencies --	1190.9595	1195.4848	1209.1009
Frequencies --	1215.0299	1223.9283	1245.7204
Frequencies --	1247.7032	1278.7205	1280.1911
Frequencies --	1294.6350	1312.1611	1317.2487
Frequencies --	1327.4624	1328.9120	1339.1453
Frequencies --	1342.2033	1352.3027	1356.4306
Frequencies --	1357.2727	1360.5600	1362.5060
Frequencies --	1369.3886	1369.8879	1376.8954
Frequencies --	1386.0816	1410.5654	1414.8441
Frequencies --	1415.3305	1422.7361	1423.4369
Frequencies --	1426.5605	1427.8150	1433.1077
Frequencies --	1433.2494	1438.0868	1443.5659
Frequencies --	1445.3637	1450.0740	1457.6721
Frequencies --	1459.9922	1461.9266	1471.1987
Frequencies --	1472.8462	1481.6159	1482.2703
Frequencies --	1482.9333	1484.2630	1487.1257
Frequencies --	1491.3097	1491.8842	1492.7878
Frequencies --	1493.2632	1497.1634	1499.6690
Frequencies --	1501.4478	1502.7361	1506.2650
Frequencies --	1508.6740	1510.5914	1514.3337
Frequencies --	1520.2288	1574.7769	1583.0154
Frequencies --	1583.7095	1596.7544	1597.3986
Frequencies --	1613.3835	1620.1904	1622.4500
Frequencies --	3000.2263	3003.7557	3010.3702
Frequencies --	3010.8922	3011.2488	3012.0554
Frequencies --	3014.3730	3016.3897	3016.9825
Frequencies --	3018.1740	3025.1292	3034.8400
Frequencies --	3060.1905	3065.7175	3074.1878
Frequencies --	3083.5307	3092.3380	3098.9394
Frequencies --	3102.6410	3104.0354	3108.3847
Frequencies --	3112.9342	3120.4180	3120.5035
Frequencies --	3143.8406	3147.5854	3153.7288
Frequencies --	3156.8107	3166.2823	3168.8585
Frequencies --	3170.6477	3173.9104	3184.3299
Frequencies --	3200.4771	3206.2711	3229.7400

proximal conformation

vacuum	toluene-like solvent	D3 dispersion
-3276.8824095	-3276.8920442	-0.66368715

Imaginary frequency corresponding to vibration along the reaction coordinate: -238 cm^{-1} .

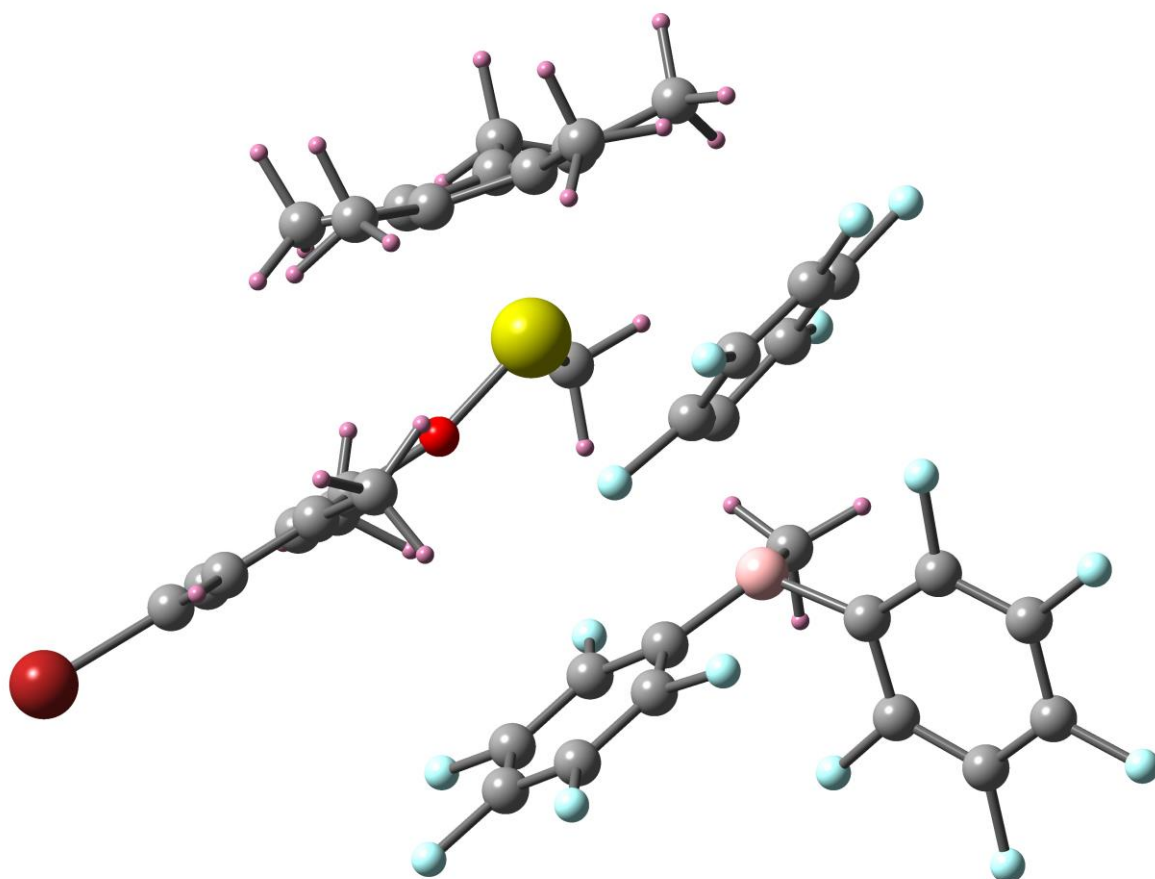
Ti	-1.65456100	1.58027000	-0.28566900
C	-1.98770700	1.16537100	-2.28829600
H	-1.55431700	0.15691200	-2.37010500
H	-3.02422300	1.13077100	-2.64003000
H	-1.41206700	1.88204900	-2.89608800
O	-2.28399600	0.06614000	0.39785500
C	-2.89891800	-0.91863800	1.17709400
C	-2.41451200	-1.06865100	2.50264700
C	-3.93688500	-1.75412500	0.65890600
C	-2.94916400	-2.05504900	3.34756400
C	-4.44702800	-2.73923600	1.54580800
C	-3.97464100	-2.89679800	2.86277900
H	-2.56177300	-2.17269900	4.36137000
H	-5.23073300	-3.40863000	1.19003600
C	-1.58173500	3.95955500	0.60955200
C	-2.04437400	4.05043900	-0.75270800
C	-2.50317100	3.12422000	1.34903700
C	-3.29155700	3.32622700	-0.84863300
C	-3.57793900	2.75491600	0.45434900
F	7.71909900	-1.56910200	-1.37361900
C	6.36311900	-1.31391700	-1.23058000
C	5.91180300	-0.08477900	-0.72821200

C	5.40857600	-2.28247100	-1.58278800
C	4.52751400	0.14930700	-0.59547000
F	6.83008300	0.89109700	-0.35717900
C	4.04006300	-1.99268600	-1.43122900
F	5.82280100	-3.51460900	-2.07500700
C	3.51532500	-0.76653500	-0.93974200
F	4.19764900	1.39636000	-0.05173200
F	3.16943800	-3.03255000	-1.79574500
B	1.84638800	-0.65046300	-0.95898200
C	1.09649200	1.25738700	-0.14182700
C	1.57331900	2.37402200	-0.87839700
C	1.28531900	1.41591800	1.25599200
C	2.26702900	3.46584600	-0.33028800
F	1.36815900	2.43242500	-2.26944200
C	1.99841000	2.45969000	1.86712100
F	0.69538200	0.48976200	2.13852700
C	2.51155300	3.48718800	1.05415100
F	2.69486100	4.53384300	-1.11575800
F	2.15799900	2.53539700	3.24789800
F	3.18343800	4.55211400	1.62454900
C	1.23768800	-1.78098400	0.04923500
C	0.18165900	-2.65432700	-0.29691600
C	1.84369300	-2.09897500	1.29124300
C	-0.23251200	-3.74790700	0.48688000
C	1.45342000	-3.16567100	2.12008500
C	0.40563800	-4.00644500	1.70964300
F	2.90153200	-1.31914800	1.77190500
F	2.08845300	-3.39661700	3.33517200
F	-0.00341300	-5.06398100	2.50836300
F	-1.27119100	-4.57287400	0.06601100
F	-0.52615300	-2.47373700	-1.49156700
C	1.39760700	-0.59106900	-2.50448900
H	0.34009000	-0.38541600	-2.66951500
H	1.98178600	0.16142200	-3.05127800
H	1.60900200	-1.56599400	-2.97129800
C	-0.54692500	4.86157200	1.23891800
H	-1.06404000	5.76880600	1.59993500
H	-0.05325400	4.41849100	2.11043500
H	0.21653300	5.19864000	0.53088500
C	-1.42119900	4.89312900	-1.84314200
H	-1.71208700	5.95087700	-1.71698400
H	-0.32418600	4.85635100	-1.83236000
H	-1.75091300	4.58365300	-2.84300400
C	-2.46978200	2.89245700	2.84354900
H	-3.02002300	1.99091600	3.13874200
H	-1.44641900	2.80280900	3.23463500
H	-2.94006800	3.74498400	3.36503100
C	-4.25602800	3.39518800	-2.00879700
H	-4.87398700	4.30540200	-1.91467300
H	-3.74604100	3.44866100	-2.97882700
H	-4.94273500	2.53932200	-2.03623800
C	-4.88209000	2.11945900	0.87195000
H	-4.75341400	1.35779500	1.64992100
H	-5.54956400	2.89730000	1.28304000
H	-5.40752100	1.65390500	0.03088700
H	-4.39439100	-3.67616900	3.50148800
H	-1.60550400	-0.42618100	2.84403600

C	-4.48604200	-1.64224000	-0.76843100
C	-4.12951600	-2.89215900	-1.63838000
C	-6.03114700	-1.41156600	-0.80313700
H	-4.01204100	-0.77388600	-1.24653900
C	-4.65370500	-2.74693800	-3.08864600
H	-4.57038700	-3.79487300	-1.18164600
H	-3.04258200	-3.04273000	-1.64674500
C	-6.55512200	-1.25578700	-2.25346800
H	-6.54502700	-2.26675500	-0.33325300
H	-6.29786700	-0.52421300	-0.20732400
C	-6.17683500	-2.47329500	-3.13251400
H	-4.41761800	-3.66420300	-3.65443700
H	-4.11728600	-1.92211800	-3.59258600
H	-7.65105700	-1.12520400	-2.23728900
H	-6.13450400	-0.33715600	-2.70405000
H	-6.50363200	-2.30514600	-4.17290800
H	-6.71919100	-3.36571400	-2.77034900

Frequencies --	-238.2057	-11.1596	10.7784
Frequencies --	16.9591	24.6565	28.1182
Frequencies --	31.2938	33.9919	37.2169
Frequencies --	42.6570	43.8035	47.3438
Frequencies --	49.6357	53.7048	57.1350
Frequencies --	61.6037	66.3347	84.4837
Frequencies --	88.0527	89.4594	96.7628
Frequencies --	97.5693	104.6232	109.4628
Frequencies --	110.9563	113.1678	118.7413
Frequencies --	122.2345	124.3022	126.5537
Frequencies --	134.0198	139.6767	144.0482
Frequencies --	151.3169	154.1194	156.8574
Frequencies --	165.0191	167.2102	174.6654
Frequencies --	177.1454	186.4614	190.5950
Frequencies --	195.8445	200.8271	203.8265
Frequencies --	211.0638	220.7697	225.2087
Frequencies --	229.0863	236.8839	237.2068
Frequencies --	243.3443	264.1720	265.6534
Frequencies --	266.4839	267.5303	269.1932
Frequencies --	272.5701	275.5327	278.0684
Frequencies --	279.2178	282.9916	287.3611
Frequencies --	292.7819	298.1127	299.3437
Frequencies --	303.6234	305.8612	310.6155
Frequencies --	314.0954	316.3234	317.9137
Frequencies --	327.3150	334.4179	337.4571
Frequencies --	349.2157	368.8064	375.1693
Frequencies --	380.7863	381.7752	383.6633
Frequencies --	399.7000	412.9209	422.0650
Frequencies --	425.0969	431.5419	434.0538
Frequencies --	436.9100	439.5069	443.0624
Frequencies --	449.9170	454.7399	483.8891
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Frequencies --	521.0346	528.0362	536.1045
Frequencies --	539.4442	542.1572	551.7286
Frequencies --	552.4906	554.3410	571.8762
Frequencies --	580.8181	589.3078	591.5098
Frequencies --	604.7734	615.4957	617.1314
Frequencies --	629.1904	637.1829	641.0111
Frequencies --	643.8694	650.5372	656.1089
Frequencies --	670.3271	690.5907	696.3489
Frequencies --	715.3442	717.8444	719.5986
Frequencies --	738.4693	742.3789	751.4096
Frequencies --	768.8193	770.7472	781.5691

Frequencies --	790.6938	802.2795	805.1032
Frequencies --	820.1831	826.8582	866.4140
Frequencies --	873.3888	886.4899	889.4581
Frequencies --	897.5045	901.0815	907.4160
Frequencies --	915.3471	924.8644	934.7672
Frequencies --	964.2620	966.0037	972.9260
Frequencies --	982.7539	987.2246	995.6936
Frequencies --	996.6750	997.8653	1031.5418
Frequencies --	1038.5867	1040.1906	1043.1443
Frequencies --	1044.8942	1045.2285	1047.8233
Frequencies --	1052.8707	1053.5288	1055.4269
Frequencies --	1058.5469	1059.6457	1085.1908
Frequencies --	1087.5729	1087.8968	1089.7008
Frequencies --	1093.2542	1115.1457	1125.6561
Frequencies --	1152.1723	1171.7362	1172.5284
Frequencies --	1175.3526	1181.3835	1184.4619
Frequencies --	1191.2175	1196.4451	1211.5562
Frequencies --	1214.3021	1223.7943	1243.1805
Frequencies --	1245.9083	1278.3760	1281.8347
Frequencies --	1292.5310	1311.1878	1312.6489
Frequencies --	1326.9379	1328.9633	1339.1741
Frequencies --	1345.0673	1347.9954	1354.5375
Frequencies --	1357.4803	1360.0483	1361.4703
Frequencies --	1364.0453	1370.3319	1379.0474
Frequencies --	1385.0931	1411.1821	1414.8741
Frequencies --	1415.6349	1423.8984	1425.3842
Frequencies --	1425.9488	1428.1100	1429.5366
Frequencies --	1432.2150	1433.4536	1444.7502
Frequencies --	1446.7193	1449.5394	1451.6497
Frequencies --	1456.7599	1462.7854	1471.5175
Frequencies --	1473.0289	1480.4446	1481.3971
Frequencies --	1482.1848	1484.9657	1488.1666
Frequencies --	1490.6546	1491.6195	1493.2419
Frequencies --	1494.6868	1495.6905	1500.7526
Frequencies --	1502.3771	1502.8074	1506.8927
Frequencies --	1508.4469	1510.6129	1514.5414
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Frequencies --	1586.0776	1596.9476	1599.2212
Frequencies --	1612.6776	1621.0885	1622.2633
Frequencies --	2992.7835	3001.5367	3004.7137
Frequencies --	3006.6967	3008.5010	3011.0341
Frequencies --	3012.1608	3012.3075	3013.8084
Frequencies --	3022.2368	3028.4242	3038.5492
Frequencies --	3059.3862	3064.2187	3075.3996
Frequencies --	3076.6341	3094.9144	3096.6180
Frequencies --	3105.0171	3108.5533	3116.9199
Frequencies --	3117.4700	3121.9013	3132.2010
Frequencies --	3134.9692	3145.8838	3146.8547
Frequencies --	3151.6915	3165.6417	3167.2192
Frequencies --	3167.9323	3178.0440	3182.9162
Frequencies --	3198.8152	3212.2005	3226.5757

Catalyst 14:

vacuum	toluene-like solvent	D3 dispersion
-3133.4832388	-3133.493375	-0.60353985

Imaginary frequency corresponding to vibration along the reaction coordinate: -241 cm^{-1} .

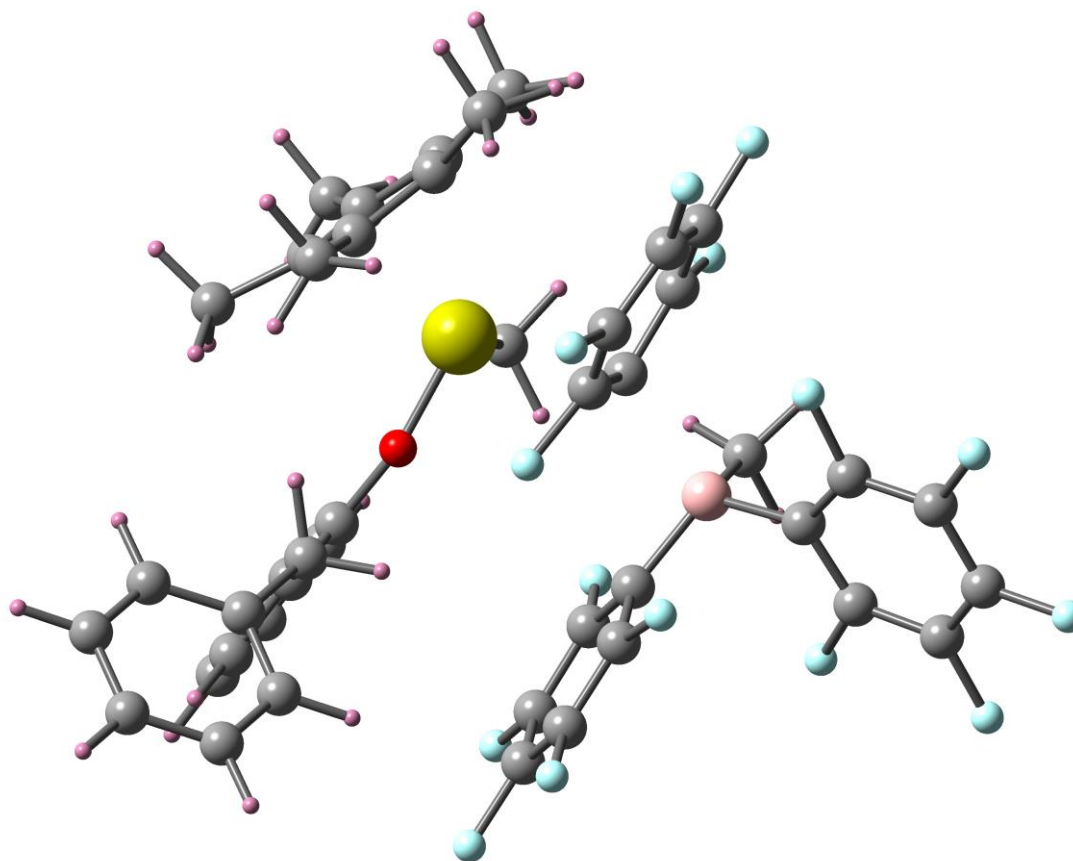
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C	-0.74351900	1.90988700	-2.69990800
H	-0.51729300	0.83627400	-2.76128800
H	-1.59520200	2.13531500	-3.34981700
H	0.12919600	2.50311800	-3.01288600
O	-2.10477100	0.77831800	-0.33819900
C	-3.20661500	-0.03536700	-0.05760400
C	-3.46273300	-0.44748400	1.28600700
C	-4.04339400	-0.45845400	-1.13935100
C	-4.60882700	-1.23963800	1.53758500
C	-5.17429900	-1.25185900	-0.84120600
C	-5.45597900	-1.62394900	0.48565000
H	-4.81704600	-1.55865500	2.55851500
H	-5.81890000	-1.58310100	-1.65432300
C	-0.83692300	4.24812900	0.65932600
C	-0.50759000	4.61365900	-0.70012500
C	-2.19170000	3.74115600	0.67347900
C	-1.66399500	4.34771000	-1.52465000
C	-2.70250200	3.79578200	-0.67775200

F	7.44282000	-3.29801000	0.03718700
C	6.21007800	-2.69621800	-0.16763000
C	5.91867800	-1.44550100	0.39659600
C	5.22500100	-3.32545100	-0.94714000
C	4.65832500	-0.85321200	0.17204300
F	6.87074000	-0.79996300	1.17713300
C	3.98569100	-2.68838200	-1.13814900
F	5.48251000	-4.56518600	-1.51964100
C	3.62637100	-1.42600900	-0.59516600
F	4.47543600	0.38492700	0.79971000
F	3.06432500	-3.39374500	-1.92988100
B	2.14064500	-0.85129400	-1.07338800
C	1.59845100	1.11803700	-0.04165800
C	2.45168300	2.17656100	-0.44422900
C	1.48019200	1.02910000	1.36722300
C	3.18348600	3.00148000	0.42813100
F	2.61800400	2.46150800	-1.81270500
C	2.18670500	1.81025700	2.29772200
F	0.57290800	0.10851300	1.92306500
C	3.06031700	2.80107700	1.81501300
F	4.00593700	4.02313600	-0.04244700
F	2.01220700	1.65959700	3.67084100
F	3.74939200	3.61249800	2.69906800
C	-2.53884300	-0.13774100	2.44954900
H	-1.96209300	0.77738800	2.30320100
H	-3.10775100	-0.04755500	3.38599600
H	-1.80986200	-0.95112800	2.58561800
C	-3.74687300	-0.12366900	-2.58973200
H	-3.66681200	0.95769300	-2.75621800
H	-2.79921300	-0.57562000	-2.91165600
H	-4.54000300	-0.50881500	-3.24425000
C	0.95963500	-1.85719400	-0.57513000
C	-0.13470600	-2.24598000	-1.38167800
C	1.02295100	-2.56128300	0.65548200
C	-1.07854700	-3.22827000	-1.02654300
C	0.09678600	-3.53871600	1.06289900
C	-0.96584600	-3.88257100	0.21009800
F	2.05493400	-2.30174200	1.56114300
F	0.22067500	-4.16804500	2.29628200
F	-1.89280300	-4.84086000	0.58912100
F	-2.12424500	-3.54996800	-1.88645400
F	-0.34569900	-1.65304000	-2.63452300
C	2.26888200	-0.41554200	-2.61590600
H	1.42681700	0.14884200	-3.01774000
H	3.18257300	0.17139700	-2.78194200
H	2.35975700	-1.33249900	-3.22234800
Br	-7.04655200	-2.71028000	0.87010700
C	-0.04571600	4.58452700	1.90307800
H	-0.48332600	5.48517800	2.36784700
H	-0.07459800	3.79305400	2.66356300
H	1.00196600	4.81653300	1.68955600
C	0.72818100	5.34148200	-1.17964300
H	0.46515400	6.38322400	-1.43166000
H	1.51618000	5.38293100	-0.42108400
H	1.16290300	4.89388700	-2.08445300
C	-3.00908400	3.47101400	1.91527700
H	-3.80256300	2.73259900	1.74939700

H	-2.39590600	3.12543400	2.75743300
H	-3.49847900	4.40731000	2.23752400
C	-1.83783300	4.83323900	-2.94297100
H	-2.10715700	5.90395300	-2.92663200
H	-0.91776400	4.74082400	-3.53449000
H	-2.63735800	4.30464300	-3.47742700
C	-4.13720900	3.55191200	-1.08392200
H	-4.61266400	2.75819900	-0.49462300
H	-4.72664200	4.47221700	-0.92596100
H	-4.23358600	3.28814500	-2.14474400

Frequencies --	-240.6227	11.5581	15.0050
Frequencies --	16.1027	17.7608	26.5659
Frequencies --	30.6557	34.7200	36.8827
Frequencies --	41.4217	46.8310	48.5222
Frequencies --	57.1863	62.2074	67.7295
Frequencies --	73.1624	84.3769	90.4697
Frequencies --	91.5326	97.0800	104.4763
Frequencies --	110.8364	112.6423	113.7756
Frequencies --	121.3095	125.5400	128.6064
Frequencies --	132.5126	135.2097	141.5601
Frequencies --	147.3968	149.5784	153.3738
Frequencies --	157.3335	162.5432	164.8704
Frequencies --	169.5174	170.1047	175.6408
Frequencies --	178.9336	183.2419	189.5140
Frequencies --	192.8996	197.7754	202.4786
Frequencies --	204.0634	221.0932	223.9920
Frequencies --	227.5759	230.0358	239.2280
Frequencies --	244.9653	260.2741	262.7708
Frequencies --	263.9294	265.7660	266.0084
Frequencies --	268.2884	269.3533	270.5288
Frequencies --	276.2201	276.7264	280.0738
Frequencies --	290.5970	291.9488	297.7396
Frequencies --	298.8010	302.6931	303.5775
Frequencies --	305.6232	316.5579	316.8337
Frequencies --	327.7945	332.1371	342.5431
Frequencies --	365.1006	368.5831	376.0876
Frequencies --	380.9047	383.6295	387.7545
Frequencies --	407.1338	408.8767	422.5821
Frequencies --	424.8082	427.0258	431.2327
Frequencies --	433.1561	439.0758	450.0630
Frequencies --	454.0582	484.2496	500.1110
Frequencies --	502.1528	515.2340	528.1672
Frequencies --	534.4085	540.0796	542.4347
Frequencies --	550.8980	552.4944	558.6795
Frequencies --	565.1379	566.7345	572.5408
Frequencies --	586.1319	587.6163	593.1669
Frequencies --	600.9288	610.8217	629.3287
Frequencies --	637.1147	642.2167	644.3041
Frequencies --	646.2949	667.6790	685.9378
Frequencies --	688.0249	711.4331	717.3943
Frequencies --	719.8128	730.3496	740.1616
Frequencies --	751.7650	783.5614	796.7879
Frequencies --	800.7313	807.7969	836.9610
Frequencies --	886.0507	886.9546	891.1472
Frequencies --	895.8438	907.7304	914.8330
Frequencies --	917.0150	951.4208	962.4767
Frequencies --	972.3035	982.7285	992.2025
Frequencies --	1000.1486	1010.6818	1030.9487
Frequencies --	1038.4954	1040.6250	1043.4350
Frequencies --	1044.7921	1046.6675	1049.2463
Frequencies --	1049.4472	1055.9875	1057.7951

Frequencies --	1062.0977	1065.6416	1085.3859
Frequencies --	1087.4641	1093.8403	1123.8223
Frequencies --	1127.5339	1171.0710	1171.6896
Frequencies --	1174.9238	1184.0913	1191.6996
Frequencies --	1216.2282	1224.9391	1244.6174
Frequencies --	1267.7524	1283.0411	1313.3247
Frequencies --	1328.1597	1341.5068	1343.6674
Frequencies --	1350.0705	1358.9743	1369.0381
Frequencies --	1375.0232	1411.4819	1414.4358
Frequencies --	1415.0045	1416.4956	1420.4381
Frequencies --	1421.7638	1422.7512	1425.3235
Frequencies --	1427.0899	1429.7303	1430.7255
Frequencies --	1432.3006	1434.6549	1436.9243
Frequencies --	1445.9779	1449.1758	1450.5392
Frequencies --	1457.2985	1461.6830	1470.4255
Frequencies --	1473.3431	1482.2482	1489.7895
Frequencies --	1491.0275	1492.3031	1492.9726
Frequencies --	1494.3667	1498.3713	1499.0893
Frequencies --	1500.4630	1503.6946	1505.6220
Frequencies --	1506.2289	1509.1297	1511.7414
Frequencies --	1517.6706	1520.6089	1576.0962
Frequencies --	1583.9803	1584.1795	1588.8743
Frequencies --	1595.9934	1597.7333	1619.2583
Frequencies --	1622.8598	3009.3323	3011.9834
Frequencies --	3013.5783	3017.0699	3018.0767
Frequencies --	3019.4775	3028.3908	3038.7370
Frequencies --	3045.7469	3103.5911	3105.0118
Frequencies --	3105.8121	3107.8355	3108.6722
Frequencies --	3115.6636	3117.9564	3142.7143
Frequencies --	3144.5404	3147.4614	3149.5563
Frequencies --	3153.4842	3157.0731	3166.3442
Frequencies --	3173.7272	3174.2528	3193.4502
Frequencies --	3198.6721	3201.8577	3205.2627

Catalyst 15:**distal conformation**

vacuum	toluene-like solvent	D3 dispersion
-3312.5761539	-3312.5868124	-0.65408415

Imaginary frequency corresponding to vibration along the reaction coordinate: -235 cm^{-1} .

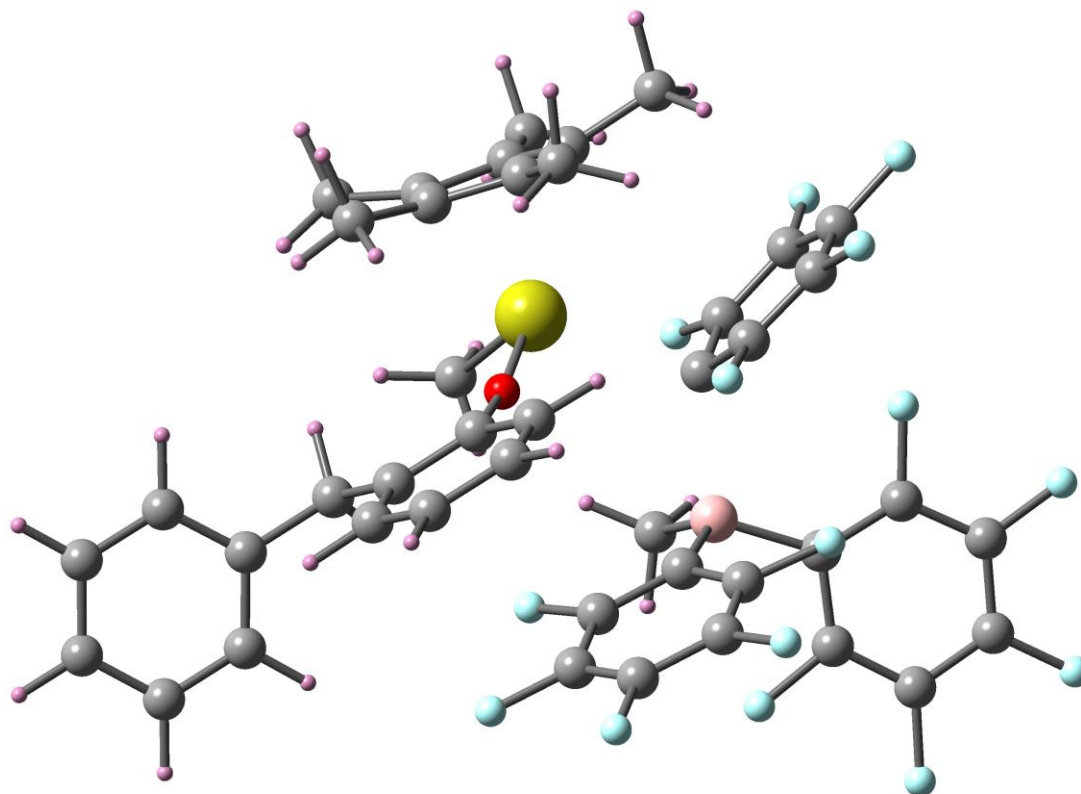
Ti	-1.26122700	1.98464000	-0.88805000
C	-0.81918100	2.04267600	-2.91014800
H	-0.33829600	1.06569000	-3.05422400
H	-1.64601800	2.13860700	-3.62303300
H	-0.09366300	2.85390400	-3.07661100
O	-2.12788000	0.43029400	-0.91613800
C	-3.02648900	-0.58586500	-1.24648400
C	-3.57413200	-1.44773500	-0.24642000
C	-3.35268400	-0.74121200	-2.61648100
C	-4.45425300	-2.46272900	-0.69360800
C	-4.23416800	-1.75809700	-3.02254400
C	-4.78767000	-2.62238400	-2.05503500
H	-4.88275500	-3.14375800	0.04046000
H	-4.47028900	-1.88140300	-4.08111000
C	-1.48346600	4.19868600	0.36494200
C	-1.53983200	4.52674100	-1.03554600
C	-2.57522300	3.29096400	0.66133100

C	-2.69635200	3.86791400	-1.60221000
C	-3.34501400	3.11121400	-0.55100500
F	7.48974300	-2.18593800	0.83712800
C	6.24720000	-1.71630400	0.43809900
C	5.64908900	-0.62581700	1.08545300
C	5.55877000	-2.31948000	-0.62748600
C	4.38537500	-0.16717100	0.65959800
F	6.30298000	-0.00503200	2.14377500
C	4.30055100	-1.81949300	-1.00993100
F	6.12502100	-3.40031400	-1.29291800
C	3.63464300	-0.72537500	-0.39337300
F	3.89011100	0.92257000	1.38769900
F	3.69911100	-2.48861900	-2.08831100
B	2.19499200	-0.26627800	-1.11015500
C	1.17388600	1.36058800	0.02120400
C	1.89598100	2.58141400	-0.06790100
C	0.80972700	1.04845600	1.35928700
C	2.33695100	3.33850300	1.02817500
F	2.21275100	3.11906600	-1.32707800
C	1.20818800	1.76541700	2.50043300
F	-0.03970200	-0.04314000	1.60316800
C	2.00554400	2.91222400	2.32622800
F	3.04995000	4.52165300	0.85796500
F	0.80697500	1.39259300	3.77917800
F	2.40067500	3.65423900	3.42138800
C	-3.19518300	-1.29108000	1.23336400
H	-2.12209700	-1.49916300	1.34270900
H	-3.31246900	-0.23163300	1.50190300
C	1.16013500	-1.53378000	-1.07465300
C	0.41660700	-1.97780900	-2.19377100
C	1.07787300	-2.41644400	0.03293500
C	-0.33179600	-3.16991100	-2.23328500
C	0.31994000	-3.60114200	0.05295600
C	-0.38906200	-3.98904600	-1.09568200
F	1.78785600	-2.14148600	1.20599800
F	0.26123700	-4.39192400	1.19773800
F	-1.14466600	-5.15178000	-1.09787700
F	-1.01820700	-3.53893100	-3.38403700
F	0.39271800	-1.23202300	-3.37884800
C	2.58600100	0.42649100	-2.51354200
H	1.77282600	0.92754300	-3.04146700
H	3.39840100	1.15331400	-2.37672600
H	2.96820400	-0.35855500	-3.18624200
C	-0.66346800	4.93209600	1.40313600
H	-1.23583500	5.82196500	1.71924700
H	-0.48045200	4.34072500	2.30667700
H	0.29604700	5.29735400	1.02153500
C	-0.64915600	5.51439200	-1.75382400
H	-1.11330100	6.51631800	-1.74467500
H	0.33536500	5.61089200	-1.28032500
H	-0.49021000	5.24469800	-2.80620100
C	-2.96523800	2.83051700	2.04804400
H	-3.54278800	1.89852000	2.03794200
H	-2.09359000	2.67190300	2.69742100
H	-3.59706600	3.59287700	2.53655900
C	-3.28525300	4.14429000	-2.96477800
H	-3.97285900	5.00561800	-2.89600300

H	-2.52229100	4.39984700	-3.71062600
H	-3.86811100	3.29727800	-3.35017400
C	-4.70615300	2.46256200	-0.65295500
H	-4.86502700	1.69716900	0.11553200
H	-5.48721200	3.23043800	-0.51441100
H	-4.88138800	1.99167300	-1.62832300
H	-5.46482200	-3.42370000	-2.35601300
H	-2.89648500	-0.08086500	-3.35124000
C	-3.97503700	-2.14506200	2.23112900
C	-5.26272700	-1.75202200	2.67828200
C	-3.41791800	-3.33594600	2.76023200
C	-5.97434600	-2.52329700	3.62136500
H	-5.71500200	-0.83639800	2.28680800
C	-4.12553800	-4.11260400	3.70445900
H	-2.42416600	-3.65821800	2.44124600
C	-5.40685500	-3.70926100	4.13900800
H	-6.96338500	-2.19894000	3.95423600
H	-3.67361900	-5.02489700	4.10074200
H	-5.95315800	-4.30671200	4.87265100

Frequencies --	-234.5283	-30.0747	10.3058
Frequencies --	13.7374	16.0062	26.6066
Frequencies --	28.2186	29.1659	33.8075
Frequencies --	35.3073	38.0112	39.9375
Frequencies --	46.0440	49.4603	53.2488
Frequencies --	56.8937	60.0347	62.1214
Frequencies --	67.2519	74.7759	85.7231
Frequencies --	91.2448	91.8816	96.9475
Frequencies --	103.1230	110.6006	113.5290
Frequencies --	116.8630	120.7176	126.0496
Frequencies --	128.4803	131.7057	135.2288
Frequencies --	144.2487	149.0567	155.6999
Frequencies --	157.8759	165.2431	166.0908
Frequencies --	167.8952	177.6691	187.0680
Frequencies --	196.9085	199.7345	204.3349
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Frequencies --	260.8787	264.0827	265.3592
Frequencies --	265.9195	269.3423	271.0180
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Frequencies --	425.4095	431.4353	434.3506
Frequencies --	441.5977	445.4423	450.2771
Frequencies --	454.3533	465.9112	485.4824
Frequencies --	486.1515	501.0366	526.3031
Frequencies --	535.0804	539.1795	539.7284
Frequencies --	542.8853	551.3582	551.4035
Frequencies --	570.9870	571.7482	580.1258
Frequencies --	589.4278	589.7105	604.1611
Frequencies --	615.5500	620.5634	624.0617
Frequencies --	628.9469	637.1952	641.2187
Frequencies --	644.1748	648.2106	653.0122
Frequencies --	672.3894	690.1116	698.0412
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Frequencies --	716.6961	719.7507	737.3811
Frequencies --	746.0321	749.9911	769.6412
Frequencies --	781.6278	799.6086	804.1392
Frequencies --	806.2322	826.3509	831.6242
Frequencies --	861.7409	867.5304	890.0889
Frequencies --	897.2216	907.4584	917.5674
Frequencies --	926.0963	930.6603	938.1147
Frequencies --	965.1355	968.0167	968.6410
Frequencies --	985.8666	986.7252	991.1080
Frequencies --	995.7557	999.7263	1005.8116
Frequencies --	1022.0880	1035.8360	1038.5332
Frequencies --	1039.9505	1041.6157	1042.1061
Frequencies --	1044.6414	1046.0020	1052.5942
Frequencies --	1054.1160	1057.2138	1059.1964
Frequencies --	1083.5361	1085.3900	1085.8855
Frequencies --	1094.8899	1104.1946	1123.4831
Frequencies --	1171.1698	1173.1701	1175.6766
Frequencies --	1181.0641	1182.8555	1187.9922
Frequencies --	1192.0157	1204.0044	1205.7549
Frequencies --	1212.3030	1213.9204	1221.5219
Frequencies --	1237.4369	1246.5954	1284.8696
Frequencies --	1311.1402	1319.2662	1326.9842
Frequencies --	1336.3174	1341.3071	1351.6579
Frequencies --	1355.6891	1369.4657	1374.1215
Frequencies --	1380.4301	1380.9502	1410.9523
Frequencies --	1414.0183	1414.8597	1422.1379
Frequencies --	1424.2295	1425.4094	1427.3815
Frequencies --	1429.4215	1431.8138	1437.7990
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Frequencies --	1476.3472	1481.8857	1490.1218
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Frequencies --	1502.2101	1505.8775	1507.1802
Frequencies --	1508.4978	1514.5645	1518.6732
Frequencies --	1574.1362	1585.6438	1586.8855
Frequencies --	1596.8891	1597.7363	1605.1511
Frequencies --	1614.0235	1619.6656	1622.4923
Frequencies --	1628.1486	3010.2081	3010.9831
Frequencies --	3011.3424	3014.6477	3016.6613
Frequencies --	3020.1694	3032.4329	3062.0682
Frequencies --	3102.0791	3103.8102	3105.0028
Frequencies --	3112.8078	3115.9570	3116.8197
Frequencies --	3117.0080	3143.9790	3146.4237
Frequencies --	3147.8868	3150.4058	3153.8973
Frequencies --	3156.3603	3159.8935	3164.8876
Frequencies --	3167.1319	3170.0878	3172.7205
Frequencies --	3177.5659	3187.3960	3192.4751
Frequencies --	3194.8197	3206.2695	3223.1213

proximal conformation

vacuum	toluene-like solvent	D3 dispersion
-3312.5802657	-3312.5909977	-0.65550947

Imaginary frequency corresponding to vibration along the reaction coordinate: -230 cm^{-1} .

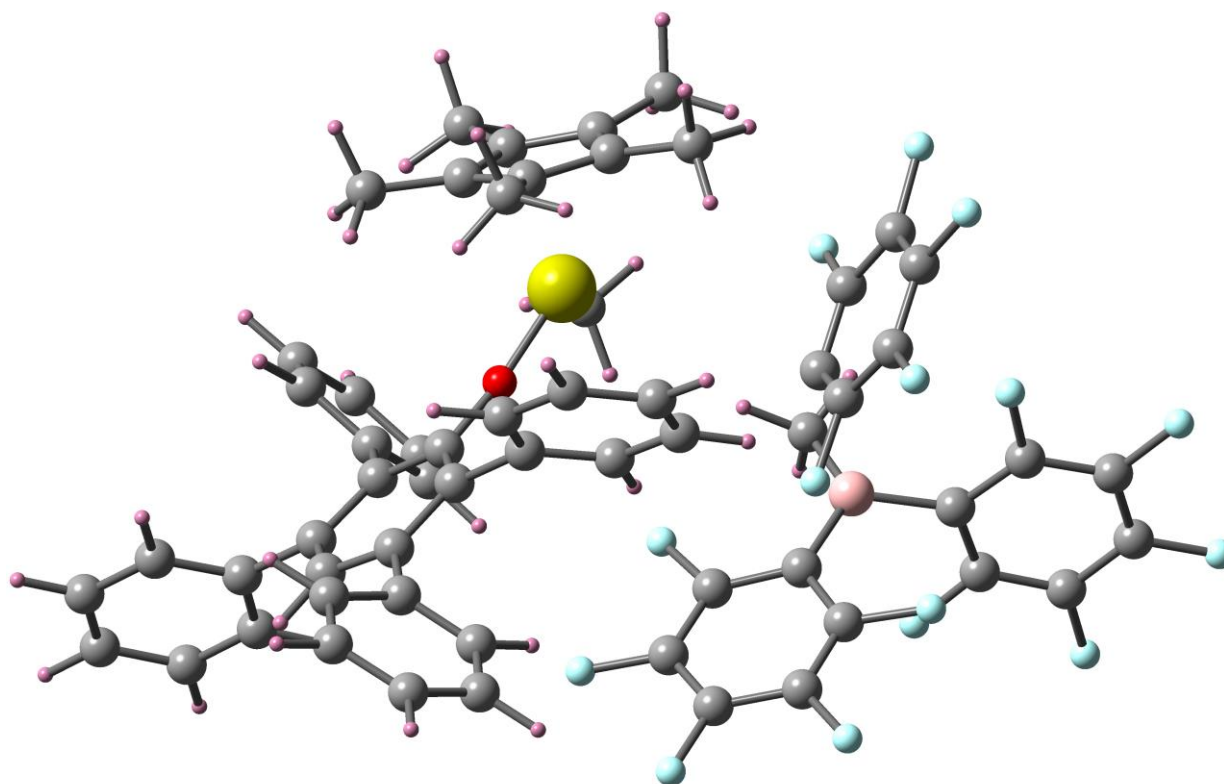
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H	-2.63136800	1.52735100	-2.63104800
H	-0.95397600	2.03495100	-3.02857600
O	-1.96128200	0.65484900	0.44695600
C	-2.74737900	-0.12464400	1.29616600
C	-2.35791300	-0.22876600	2.65342400
C	-3.89322600	-0.81209700	0.78915200
C	-3.11154400	-1.01774800	3.54188400
C	-4.62882600	-1.59191400	1.71223400
C	-4.25375300	-1.69820200	3.06872500
H	-2.80127800	-1.10674500	4.58472500
H	-5.50451900	-2.13503600	1.35967300
C	-0.63101500	4.34649700	0.34982900
C	-1.05823000	4.42452200	-1.02497600
C	-1.69634200	3.74448400	1.12345100
C	-2.41447800	3.92942700	-1.09881100
C	-2.81118500	3.51002700	0.23190400
F	7.33727300	-3.11827400	-1.00227400
C	6.06690000	-2.56370100	-0.95299700

C	5.87398500	-1.24594000	-0.51405000
C	4.94144500	-3.30998100	-1.33976900
C	4.57171800	-0.70574700	-0.47491200
F	6.96498200	-0.48290600	-0.11350600
C	3.66616200	-2.71887500	-1.28166500
F	5.09683300	-4.62105900	-1.77401500
C	3.40071700	-1.39028100	-0.85172000
F	4.50308700	0.60719600	0.00797800
F	2.60788700	-3.55122300	-1.68095800
B	1.80627900	-0.90607600	-0.98599900
C	1.46420200	1.13883900	-0.23133400
C	2.15312900	2.10796200	-1.01018000
C	1.68687100	1.31210100	1.16134100
C	3.05255100	3.06070100	-0.50387300
F	1.95118400	2.15678300	-2.40099800
C	2.58326900	2.23040500	1.73263900
F	0.94814900	0.54287200	2.07847500
C	3.28852100	3.10087900	0.88175100
F	3.68591100	3.98397700	-1.33194600
F	2.75198000	2.33527200	3.11007700
F	4.15111800	4.04120800	1.41205300
C	-4.27079600	-0.70856200	-0.69562300
H	-4.38547800	0.35674700	-0.94559500
H	-3.41344100	-1.06151700	-1.28619500
C	0.88380800	-1.85758500	-0.02980100
C	-0.32397300	-2.45937700	-0.45158300
C	1.32145600	-2.31563200	1.23950500
C	-1.02837800	-3.42901200	0.28597800
C	0.64119700	-3.26404600	2.02466100
C	-0.54670800	-3.83548100	1.53940300
F	2.50838200	-1.82221200	1.79075400
F	1.13081500	-3.64428800	3.26874800
F	-1.23874400	-4.77163000	2.29191000
F	-2.20386500	-3.98462800	-0.21336000
F	-0.90428500	-2.11673700	-1.68128300
C	1.49464400	-0.77835300	-2.56238500
H	0.54597900	-0.30443100	-2.81562400
H	2.29468700	-0.22575500	-3.07351500
H	1.47235800	-1.79045000	-2.99697600
C	0.54764500	5.07887900	0.94715500
H	0.20566100	6.08588100	1.24643500
H	0.94165500	4.60331700	1.85230700
H	1.36965900	5.22688600	0.23938200
C	-0.29521300	5.06683700	-2.16129100
H	-0.55420500	6.13817200	-2.23212500
H	0.79165100	5.00463100	-2.02767900
H	-0.53563100	4.61349900	-3.13213200
C	-1.71230900	3.61749500	2.63061500
H	-2.47683800	2.91438700	2.98092100
H	-0.74478600	3.29005100	3.03740900
H	-1.93687400	4.59820800	3.08576400
C	-3.33639100	4.09082900	-2.28371900
H	-3.77455300	5.10428000	-2.26839400
H	-2.81491500	3.97800900	-3.24254700
H	-4.17053800	3.37753200	-2.26948200
C	-4.21130100	3.13153700	0.65575700
H	-4.22469900	2.43509300	1.50233400

H	-4.75489500	4.03942200	0.97107800
H	-4.78837000	2.67890000	-0.16021400
H	-4.84342500	-2.31897400	3.74585900
H	-1.46047600	0.28524500	2.99068100
C	-5.52502500	-1.45842200	-1.13980600
C	-5.44117800	-2.78738300	-1.62759500
C	-6.79944400	-0.83762000	-1.10164400
C	-6.59522100	-3.47503000	-2.06212500
H	-4.47085300	-3.28607200	-1.66736000
C	-7.95702600	-1.52065700	-1.53416600
H	-6.89000100	0.18725400	-0.73066700
C	-7.85842700	-2.84459800	-2.01700600
H	-6.50637200	-4.49750100	-2.43676100
H	-8.92850700	-1.02156200	-1.49843500
H	-8.75137800	-3.37498400	-2.35607200

Frequencies --	-229.9878	8.6224	14.9939
Frequencies --	17.0644	21.1321	26.9107
Frequencies --	28.2965	32.5350	35.0262
Frequencies --	38.1742	41.7645	43.4047
Frequencies --	49.0041	54.0732	56.5440
Frequencies --	60.0518	63.0385	67.8083
Frequencies --	81.5257	88.6443	92.8512
Frequencies --	101.7267	104.6741	109.5134
Frequencies --	115.2086	120.3324	124.2202
Frequencies --	127.6050	132.2913	135.3770
Frequencies --	142.8621	147.7582	150.2686
Frequencies --	156.0771	157.7210	158.1061
Frequencies --	164.9302	167.1488	177.1462
Frequencies --	179.2465	182.9498	191.0132
Frequencies --	192.1999	201.0162	202.8189
Frequencies --	209.7059	219.4091	221.2883
Frequencies --	226.5728	237.0792	242.3127
Frequencies --	261.5905	262.5523	264.2085
Frequencies --	265.6962	266.6758	271.5648
Frequencies --	271.8704	275.8300	278.2012
Frequencies --	281.1122	288.2860	291.7060
Frequencies --	296.0142	300.3687	301.8634
Frequencies --	303.2746	306.5761	314.2794
Frequencies --	317.5804	326.6882	327.9988
Frequencies --	330.5093	331.7633	333.6926
Frequencies --	370.7436	374.5549	377.4869
Frequencies --	381.6662	384.3549	402.2523
Frequencies --	405.5531	410.3532	421.7599
Frequencies --	424.2317	431.3339	434.2019
Frequencies --	441.2535	447.6402	450.2687
Frequencies --	454.7480	468.0404	485.2711
Frequencies --	486.1284	508.5919	527.6759
Frequencies --	535.7938	539.3034	542.0781
Frequencies --	542.9972	551.3633	551.7145
Frequencies --	569.8520	570.8442	583.3720
Frequencies --	591.1348	591.6062	606.9951
Frequencies --	617.0011	622.0172	623.9708
Frequencies --	628.8020	637.5329	641.4896
Frequencies --	643.7935	649.1861	653.0518
Frequencies --	671.3809	690.2886	698.0011
Frequencies --	706.9666	710.9521	714.9131
Frequencies --	716.9861	719.6242	737.8227
Frequencies --	746.2658	749.5020	770.8778
Frequencies --	782.1864	800.6087	804.8097
Frequencies --	806.7269	828.8724	832.4555

Frequencies --	863.7091	871.8009	888.1749
Frequencies --	895.7614	907.1696	914.8043
Frequencies --	932.1391	934.7818	938.5613
Frequencies --	965.1946	970.2323	970.4385
Frequencies --	984.5887	988.3700	990.7186
Frequencies --	997.5270	1000.2518	1006.9393
Frequencies --	1022.0933	1033.2508	1036.3472
Frequencies --	1041.9303	1042.0797	1046.0855
Frequencies --	1047.3644	1048.4039	1053.1147
Frequencies --	1053.9404	1056.5498	1059.5715
Frequencies --	1086.0415	1087.1996	1088.4159
Frequencies --	1094.0018	1105.8475	1124.9285
Frequencies --	1171.3656	1173.0939	1175.6356
Frequencies --	1180.6178	1182.1877	1188.7167
Frequencies --	1191.8367	1203.6728	1209.4675
Frequencies --	1214.2719	1215.2715	1221.8831
Frequencies --	1237.4752	1244.4947	1287.9009
Frequencies --	1310.9828	1320.5909	1327.4023
Frequencies --	1336.0102	1342.8217	1351.6476
Frequencies --	1357.3340	1367.4789	1374.8153
Frequencies --	1378.6983	1379.8977	1411.5510
Frequencies --	1413.5140	1414.5454	1422.3656
Frequencies --	1423.4359	1426.3639	1428.6243
Frequencies --	1431.1406	1431.2172	1434.6884
Frequencies --	1445.3768	1446.6663	1448.0289
Frequencies --	1450.0194	1455.1034	1457.5929
Frequencies --	1463.5366	1471.5491	1473.5155
Frequencies --	1478.0257	1483.4672	1491.3806
Frequencies --	1491.9548	1493.1339	1495.9427
Frequencies --	1499.6278	1500.3625	1501.7164
Frequencies --	1502.4155	1506.8944	1508.2517
Frequencies --	1511.5390	1515.6185	1518.4505
Frequencies --	1573.9349	1584.8655	1585.4860
Frequencies --	1596.9452	1597.9979	1604.0492
Frequencies --	1614.0660	1620.7671	1622.7071
Frequencies --	1627.5016	3008.8130	3009.1557
Frequencies --	3011.4281	3012.3323	3013.0091
Frequencies --	3014.2221	3037.2909	3049.5510
Frequencies --	3096.9628	3103.8060	3104.4618
Frequencies --	3105.5422	3112.0061	3113.1814
Frequencies --	3121.1064	3138.8742	3143.4069
Frequencies --	3146.7914	3150.2422	3152.7530
Frequencies --	3156.7769	3159.1670	3164.6339
Frequencies --	3168.7146	3169.8873	3171.8450
Frequencies --	3181.5674	3187.7495	3194.1676
Frequencies --	3206.6456	3207.2903	3228.9285

Catalyst 16:

vacuum	toluene-like solvent	D3 dispersion
-3966.1030953	-3966.119655	-0.84422840

Imaginary frequency corresponding to vibration along the reaction coordinate: -98 cm^{-1} .

Ti	-1.15116100	2.24154600	-1.08666000
C	-0.18934700	1.31126600	-2.63897100
H	0.11882500	0.37176400	-2.14487600
H	-0.84596400	1.06742600	-3.48427500
H	0.69844000	1.85365900	-2.98805700
O	-2.25478100	0.97133200	-0.48868500
C	-3.24029200	0.09848700	-0.02482000
C	-3.52837000	0.07585700	1.37884800
C	-3.94116700	-0.70321300	-0.98056000
C	-4.58524800	-0.77694900	1.82536300
C	-5.02616400	-1.50085100	-0.51202900
C	-5.32634400	-1.50730200	0.86857000
C	-0.68087700	4.57742000	-0.69273100
C	-0.40804200	4.40562300	-2.10507000
C	-2.08633600	4.30193400	-0.46720100
C	-1.62271400	3.95823800	-2.74091100
C	-2.66659700	3.88847300	-1.72480300
F	9.55233300	-2.27214600	-0.19462000
C	8.19732600	-2.02628100	-0.36493900
C	7.64733600	-0.78535400	0.00093600
C	7.35820100	-3.01478900	-0.90965200
C	6.26883100	-0.54979300	-0.18224500
F	8.46650500	0.19724400	0.54209300

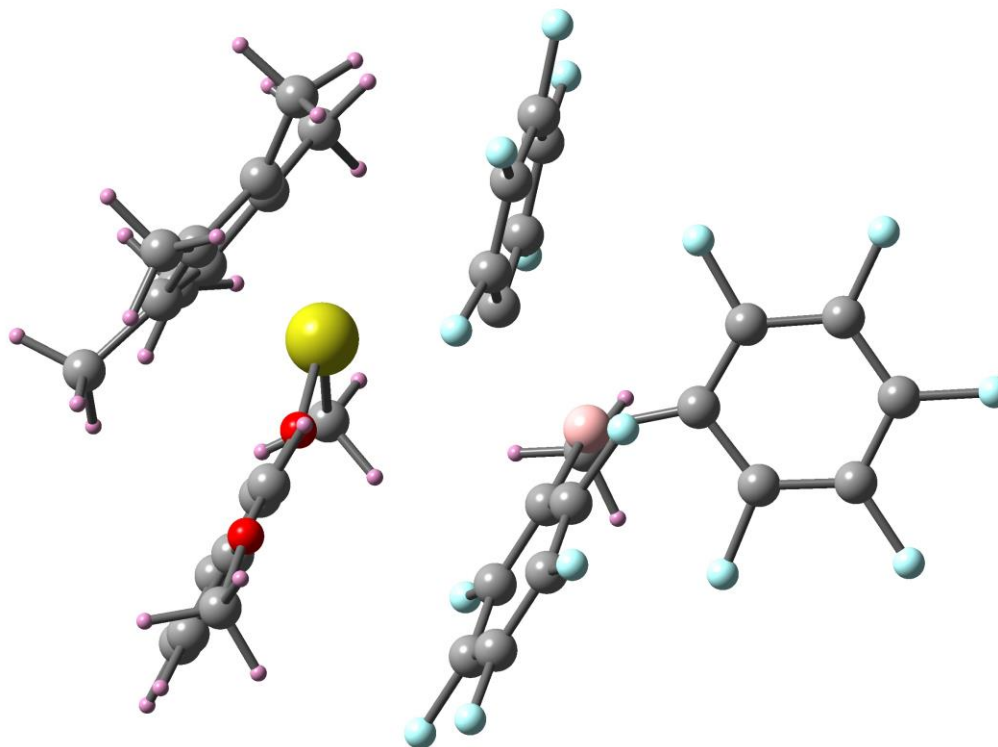
C	5.99022500	-2.73124500	-1.06889800
F	7.88289800	-4.24655100	-1.28155500
C	5.38361300	-1.50562300	-0.71570600
F	5.79837900	0.70215600	0.21464800
F	5.18755400	-3.74605500	-1.61994200
B	3.81021800	-1.34961600	-1.07705900
C	2.74772500	1.13965200	0.03335400
C	3.28835000	2.27198200	-0.57257900
C	2.66910400	1.20851700	1.42095600
C	3.76703700	3.39646800	0.12504900
F	3.37470700	2.34992900	-1.99970300
C	3.13213800	2.28733100	2.19835900
F	2.05720700	0.13670500	2.15098200
C	3.69552000	3.39378800	1.53215700
F	4.27128900	4.53467200	-0.52963000
F	3.02730400	2.31357500	3.59908500
F	4.13672700	4.49929000	2.25812300
C	2.77929300	-2.18906800	-0.19216800
C	1.52997300	-2.65129200	-0.67631000
C	3.05781800	-2.59529000	1.14047900
C	0.63068100	-3.42499000	0.07855400
C	2.18461900	-3.36136800	1.93335100
C	0.95527100	-3.78127300	1.39815000
F	4.23926300	-2.19912700	1.76112800
F	2.51667900	-3.69802100	3.23781300
F	0.07304100	-4.53199300	2.15947400
F	-0.58336000	-3.83676300	-0.47077700
F	1.10755100	-2.35065600	-1.97662800
C	3.55174400	-0.88628800	-2.56818900
H	2.54716700	-0.50113800	-2.75754800
H	4.28136300	-0.12553200	-2.87695500
H	3.70217900	-1.76800300	-3.22229100
C	0.28168100	5.09241000	0.35628000
H	-0.03135600	6.09641000	0.68821600
H	0.31777700	4.45902400	1.25648300
H	1.30290100	5.17891300	-0.02806300
C	0.88458000	4.73886200	-2.80964100
H	0.86636900	5.79996300	-3.11497900
H	1.76759900	4.59787600	-2.17827500
H	1.03176100	4.14299500	-3.71886800
C	-2.84258900	4.56728500	0.81180200
H	-3.60920600	3.81185300	1.01916000
H	-2.18157900	4.61294600	1.68480600
H	-3.35361700	5.54312600	0.73302400
C	-1.83175500	3.77897800	-4.22497400
H	-2.11472300	4.74581500	-4.67708600
H	-0.92330400	3.43514900	-4.73516700
H	-2.63380100	3.06427500	-4.44993200
C	-4.13788600	3.65411100	-1.97839400
H	-4.64922300	3.24583400	-1.09622700
H	-4.62753600	4.61137700	-2.22884900
H	-4.31214400	2.96769600	-2.81553200
H	-6.12139700	-2.16332800	1.22009500
C	-4.93174900	-0.99631800	3.27417600
C	-3.97493600	-1.49870700	4.19430100
C	-6.25882500	-0.78613500	3.73244400
C	-4.33209400	-1.77365300	5.53040700

H	-2.95339600	-1.69017500	3.86384200
C	-6.61672600	-1.05230100	5.07108300
H	-7.01311900	-0.40245000	3.04157600
C	-5.65316500	-1.54773500	5.97673400
H	-3.58059800	-2.16774300	6.21830500
H	-7.64235400	-0.87515600	5.40359500
H	-5.92797200	-1.75944900	7.01259500
C	-5.86487100	-2.37475300	-1.40884400
C	-7.24844500	-2.10053400	-1.56570000
C	-5.32865500	-3.52134900	-2.04874100
C	-8.07024900	-2.93609500	-2.35201100
H	-7.68214800	-1.22542100	-1.07603500
C	-6.14952500	-4.36244800	-2.82886400
H	-4.27343400	-3.76695900	-1.92557900
C	-7.52255600	-4.07176600	-2.98794800
H	-9.13162600	-2.70228600	-2.46478600
H	-5.71722600	-5.24462600	-3.30677900
H	-8.15659300	-4.72325800	-3.59377700
C	-2.77419300	0.93511000	2.35506700
C	-1.36891700	0.81716000	2.52803200
C	-3.47728300	1.84519100	3.18867900
C	-0.69456700	1.56915700	3.51577800
H	-0.80084500	0.09968200	1.93337600
C	-2.80594900	2.60385100	4.16837000
H	-4.55795300	1.94606200	3.08160300
C	-1.41089200	2.46556300	4.33893800
H	0.37595300	1.43106400	3.65688000
H	-3.37230600	3.28830400	4.80438600
H	-0.88845600	3.03515700	5.11074300
C	-3.55565300	-0.73428900	-2.43601500
C	-4.34955200	-0.10123800	-3.42508700
C	-2.43402800	-1.49460000	-2.85234800
C	-4.02862600	-0.22032600	-4.79434600
H	-5.23609400	0.46137100	-3.12579600
C	-2.11367300	-1.62129500	-4.22008100
H	-1.83140400	-2.00911400	-2.10444300
C	-2.90931900	-0.98254600	-5.19698300
H	-4.66097000	0.26254600	-5.54346300
H	-1.25003900	-2.21977400	-4.51779100
H	-2.66730100	-1.08672500	-6.25712800

Frequencies --	-98.4603	-4.4148	8.2376
Frequencies --	9.4647	12.2855	12.8777
Frequencies --	14.9423	18.1594	21.1269
Frequencies --	23.0995	26.5498	30.1075
Frequencies --	32.1406	34.4240	35.8813
Frequencies --	39.2834	42.7842	43.6901
Frequencies --	46.6497	48.6664	51.3021
Frequencies --	56.4056	59.2476	63.6744
Frequencies --	64.3058	70.0721	72.0806
Frequencies --	78.2608	89.2355	91.9161
Frequencies --	102.0285	104.7286	108.0534
Frequencies --	113.1177	115.3677	116.5933
Frequencies --	118.5804	120.1037	123.3352
Frequencies --	125.2845	134.1518	137.7029
Frequencies --	140.4782	141.5951	143.6079
Frequencies --	144.0119	152.0077	153.7817
Frequencies --	155.6925	160.1008	163.3110

Frequencies --	176.4441	178.5217	183.1290
Frequencies --	194.2547	195.0802	198.0378
Frequencies --	209.4842	210.4730	211.2212
Frequencies --	213.1915	218.8621	228.7080
Frequencies --	248.9618	253.4460	254.9270
Frequencies --	257.6090	259.2595	263.9319
Frequencies --	264.9090	265.7499	268.6352
Frequencies --	276.9276	277.6805	284.8811
Frequencies --	288.3463	289.4393	290.7207
Frequencies --	293.9201	297.7286	302.1484
Frequencies --	304.5392	308.6138	316.9506
Frequencies --	321.9576	327.1432	333.7189
Frequencies --	334.1542	348.3695	373.6326
Frequencies --	378.9846	379.2211	389.7144
Frequencies --	395.1618	402.6952	404.4017
Frequencies --	405.5648	405.9342	408.1638
Frequencies --	412.8672	415.8530	419.7589
Frequencies --	420.7107	425.0434	430.4156
Frequencies --	431.1331	446.1378	448.0680
Frequencies --	453.1619	482.3874	486.6150
Frequencies --	507.3012	517.3958	527.5267
Frequencies --	527.8317	531.7442	536.3873
Frequencies --	539.3266	542.0346	545.5108
Frequencies --	549.4024	550.2320	551.8716
Frequencies --	556.3882	581.1967	587.6037
Frequencies --	598.1179	608.5721	613.3075
Frequencies --	615.9357	617.1842	619.7662
Frequencies --	623.9362	628.2743	629.3660
Frequencies --	630.9720	633.3974	637.0235
Frequencies --	639.2161	640.1911	647.2422
Frequencies --	656.4172	665.8695	672.2665
Frequencies --	689.9520	695.1570	697.8513
Frequencies --	709.4809	709.5265	716.3959
Frequencies --	716.6640	720.8694	722.2885
Frequencies --	746.0039	746.3240	748.1157
Frequencies --	765.1297	765.7421	774.2689
Frequencies --	784.2017	791.6664	795.9412
Frequencies --	800.1972	805.1456	806.1231
Frequencies --	844.2453	858.2654	858.9943
Frequencies --	859.9504	861.7676	871.7507
Frequencies --	876.5682	879.4107	908.6820
Frequencies --	914.4378	915.2567	933.7980
Frequencies --	937.1219	938.3844	944.1655
Frequencies --	948.0445	961.8785	965.4843
Frequencies --	976.0229	978.2340	984.4520
Frequencies --	987.8015	994.6012	995.9249
Frequencies --	999.0812	1000.8112	1004.8789
Frequencies --	1007.0976	1010.2135	1013.2315
Frequencies --	1014.1427	1019.7958	1022.3105
Frequencies --	1026.8693	1040.0119	1040.2408
Frequencies --	1044.4195	1045.2786	1045.8035
Frequencies --	1047.5396	1049.9310	1050.2949
Frequencies --	1052.7983	1053.6683	1058.4504
Frequencies --	1062.5990	1089.3505	1089.6704
Frequencies --	1090.1398	1090.8007	1092.0190
Frequencies --	1092.1485	1100.4036	1125.2263
Frequencies --	1126.9246	1129.1389	1130.0692
Frequencies --	1136.2934	1171.4802	1175.0102
Frequencies --	1183.2997	1184.0235	1184.1572
Frequencies --	1187.6654	1192.2199	1204.6657
Frequencies --	1206.4781	1207.0897	1208.0140
Frequencies --	1217.9137	1228.0867	1232.2073
Frequencies --	1243.8641	1257.4965	1281.5118

Frequencies --	1305.2874	1318.3889	1328.3780
Frequencies --	1332.1007	1332.2685	1333.9162
Frequencies --	1335.4025	1338.5475	1346.1533
Frequencies --	1357.7042	1362.8679	1363.6637
Frequencies --	1366.8430	1368.4456	1369.8359
Frequencies --	1371.0758	1378.6532	1385.2533
Frequencies --	1408.7677	1411.0283	1414.7711
Frequencies --	1419.8776	1421.3283	1425.6604
Frequencies --	1426.2750	1429.3232	1429.9068
Frequencies --	1430.1397	1432.0139	1436.1221
Frequencies --	1441.5058	1443.3502	1445.3086
Frequencies --	1447.4973	1448.2315	1449.6956
Frequencies --	1456.8582	1459.3221	1460.3831
Frequencies --	1471.0138	1472.9849	1480.1447
Frequencies --	1489.4586	1490.7546	1494.0719
Frequencies --	1495.5460	1497.0806	1497.2458
Frequencies --	1498.8554	1502.1624	1502.8294
Frequencies --	1506.6959	1508.9614	1509.8735
Frequencies --	1512.5361	1519.3976	1526.9971
Frequencies --	1575.8444	1586.9936	1588.1931
Frequencies --	1593.5966	1594.7224	1596.1523
Frequencies --	1597.0099	1598.3044	1598.5069
Frequencies --	1619.1971	1619.3249	1623.2066
Frequencies --	1623.6409	1624.1313	1624.3247
Frequencies --	2992.2946	2997.5980	3011.6944
Frequencies --	3012.0243	3013.1491	3016.6662
Frequencies --	3017.5670	3091.9808	3106.3571
Frequencies --	3108.1869	3110.1143	3116.4666
Frequencies --	3118.6857	3126.0913	3148.3876
Frequencies --	3151.5363	3152.6423	3153.0810
Frequencies --	3154.2348	3157.9033	3160.0400
Frequencies --	3161.7619	3163.6698	3166.3246
Frequencies --	3166.4624	3168.2979	3172.2214
Frequencies --	3173.5378	3176.8111	3177.4421
Frequencies --	3178.3835	3180.7405	3185.6171
Frequencies --	3185.9165	3189.3687	3191.6771
Frequencies --	3192.6566	3194.7514	3197.9322
Frequencies --	3198.1667	3209.1120	3227.8202

Catalyst 17:**distal conformation**

vacuum	toluene-like solvent	D3 dispersion
-3156.8201207	-3156.8305403	-0.57958918

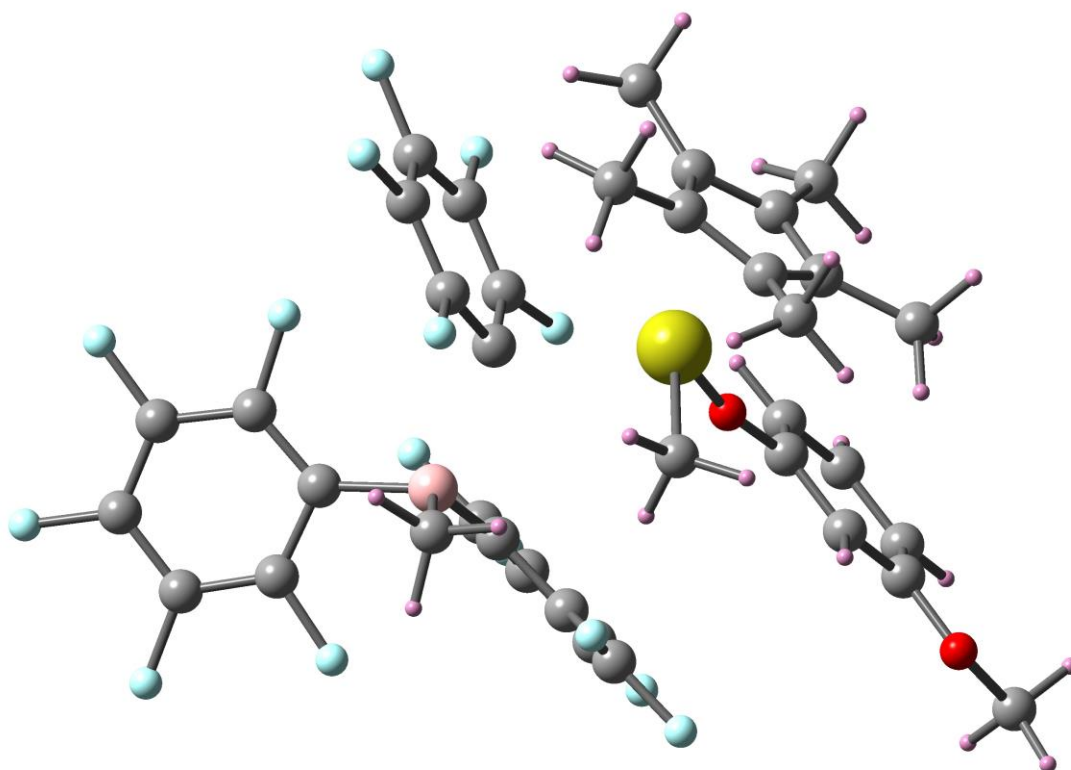
Imaginary frequency corresponding to vibration along the reaction coordinate: -226 cm^{-1} .

Ti	2.02048400	-1.34657500	-0.77354800
C	1.94372600	-1.14770500	-2.83689700
H	1.30772400	-0.25981400	-2.95772700
H	2.89789400	-0.96903200	-3.34784000
H	1.45445600	-2.03355300	-3.27341900
O	2.44300000	0.33478800	-0.41368200
C	3.05011600	1.55163200	-0.13345900
C	2.95469300	2.09239500	1.16351300
C	3.71796100	2.24601400	-1.17460800
C	3.53412700	3.35631600	1.43028300
C	4.29104300	3.49716200	-0.88745800
C	4.20957400	4.06401500	0.40373000
H	4.79553900	4.05009900	-1.68228400
C	2.81251900	-3.23643100	0.65042800
C	2.68808900	-3.77569700	-0.68520500
C	3.79552100	-2.17545900	0.61977700
C	3.62027900	-3.07320100	-1.53559200
C	4.29971100	-2.07679100	-0.73204900
F	-7.58366500	0.41044300	0.02225000
C	-6.21414300	0.31884500	-0.17890400

C	-5.45801400	-0.67441600	0.45986200
C	-5.55046100	1.22046400	-1.02729700
C	-4.06729600	-0.74695100	0.23593800
F	-6.08166000	-1.57705800	1.31419400
C	-4.16135500	1.09998000	-1.21443800
F	-6.26938400	2.22032100	-1.67185100
C	-3.33682200	0.11719100	-0.60191100
F	-3.41887800	-1.76416100	0.94846900
F	-3.59487900	2.05388900	-2.07558200
B	-1.73582300	0.12918800	-1.08842400
C	-0.52433900	-1.36180000	-0.03843100
C	-0.92805200	-2.69011700	-0.34541400
C	-0.38840000	-1.15192000	1.36241900
C	-1.26773900	-3.67247200	0.59985300
F	-1.00183600	-3.10017500	-1.68826200
C	-0.73142000	-2.08069600	2.35879300
F	0.16045900	0.05245700	1.82951900
C	-1.19047500	-3.35137800	1.96679500
F	-1.65181800	-4.95530000	0.21976100
F	-0.57763400	-1.79749700	3.71150400
F	-1.50059100	-4.30194900	2.92092700
C	-1.07654400	1.57142900	-0.68482100
C	-0.29976600	2.35918600	-1.56592200
C	-1.39373700	2.23818300	0.52652200
C	0.12074700	3.67532200	-1.29571400
C	-0.97996400	3.54217300	0.85298200
C	-0.21616900	4.27280100	-0.07167900
F	-2.17442300	1.59768900	1.49469700
F	-1.31992500	4.11599200	2.07267200
F	0.21403700	5.55818900	0.22821100
F	0.87430600	4.38521400	-2.22492900
F	0.10279100	1.85663300	-2.80993500
C	-1.72392400	-0.37674500	-2.62082600
H	-0.74005600	-0.60206400	-3.03285200
H	-2.35315100	-1.26922100	-2.74129700
H	-2.16166700	0.41442900	-3.25002700
C	2.27217000	-3.84893900	1.92197100
H	3.05968100	-4.48261200	2.36653200
H	2.00437800	-3.10387300	2.68187700
H	1.40734900	-4.49754700	1.75121200
C	1.89183900	-4.99026400	-1.10938200
H	2.57548400	-5.83719200	-1.29226700
H	1.17544700	-5.31244900	-0.34614700
H	1.33108000	-4.82516900	-2.04050900
C	4.33134300	-1.45597200	1.83604400
H	4.82609500	-0.51178000	1.58103000
H	3.54681700	-1.22994800	2.57193000
H	5.07747300	-2.09178900	2.34449600
C	4.00190400	-3.50135100	-2.93163000
H	4.71423900	-4.34306300	-2.87116600
H	3.13937500	-3.84835500	-3.51614000
H	4.49398000	-2.70161700	-3.49913100
C	5.45558500	-1.22013700	-1.19385000
H	5.59344600	-0.33003900	-0.56923200
H	6.39197000	-1.80325600	-1.14615700
H	5.33715500	-0.88268700	-2.23267000
H	4.65336900	5.04016900	0.58800800

H	2.41744200	1.57279000	1.95276200
H	3.75745100	1.82327200	-2.17677900
O	3.37039600	3.80286100	2.74462200
C	3.80469500	5.16025500	3.09461100
H	3.28769700	5.91497900	2.47921100
H	3.51904200	5.28226600	4.14616600
H	4.89735500	5.27287800	2.99205900
Frequencies --	-225.5713	6.2327	13.8412
Frequencies --	15.2591	21.5948	27.6943
Frequencies --	33.0047	35.2620	39.6945
Frequencies --	44.3191	47.9183	53.0282
Frequencies --	56.9113	59.6970	63.6077
Frequencies --	78.3379	85.4485	91.5481
Frequencies --	94.2868	100.8347	106.7288
Frequencies --	110.1086	111.9365	115.8408
Frequencies --	119.1890	120.7059	127.7404
Frequencies --	128.3574	135.7710	143.1653
Frequencies --	144.2574	145.6389	150.0887
Frequencies --	157.2287	159.3870	164.9409
Frequencies --	166.6816	173.5486	185.3837
Frequencies --	194.9972	198.0264	198.3859
Frequencies --	203.3923	211.5012	222.5747
Frequencies --	235.2844	236.1566	241.9599
Frequencies --	256.0225	258.3835	263.9043
Frequencies --	265.9187	267.2200	267.5615
Frequencies --	271.4071	275.1403	275.5877
Frequencies --	277.6170	280.3908	285.8589
Frequencies --	291.2094	294.6317	297.2418
Frequencies --	301.2137	304.0669	306.2224
Frequencies --	313.9978	316.5801	321.0892
Frequencies --	324.9724	329.1359	333.5574
Frequencies --	370.7879	374.0972	375.1854
Frequencies --	381.7683	386.2623	399.8682
Frequencies --	407.6323	413.2948	422.7745
Frequencies --	425.0149	431.0001	434.0116
Frequencies --	441.8108	450.5662	455.2737
Frequencies --	457.2326	478.1789	485.3538
Frequencies --	508.7971	529.8888	535.0226
Frequencies --	539.7338	542.6186	551.1329
Frequencies --	552.5095	558.6745	571.2000
Frequencies --	585.1776	592.6416	594.1386
Frequencies --	605.0755	605.8696	614.9389
Frequencies --	628.8634	637.5828	642.3935
Frequencies --	644.6430	650.0717	651.6842
Frequencies --	673.2850	677.9468	692.3173
Frequencies --	697.6215	714.5528	716.7979
Frequencies --	719.5065	737.5731	749.8423
Frequencies --	762.7815	781.4672	784.6324
Frequencies --	798.7280	806.5339	830.4336
Frequencies --	841.6899	870.5702	890.2663
Frequencies --	897.5912	907.4998	917.3091
Frequencies --	950.3898	963.7513	964.2100
Frequencies --	969.8635	986.0097	988.5731
Frequencies --	991.2077	996.0124	1024.9563
Frequencies --	1036.3352	1038.2027	1040.5520
Frequencies --	1040.8522	1044.6960	1048.2111
Frequencies --	1048.7866	1057.3371	1058.9829
Frequencies --	1084.8868	1085.8941	1086.7589
Frequencies --	1098.3461	1123.0661	1127.2691
Frequencies --	1163.7583	1172.2229	1173.1087
Frequencies --	1174.9454	1176.0721	1189.4934

Frequencies --	1200.9923	1213.4435	1221.8785
Frequencies --	1246.3417	1268.7075	1303.3695
Frequencies --	1310.1371	1326.6372	1334.4814
Frequencies --	1342.0329	1356.6471	1370.0800
Frequencies --	1379.5869	1384.9779	1410.8852
Frequencies --	1413.4183	1413.6869	1422.6128
Frequencies --	1423.5763	1425.8085	1428.6774
Frequencies --	1431.8288	1433.6180	1438.0297
Frequencies --	1445.4591	1447.9026	1450.4335
Frequencies --	1453.9081	1456.1217	1457.4599
Frequencies --	1463.0964	1470.1836	1472.8041
Frequencies --	1481.9176	1483.6125	1485.4255
Frequencies --	1488.6243	1490.7121	1491.8642
Frequencies --	1492.5596	1496.6304	1499.3474
Frequencies --	1503.1928	1504.5558	1505.4675
Frequencies --	1508.6044	1514.4674	1519.3806
Frequencies --	1573.9123	1585.6893	1588.8107
Frequencies --	1596.7330	1598.2055	1618.1115
Frequencies --	1619.5200	1622.1310	2996.9998
Frequencies --	3008.3195	3009.4335	3010.4834
Frequencies --	3011.7771	3014.2779	3015.4664
Frequencies --	3037.1388	3097.7139	3097.7587
Frequencies --	3100.0583	3100.4718	3102.9335
Frequencies --	3108.3569	3120.5428	3138.5340
Frequencies --	3145.7057	3149.7298	3156.0005
Frequencies --	3158.4502	3159.8431	3161.3038
Frequencies --	3169.7339	3176.5460	3206.4167
Frequencies --	3214.1254	3221.8089	3236.9700

proximal conformation

vacuum	toluene-like solvent	D3 dispersion
-3156.820176	-3156.8308366	-0.57800022

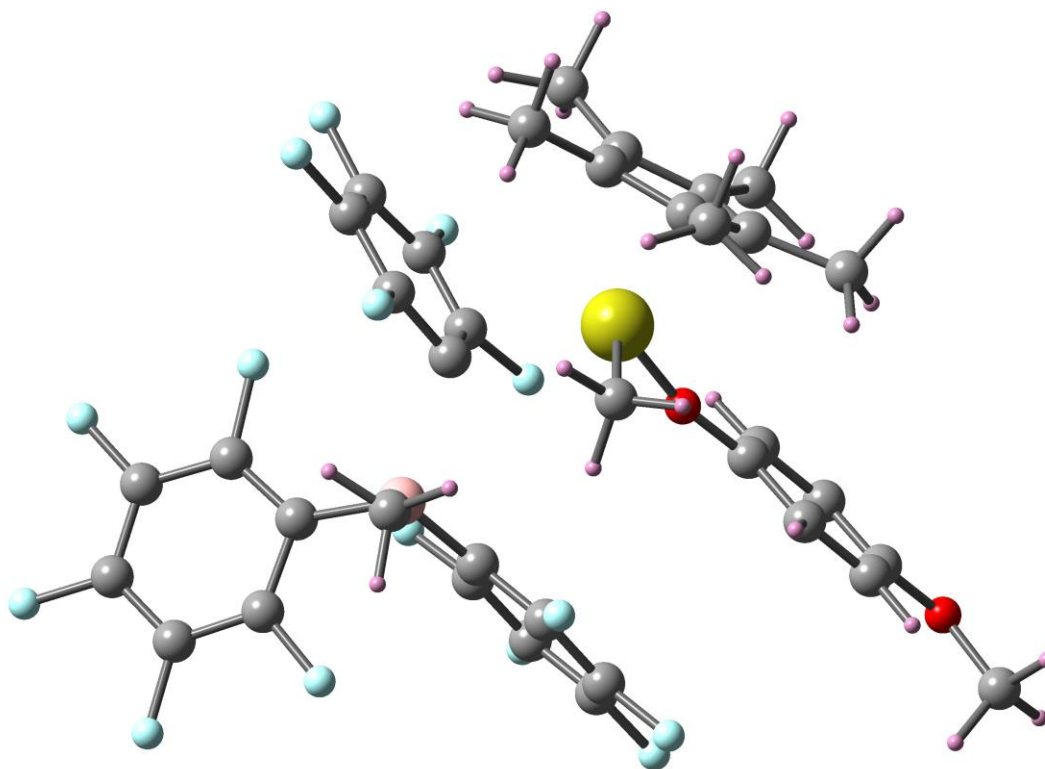
Imaginary frequency corresponding to vibration along the reaction coordinate: -230 cm^{-1} .

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C	1.96405000	-1.03478500	-2.63777900
H	1.46824500	-0.05417000	-2.65341600
H	2.97022500	-0.92612500	-3.06057900
H	1.39127500	-1.76555800	-3.23218800
O	2.43982800	-0.01104700	0.01754800
C	3.16475900	1.05273700	0.53801600
C	3.02604900	1.40061100	1.90599800
C	3.99984300	1.79010200	-0.32434400
C	3.74488200	2.50843700	2.39032700
C	4.71762900	2.89865900	0.18403900
C	4.59222400	3.26309600	1.54872100
H	3.63863400	2.79790600	3.43780500
C	2.16669900	-3.76050600	0.47777500
C	2.16358400	-4.02182100	-0.94338800
C	3.25986000	-2.85974900	0.77041400
C	3.28403900	-3.32047900	-1.52611300
C	3.95754300	-2.59266800	-0.46860000
F	-7.52797000	1.41197300	-0.38028900
C	-6.16615000	1.16660100	-0.47844200
C	-5.59936000	0.01908900	0.09455200
C	-5.32072000	2.06331700	-1.15256500

C	-4.21217400	-0.20751900	-0.02080900
F	-6.40603800	-0.88399600	0.77815300
C	-3.94420800	1.78521000	-1.23844100
F	-5.84955800	3.21373500	-1.72613300
C	-3.30671900	0.64108100	-0.68604200
F	-3.76001900	-1.36984100	0.61724700
F	-3.18600600	2.74884200	-1.92277400
B	-1.67562700	0.49901200	-1.02926900
C	-0.76547200	-1.26058200	-0.07959000
C	-1.30737600	-2.47760900	-0.57444900
C	-0.72582300	-1.22901300	1.34221900
C	-1.85359900	-3.50227500	0.21639000
F	-1.31321200	-2.72079300	-1.95924300
C	-1.26767800	-2.20929600	2.19031900
F	-0.07971100	-0.16622200	1.99336600
C	-1.85468500	-3.35063200	1.61415400
F	-2.36371900	-4.67019300	-0.34499100
F	-1.19595500	-2.10313500	3.57560000
F	-2.36810300	-4.34908800	2.41996000
C	-0.88681200	1.77668900	-0.37969000
C	0.07788800	2.54737700	-1.06989700
C	-1.24319500	2.32827400	0.87789300
C	0.63946200	3.74283400	-0.58231500
C	-0.70022500	3.50870000	1.41602400
C	0.25043500	4.22915500	0.67490300
F	-2.19616100	1.68968600	1.67865400
F	-1.09148400	3.96865600	2.66866800
F	0.80958400	5.39230500	1.18491500
F	1.58255200	4.44132600	-1.32913600
F	0.54254100	2.15126300	-2.33007500
C	-1.56884800	0.18319500	-2.60823400
H	-0.58208600	-0.11317900	-2.96423500
H	-2.28177100	-0.60155300	-2.89647400
H	-1.84849100	1.09256000	-3.16362600
C	1.39025500	-4.52186200	1.52719800
H	2.02590700	-5.34433700	1.90038100
H	1.12499800	-3.91148500	2.39936600
H	0.47921800	-4.98445400	1.13491600
C	1.28516600	-5.00590500	-1.68321600
H	1.81692700	-5.96705700	-1.79750600
H	0.34590900	-5.21554200	-1.16019000
H	1.02851300	-4.65902100	-2.69382400
C	3.70164100	-2.44621600	2.15590100
H	4.31117900	-1.53505000	2.14626100
H	2.85222500	-2.27142900	2.83112400
H	4.31396600	-3.24648700	2.60719900
C	3.81108600	-3.54275200	-2.92280100
H	4.38436700	-4.48619500	-2.94847000
H	3.01014800	-3.63085300	-3.66863200
H	4.48847200	-2.74368800	-3.24908000
C	5.26647600	-1.85177700	-0.61151100
H	5.41184500	-1.10200800	0.17466200
H	6.10558200	-2.56634400	-0.54361600
H	5.35622000	-1.33913700	-1.57880500
H	5.12703800	4.11780400	1.95768400
H	2.35659000	0.83490500	2.54969300
H	4.08452500	1.53706300	-1.37872200

O	5.51893600	3.55294200	-0.75607100
C	6.19852600	4.79400600	-0.36817800
H	6.70868400	5.13018800	-1.27872900
H	5.47482400	5.55965000	-0.04356900
H	6.94123600	4.61506400	0.42767500
Frequencies --	-230.3405	12.5821	17.5401
Frequencies --	19.3263	21.3563	28.6708
Frequencies --	34.6845	36.6179	41.4301
Frequencies --	47.3382	48.4678	51.3100
Frequencies --	56.0670	57.6556	62.3787
Frequencies --	72.4492	81.5589	91.2549
Frequencies --	94.7145	103.9592	109.9716
Frequencies --	110.4429	115.9322	120.8715
Frequencies --	124.8225	126.9630	129.2815
Frequencies --	133.2653	137.6658	143.1163
Frequencies --	147.3942	149.6617	154.2571
Frequencies --	157.5500	162.9626	164.5870
Frequencies --	167.2300	175.5859	183.9403
Frequencies --	186.0854	195.3703	200.1739
Frequencies --	203.7237	209.6339	222.0540
Frequencies --	230.0565	234.8804	243.3130
Frequencies --	252.7482	261.0798	264.1786
Frequencies --	265.2896	267.1299	268.0795
Frequencies --	271.6728	274.3074	277.7456
Frequencies --	280.6159	282.6498	289.2348
Frequencies --	295.0976	297.5677	300.9720
Frequencies --	302.0139	305.5678	308.8936
Frequencies --	311.8410	317.0809	319.5556
Frequencies --	323.4037	330.1292	333.6665
Frequencies --	364.8900	371.2641	375.5461
Frequencies --	381.0691	387.9522	397.7549
Frequencies --	407.4288	410.1373	422.7613
Frequencies --	424.6233	431.9303	434.1240
Frequencies --	441.0770	450.3503	454.7738
Frequencies --	456.0567	478.6743	485.0397
Frequencies --	508.2483	529.3422	535.6479
Frequencies --	540.1988	542.6113	551.3769
Frequencies --	551.6217	558.9667	571.4422
Frequencies --	585.2755	590.9224	593.4845
Frequencies --	603.6378	606.1074	615.9515
Frequencies --	629.2691	637.3390	642.1760
Frequencies --	644.7317	647.2550	649.5619
Frequencies --	672.4226	676.6005	690.8133
Frequencies --	692.8409	714.0987	717.1880
Frequencies --	719.8882	738.2410	751.5228
Frequencies --	765.8938	781.6343	784.5295
Frequencies --	799.7416	805.4802	828.9915
Frequencies --	835.8895	874.9381	889.5606
Frequencies --	897.6753	907.7681	917.5608
Frequencies --	951.0987	965.5572	966.9379
Frequencies --	970.2537	986.0121	988.6109
Frequencies --	991.0761	995.6370	1022.9529
Frequencies --	1035.2766	1038.3378	1040.4293
Frequencies --	1041.1129	1045.3681	1046.9703
Frequencies --	1048.8827	1057.9322	1059.4398
Frequencies --	1084.5051	1085.7202	1087.4014
Frequencies --	1100.2723	1123.3083	1125.1702
Frequencies --	1160.4952	1171.3689	1173.4645
Frequencies --	1174.1458	1176.0368	1191.8380
Frequencies --	1201.9473	1213.8483	1222.1253
Frequencies --	1245.7515	1269.0306	1300.4195

Frequencies --	1311.1409	1327.6361	1334.7542
Frequencies --	1342.2058	1356.8397	1368.6182
Frequencies --	1378.6957	1385.1351	1410.7580
Frequencies --	1414.8582	1415.0520	1422.9547
Frequencies --	1423.6310	1426.4869	1428.0936
Frequencies --	1430.8828	1432.3656	1435.8230
Frequencies --	1445.6441	1447.4997	1450.0374
Frequencies --	1454.4806	1456.2920	1457.4898
Frequencies --	1462.1429	1471.3723	1472.9362
Frequencies --	1481.8657	1483.8456	1484.8860
Frequencies --	1488.6638	1491.9669	1492.6031
Frequencies --	1494.7528	1498.3494	1500.9643
Frequencies --	1504.4707	1506.1578	1506.8563
Frequencies --	1508.6678	1515.7658	1516.9445
Frequencies --	1574.0548	1585.4285	1588.4934
Frequencies --	1597.3242	1598.6701	1617.5074
Frequencies --	1620.1821	1622.2205	2997.7765
Frequencies --	3008.7284	3009.9744	3010.3171
Frequencies --	3010.8772	3012.3196	3014.7499
Frequencies --	3036.8621	3098.7136	3100.5384
Frequencies --	3101.4233	3102.9835	3105.0148
Frequencies --	3110.5431	3119.0448	3137.4595
Frequencies --	3145.4244	3150.1883	3156.7736
Frequencies --	3159.4774	3160.9863	3161.2218
Frequencies --	3170.4082	3175.7992	3212.9272
Frequencies --	3216.4425	3225.7262	3233.1243

Catalyst 18:

vacuum	toluene-like solvent	D3 dispersion
-3156.8203557	-3156.8310842	-0.57737150

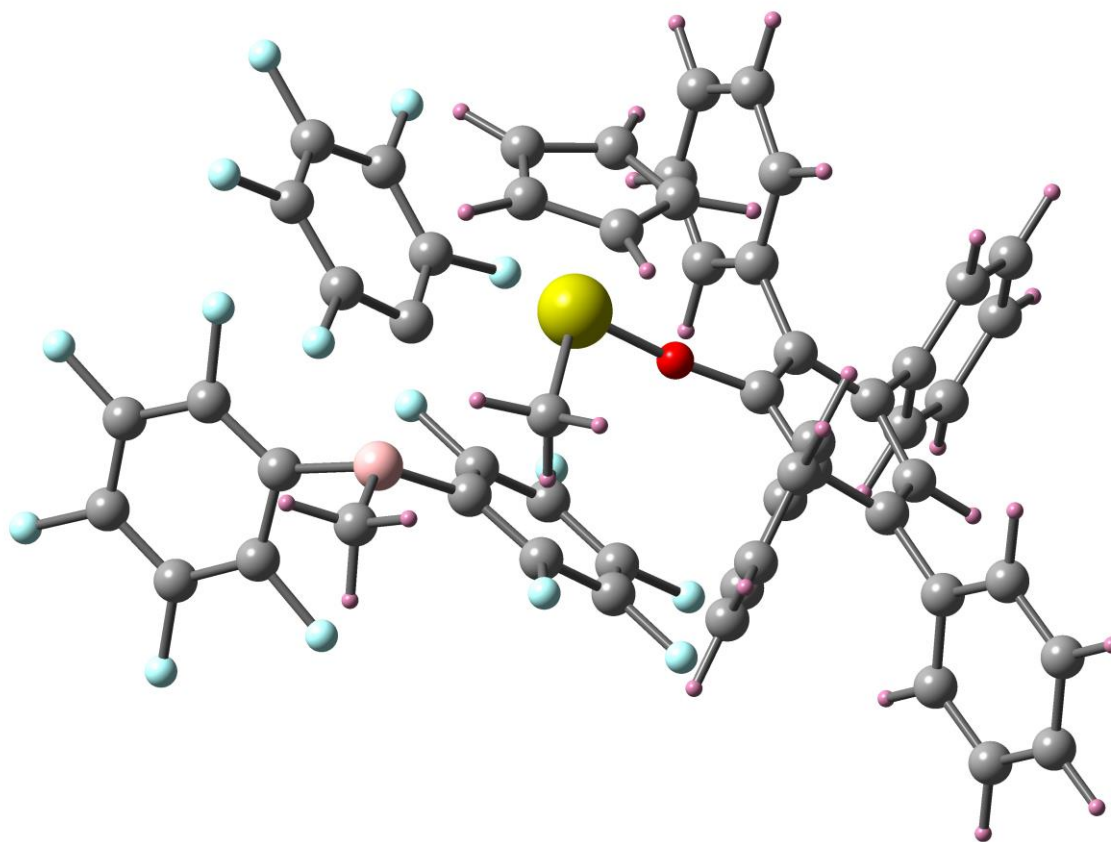
Imaginary frequency corresponding to vibration along the reaction coordinate: -233 cm^{-1} .

Ti	1.74033100	-1.67065800	-0.72974700
C	1.77303800	-1.29127500	-2.76892700
H	1.28969400	-0.30584200	-2.82128400
H	2.75934100	-1.22493300	-3.24484000
H	1.16300000	-2.04601000	-3.29166400
O	2.42478400	-0.12547000	-0.20016000
C	3.19951200	0.93759700	0.23622500
C	3.20884800	1.30121400	1.60811200
C	3.95341500	1.68131200	-0.69968300
C	3.97384900	2.39670700	2.03037900
C	4.72199800	2.78226800	-0.27584500
C	4.73617500	3.14613300	1.09495100
H	3.98404000	2.70162600	3.07645900
H	5.28170800	3.34831000	-1.01816500
C	2.06667100	-3.84800600	0.47800200
C	1.98697300	-4.17820100	-0.92591400
C	3.19715300	-2.96711400	0.67335100
C	3.09786600	-3.54196000	-1.59493300
C	3.84125200	-2.78235500	-0.60861500
F	-7.47511100	1.65294100	-0.05446900
C	-6.13381100	1.34699700	-0.23233600
C	-5.56511700	0.22275200	0.38343300

C	-5.31165900	2.15712500	-1.03298200
C	-4.19925800	-0.06743300	0.18483400
F	-6.34829400	-0.59461800	1.19084900
C	-3.95600300	1.81857400	-1.19727900
F	-5.84265000	3.28192700	-1.65344400
C	-3.31841100	0.69352100	-0.60728700
F	-3.74107600	-1.19738300	0.87406400
F	-3.21893600	2.69669300	-2.00851000
B	-1.72540100	0.46239600	-1.05757600
C	-0.80384600	-1.26964700	-0.04167100
C	-1.41820900	-2.49393500	-0.41929400
C	-0.67233500	-1.14645400	1.36914100
C	-1.94606800	-3.44382500	0.47099000
F	-1.52399100	-2.82660500	-1.78170600
C	-1.18728500	-2.05062900	2.31336300
F	0.04526700	-0.06561600	1.90647800
C	-1.84817200	-3.20398100	1.85293600
F	-2.53100000	-4.62537900	0.02209800
F	-1.02143700	-1.85856400	3.68147100
F	-2.33838000	-4.12970200	2.75452600
C	-0.84295400	1.74923100	-0.56710800
C	0.08870800	2.42795300	-1.38689200
C	-1.07690300	2.40496400	0.66916500
C	0.73134200	3.62973700	-1.03490800
C	-0.44755400	3.59603700	1.07432800
C	0.46670300	4.22011700	0.20984200
F	-1.98958900	1.87002600	1.58389100
F	-0.72039300	4.16147500	2.31455200
F	1.10866000	5.39131100	0.58499900
F	1.63483800	4.23303900	-1.90546200
F	0.43302100	1.92751000	-2.64931100
C	-1.74270500	0.02233000	-2.60907500
H	-0.79393200	-0.34130800	-3.00457800
H	-2.50147200	-0.75210100	-2.78609600
H	-2.02816500	0.89755200	-3.21418100
C	1.32227100	-4.53491200	1.59963300
H	1.94874000	-5.36303700	1.97571300
H	1.12596500	-3.87800100	2.45598700
H	0.37623800	-4.98038700	1.27671200
C	1.04071600	-5.16531900	-1.57238900
H	1.53796200	-6.14536800	-1.68106300
H	0.13003600	-5.32721600	-0.98515600
H	0.73122800	-4.84875800	-2.57818500
C	3.71514200	-2.50364800	2.01581500
H	4.35106300	-1.61467200	1.93413000
H	2.90423000	-2.27074700	2.72071300
H	4.32362900	-3.30150800	2.47686000
C	3.55084900	-3.85374800	-3.00053000
H	4.09217000	-4.81622000	-3.00163700
H	2.71282100	-3.95386100	-3.70284300
H	4.23685700	-3.09651200	-3.40024800
C	5.15911100	-2.08379600	-0.85178400
H	5.35621400	-1.29348100	-0.11796100
H	5.98562000	-2.81240400	-0.77940200
H	5.21426500	-1.63068000	-1.85115800
H	2.60229500	0.74501400	2.32034500
H	3.92185600	1.41006000	-1.75466500

O	5.45105900	4.21451100	1.63922100
C	6.18438400	5.11329600	0.74026000
H	5.50697100	5.58817600	0.01149200
H	6.61422600	5.87784000	1.39820000
H	6.99388800	4.58136700	0.21225500
Frequencies --	-232.5143	12.2048	17.0736
Frequencies --	19.6582	21.7160	28.2632
Frequencies --	33.9026	35.8055	41.2931
Frequencies --	42.8068	48.1332	50.7645
Frequencies --	54.9382	56.8118	62.5453
Frequencies --	73.8491	86.6179	90.4832
Frequencies --	92.0287	96.4410	103.3916
Frequencies --	110.5520	114.8643	117.0903
Frequencies --	121.1897	125.2515	128.4762
Frequencies --	130.8977	135.7683	136.9775
Frequencies --	143.1919	144.1611	148.7697
Frequencies --	157.0653	157.4810	164.8670
Frequencies --	168.5621	173.9894	183.4121
Frequencies --	190.1761	199.9733	200.8731
Frequencies --	207.1515	217.4318	223.2657
Frequencies --	227.2605	234.4519	236.5319
Frequencies --	242.8231	261.8306	264.3726
Frequencies --	266.0063	266.8662	269.6984
Frequencies --	271.8108	272.4285	275.7325
Frequencies --	277.6555	281.7006	289.6654
Frequencies --	292.0494	296.2681	300.6401
Frequencies --	303.3603	304.1351	306.7119
Frequencies --	309.5230	315.5308	318.8786
Frequencies --	328.4559	333.0953	348.0267
Frequencies --	369.8056	374.9124	380.6849
Frequencies --	383.6451	398.9347	408.6958
Frequencies --	414.2949	418.0273	422.1145
Frequencies --	424.4521	431.2099	433.0967
Frequencies --	433.8044	441.2763	450.3875
Frequencies --	454.5916	483.6517	484.6844
Frequencies --	503.9405	521.3210	529.8521
Frequencies --	535.7583	539.3255	542.6234
Frequencies --	551.2184	552.1794	570.9057
Frequencies --	578.5497	585.6394	590.0643
Frequencies --	591.2541	604.3099	610.2114
Frequencies --	628.6568	637.3610	637.6609
Frequencies --	641.4776	644.0314	647.5023
Frequencies --	672.2205	683.7007	691.1804
Frequencies --	712.7592	714.2552	716.6500
Frequencies --	719.6734	737.6573	751.0355
Frequencies --	769.1334	781.8827	800.0214
Frequencies --	806.7380	807.2350	828.8821
Frequencies --	830.7584	889.2437	897.4052
Frequencies --	907.5997	917.0854	924.6106
Frequencies --	949.9023	964.5588	972.5216
Frequencies --	973.5015	985.6462	990.2871
Frequencies --	990.7927	997.2904	1010.8786
Frequencies --	1034.8244	1038.2787	1040.8302
Frequencies --	1042.1575	1046.1891	1047.0300
Frequencies --	1047.9585	1057.2157	1059.3983
Frequencies --	1085.8175	1086.5606	1087.7325
Frequencies --	1123.4510	1124.8484	1126.2456
Frequencies --	1171.9571	1173.1142	1173.8369
Frequencies --	1175.9446	1185.2175	1188.4248
Frequencies --	1214.0260	1221.8361	1228.0072
Frequencies --	1245.8694	1259.6162	1311.0962

Frequencies --	1317.6009	1326.9051	1335.8000
Frequencies --	1342.0401	1357.0234	1361.0191
Frequencies --	1368.8998	1378.5716	1412.3927
Frequencies --	1414.4519	1414.5937	1422.1106
Frequencies --	1423.7850	1425.7868	1428.9502
Frequencies --	1430.6701	1431.9045	1435.6240
Frequencies --	1438.3752	1446.9876	1450.2997
Frequencies --	1454.6840	1455.9080	1457.1367
Frequencies --	1462.6393	1471.2108	1472.9295
Frequencies --	1482.7745	1485.5041	1487.0775
Frequencies --	1489.9677	1490.5372	1493.4632
Frequencies --	1499.0068	1500.1518	1501.2726
Frequencies --	1502.0254	1506.2111	1507.3886
Frequencies --	1508.9491	1516.2750	1518.1600
Frequencies --	1574.6162	1580.1639	1585.2317
Frequencies --	1596.9332	1597.8060	1620.1885
Frequencies --	1622.1695	1624.3750	2998.0224
Frequencies --	3008.3288	3008.6452	3009.6456
Frequencies --	3010.2173	3012.0025	3015.1257
Frequencies --	3037.1135	3097.1596	3099.0978
Frequencies --	3100.8047	3101.3553	3103.4140
Frequencies --	3111.3454	3120.5704	3136.7782
Frequencies --	3146.2434	3150.1744	3155.6427
Frequencies --	3157.5332	3158.2789	3162.3872
Frequencies --	3170.3583	3196.7179	3202.9066
Frequencies --	3205.0495	3217.9245	3226.9207

Catalyst 19:

vacuum	toluene-like solvent	D3 dispersion
-3769.6474055	-3769.6617719	-0.79700999

Imaginary frequency corresponding to vibration along the reaction coordinate: -214 cm^{-1} .

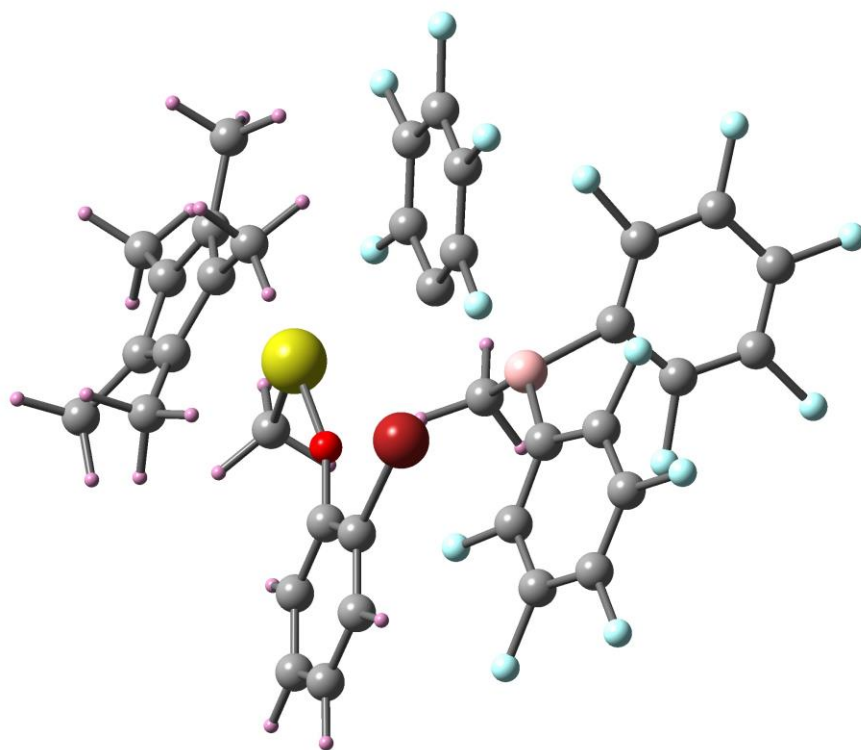
Ti	0.07437800	2.42530100	0.48442900
C	-0.01169300	3.25899500	-1.39686300
H	-0.08788300	2.36196400	-2.02731900
H	-0.83938800	3.93257500	-1.63324400
H	0.94758200	3.77549900	-1.55383200
O	-1.32542000	1.31949300	0.42389600
C	-2.52919600	0.60345700	0.44806900
C	-2.73516700	-0.39472300	1.45845200
C	-3.47648100	0.83608000	-0.60374700
C	-3.83244600	-1.29309800	1.29246600
C	-4.56483300	-0.07521500	-0.73721400
C	-4.68924500	-1.14075400	0.18025700
C	1.14248100	3.83820100	2.24532300
C	0.81005700	4.74982000	1.19597500
C	-0.06654400	3.22069700	2.71125200
C	-0.61154800	4.70917000	1.01121600
C	-1.15737200	3.77249000	1.95576900
F	7.69046900	-3.02932200	-2.34633100
C	6.52363200	-2.32715300	-2.08418700
C	6.46015200	-1.40709700	-1.02762300

C	5.37659600	-2.51984000	-2.87218500
C	5.26161400	-0.70499000	-0.78300300
F	7.57569700	-1.19556900	-0.22584000
C	4.20922300	-1.79020000	-2.58339400
F	5.40485600	-3.42627800	-3.92517000
C	4.07608400	-0.84619900	-1.52928800
F	5.31458700	0.17295300	0.30725600
F	3.11759400	-2.05527500	-3.42731700
B	2.61800100	-0.03498300	-1.48039300
C	2.45102700	1.30907800	0.25807700
C	3.37807800	2.38762800	0.18202400
C	2.48797900	0.66118900	1.52362100
C	4.29951400	2.73300400	1.18553200
F	3.41185300	3.20450900	-0.95689000
C	3.38491100	0.95026600	2.56689900
F	1.53830200	-0.33031600	1.79743400
C	4.31391500	1.99138500	2.38258900
F	5.18219100	3.79610400	1.03074200
F	3.35826000	0.25935200	3.77214400
F	5.20970000	2.30845800	3.38531600
C	1.40585300	-1.11659200	-1.27777300
C	0.20298500	-1.09855600	-2.02170500
C	1.54428700	-2.27497800	-0.47052200
C	-0.77228800	-2.11327300	-1.98397600
C	0.59391900	-3.30886600	-0.38923500
C	-0.57734600	-3.23160000	-1.16017600
F	2.68518800	-2.45047900	0.31722500
F	0.79438500	-4.39855800	0.45117800
F	-1.53738900	-4.23238300	-1.08958800
F	-1.92979000	-2.01589900	-2.75312200
F	-0.09122600	-0.03166100	-2.87871500
C	2.60636500	0.96769300	-2.74276900
H	1.79294800	1.69351100	-2.76095400
H	3.55424300	1.51859200	-2.81290500
H	2.51740100	0.36339500	-3.66028800
H	-5.52345600	-1.83177300	0.06621300
C	-4.15248300	-2.41001000	2.25480800
C	-4.03114800	-3.75931900	1.83265000
C	-4.65603600	-2.15269900	3.55510800
C	-4.38714800	-4.82125100	2.69140400
H	-3.64861100	-3.98129000	0.83461000
C	-5.01810400	-3.21255600	4.41289400
H	-4.77376800	-1.12316300	3.89605500
C	-4.88207400	-4.55202900	3.98605200
H	-4.27595700	-5.85281500	2.34919200
H	-5.40674800	-2.99191400	5.40997100
H	-5.15955100	-5.37299000	4.65127900
C	-5.61534900	0.03852900	-1.81325200
C	-6.59878200	1.05958300	-1.78300500
C	-5.68292200	-0.93516600	-2.84279600
C	-7.61734600	1.11137900	-2.75772100
H	-6.57464000	1.81093200	-0.99208900
C	-6.69745800	-0.88156100	-3.82283700
H	-4.93295200	-1.72776100	-2.88321200
C	-7.66938100	0.14229300	-3.78392000
H	-8.36854400	1.90367100	-2.71362600
H	-6.72664400	-1.63634600	-4.61227400

H	-8.45677000	0.18278200	-4.54020700
C	-1.88669600	-0.50005600	2.69904900
C	-1.01700200	-1.59528900	2.92053600
C	-2.05413700	0.44422100	3.74504300
C	-0.31911800	-1.73387700	4.13708900
H	-0.88614700	-2.34676000	2.14337500
C	-1.36601300	0.30424100	4.96923500
H	-2.75594100	1.27146800	3.61655900
C	-0.48831100	-0.78428500	5.16734000
H	0.35698700	-2.57973100	4.27586100
H	-1.52503400	1.03353100	5.76764100
H	0.05026300	-0.89450800	6.11100500
C	-3.39193500	2.01931300	-1.53227700
C	-3.76668800	3.30585300	-1.06557500
C	-3.06432600	1.86964700	-2.90257700
C	-3.81958100	4.41075900	-1.94170200
H	-4.05573500	3.43637400	-0.02011300
C	-3.11000600	2.97278000	-3.78005500
H	-2.77846700	0.89027200	-3.28487700
C	-3.49097000	4.24726400	-3.30579300
H	-4.13335200	5.38797800	-1.56581600
H	-2.85481000	2.83413600	-4.83295600
H	-3.53895100	5.09747500	-3.98992900
H	2.12922900	3.67086200	2.65351200
H	1.50940400	5.35079900	0.62223800
H	-0.14506200	2.49116800	3.50798300
H	-1.17813000	5.28929300	0.29247900
H	-2.20556700	3.52169500	2.07276700
Frequencies --	-214.2738	11.8705	14.9190
Frequencies --	20.8417	22.9484	25.8953
Frequencies --	29.9370	32.3859	35.3777
Frequencies --	37.9387	39.5932	43.6233
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Frequencies --	53.3406	54.9163	56.4920
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Frequencies --	71.6538	73.1640	80.4645
Frequencies --	86.3619	89.2033	98.5953
Frequencies --	103.1302	108.8595	112.7097
Frequencies --	118.0274	119.2471	122.7843
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Frequencies --	142.9598	145.4331	151.0297
Frequencies --	157.3300	165.9240	177.9922
Frequencies --	191.5973	193.4425	197.6532
Frequencies --	203.3483	210.6172	211.9558
Frequencies --	221.2141	229.0747	230.0281
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Frequencies --	250.9430	254.4360	263.1324
Frequencies --	265.1170	265.5016	267.1284
Frequencies --	268.5103	270.9452	276.4314
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Frequencies --	296.5298	303.5061	304.8820
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Frequencies --	322.9281	328.8205	333.4750
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Frequencies --	375.8719	379.8370	405.5300
Frequencies --	405.8610	407.0233	408.8081
Frequencies --	409.3121	410.6905	412.3113
Frequencies --	423.6440	425.9336	431.8584
Frequencies --	433.8303	437.2105	442.9034

Frequencies --	451.5385	455.2459	486.5040
Frequencies --	494.9865	506.1744	521.0826
Frequencies --	525.9126	540.7502	542.9906
Frequencies --	544.9425	550.0459	551.5176
Frequencies --	563.1125	571.0200	574.7613
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Frequencies --	617.5024	619.7945	623.6994
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Frequencies --	637.5300	640.5324	642.2566
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Frequencies --	674.0257	683.8126	689.7182
Frequencies --	694.2653	702.4602	711.1987
Frequencies --	712.0901	714.0906	715.1251
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Frequencies --	738.1457	741.1432	744.8380
Frequencies --	750.5437	766.8039	773.7245
Frequencies --	782.5532	782.9501	795.9426
Frequencies --	806.6237	812.7434	816.0109
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Frequencies --	846.5920	857.9361	859.8233
Frequencies --	862.0144	867.1599	869.1646
Frequencies --	887.0538	894.5172	899.1315
Frequencies --	907.8727	913.4867	914.1958
Frequencies --	920.7785	935.6127	936.8875
Frequencies --	941.6724	943.7083	963.0733
Frequencies --	986.2495	987.9288	988.7330
Frequencies --	992.5921	993.3892	994.9271
Frequencies --	996.2023	996.7819	1004.2369
Frequencies --	1006.1793	1009.7496	1010.9344
Frequencies --	1015.6530	1020.1201	1025.2361
Frequencies --	1033.9807	1036.4306	1040.4989
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Frequencies --	1050.3723	1054.5459	1054.7060
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Frequencies --	1090.1279	1090.5467	1091.1963
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Frequencies --	1119.4766	1127.5243	1133.7028
Frequencies --	1178.3353	1183.0737	1183.2599
Frequencies --	1183.4003	1184.1501	1194.8910
Frequencies --	1204.5168	1205.6218	1207.6200
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Frequencies --	1328.2615	1330.5685	1333.9100
Frequencies --	1335.2360	1336.6816	1341.9927
Frequencies --	1356.8014	1366.4004	1368.3629
Frequencies --	1369.8321	1370.6912	1373.7332
Frequencies --	1377.5473	1379.0528	1395.3983
Frequencies --	1402.4564	1414.4330	1422.1669
Frequencies --	1427.4859	1440.5277	1443.2213
Frequencies --	1444.8578	1445.6115	1447.0367
Frequencies --	1448.8057	1450.5686	1452.2069
Frequencies --	1452.8541	1469.5512	1473.0914
Frequencies --	1494.4658	1496.1973	1497.1224
Frequencies --	1502.1237	1503.0341	1507.4871
Frequencies --	1524.4615	1571.1296	1582.6391
Frequencies --	1588.0600	1594.0264	1595.6160
Frequencies --	1596.3159	1596.9322	1598.0276
Frequencies --	1598.5710	1619.1469	1622.6101
Frequencies --	1623.3046	1623.9707	1624.2981
Frequencies --	1624.7495	3021.2921	3035.0156
Frequencies --	3118.9059	3148.2924	3148.5072

Frequencies --	3149.8557	3153.2296	3154.0637
Frequencies --	3161.2714	3161.8076	3163.0228
Frequencies --	3165.4333	3171.7144	3174.9338
Frequencies --	3175.0966	3177.2242	3183.3902
Frequencies --	3185.8026	3187.6291	3189.0487
Frequencies --	3190.8992	3192.8687	3194.2040
Frequencies --	3195.7005	3208.3917	3210.1760
Frequencies --	3216.2223	3249.9542	3264.5762
Frequencies --	3281.1157	3288.6358	3310.9688

Catalyst 20:**distal conformation**

vacuum	toluene-like solvent	D3 dispersion
-3054.8968084	-3054.9073465	-0.57255246

Imaginary frequency corresponding to vibration along the reaction coordinate: -233 cm^{-1} .

Ti	1.98123500	-1.17761200	-0.76171800
C	1.83090500	-0.89486600	-2.80808400
H	1.17512100	-0.01568500	-2.86436700
H	2.74424000	-0.69792800	-3.37946700
H	1.32063700	-1.77782300	-3.22397900
O	2.43879200	0.50979400	-0.37517300
C	3.10467500	1.71923600	-0.37364600
C	3.35198800	2.46118300	0.81376100
C	3.54263300	2.25378300	-1.61490500
C	4.01470100	3.70533600	0.75215300
C	4.20934100	3.48902700	-1.67332400
C	4.44758000	4.21841200	-0.48809700
H	4.18582100	4.26972800	1.66892000
H	4.52445600	3.88656900	-2.63955700
C	2.59118700	-3.50716300	0.01649900
C	2.97128900	-3.43682800	-1.37069100
C	3.32172100	-2.48524200	0.73960800
C	3.98097100	-2.40948000	-1.50485000
C	4.20526200	-1.82589100	-0.19891100
F	-7.72888200	0.29988700	-0.02639400

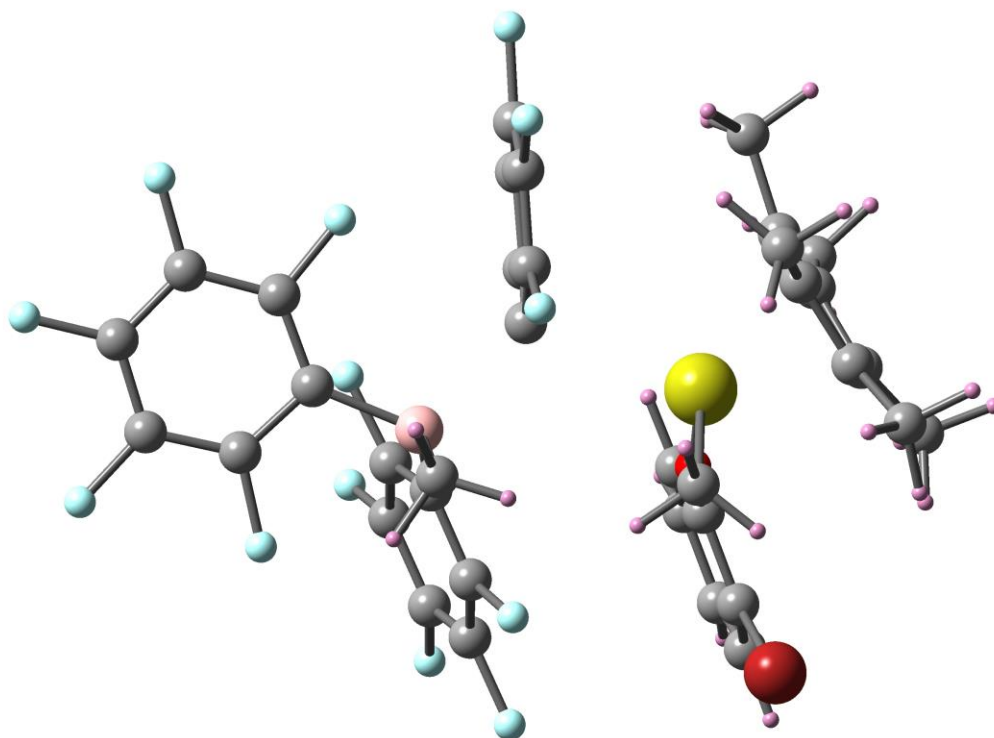
C	-6.35722200	0.24671200	-0.22606100
C	-5.59245600	-0.80001400	0.30835700
C	-5.69981500	1.24112400	-0.96924300
C	-4.19958300	-0.83108700	0.08871200
F	-6.20939300	-1.79666800	1.05631800
C	-4.30811500	1.15809500	-1.15753400
F	-6.42742400	2.29479300	-1.50991100
C	-3.47448200	0.12659200	-0.64555100
F	-3.54262300	-1.91150300	0.69183500
F	-3.74895300	2.20387600	-1.91012500
B	-1.86876100	0.20991300	-1.11063300
C	-0.64089600	-1.35676700	-0.19889900
C	-1.00069700	-2.65014300	-0.66911800
C	-0.54818100	-1.30786200	1.22037700
C	-1.36087400	-3.73472800	0.14598500
F	-1.00314800	-2.91619500	-2.05012700
C	-0.88437400	-2.35809600	2.09307200
F	-0.05785300	-0.14767200	1.83315700
C	-1.31813400	-3.57783900	1.54300400
F	-1.71032900	-4.97033000	-0.39153800
F	-0.76570400	-2.23289100	3.47325800
F	-1.63534900	-4.63873300	2.36986500
C	-1.23731600	1.61569500	-0.56142700
C	-0.45848100	2.49335700	-1.35078400
C	-1.58763200	2.16374300	0.69963600
C	-0.06645000	3.78579200	-0.95390400
C	-1.20366600	3.43930100	1.15106800
C	-0.43700800	4.26445100	0.31209900
F	-2.37562200	1.42737600	1.58969800
F	-1.57689300	3.89301300	2.41020200
F	-0.03996000	5.52546700	0.73257400
F	0.68720700	4.59178700	-1.80188700
F	-0.02505200	2.11321300	-2.62871000
C	-1.84096500	-0.14095600	-2.68625400
H	-0.85318700	-0.30000700	-3.12038800
H	-2.44844200	-1.03219400	-2.89625200
H	-2.29975300	0.69734400	-3.23452600
C	1.84790600	-4.65757600	0.65441700
H	2.58057300	-5.45242500	0.88232800
H	1.37429700	-4.39167000	1.60519300
H	1.09424600	-5.10421600	-0.00320500
C	2.51173900	-4.38133600	-2.45714300
H	3.13178700	-5.29510100	-2.45019400
H	1.46816300	-4.69640000	-2.32355400
H	2.60003600	-3.93889400	-3.45735300
C	3.33188600	-2.30891000	2.24130400
H	3.62142100	-1.29514500	2.53970600
H	2.35695200	-2.52095500	2.70003200
H	4.05950700	-3.00617600	2.69306600
C	4.84307500	-2.16930800	-2.72142300
H	5.75107300	-2.79401400	-2.65269300
H	4.33704200	-2.43802300	-3.65667100
H	5.17713000	-1.12605100	-2.80259700
C	5.32984900	-0.88279100	0.15792000
H	5.11953200	-0.30331100	1.06386500
H	6.24603400	-1.46834400	0.35047400
H	5.56225100	-0.17366200	-0.64672200

H	3.33049400	1.69607400	-2.52495000
H	4.95377000	5.18427500	-0.52234100
Br	2.77859300	1.80757300	2.56614100

Frequencies --	-232.8419	11.4178	13.3221
Frequencies --	15.8869	27.4853	31.0272
Frequencies --	32.8797	34.3086	38.2984
Frequencies --	42.1078	46.9793	53.4844
Frequencies --	55.6651	59.5242	62.0788
Frequencies --	75.6033	83.1399	88.6652
Frequencies --	92.8235	95.7340	110.3132
Frequencies --	114.9393	115.6659	120.5980
Frequencies --	125.3240	125.7004	127.8825
Frequencies --	132.4593	133.8146	143.1551
Frequencies --	149.4667	154.8804	156.5806
Frequencies --	164.4995	168.0299	170.0579
Frequencies --	172.8289	181.2336	185.5935
Frequencies --	189.4715	198.7617	202.3759
Frequencies --	209.3522	220.8461	222.8210
Frequencies --	235.8752	243.8562	259.5600
Frequencies --	263.8546	265.1252	266.3850
Frequencies --	268.8122	270.7056	275.0638
Frequencies --	277.6545	283.3122	287.7979
Frequencies --	288.9255	295.0622	297.8138
Frequencies --	301.1759	301.4910	302.8809
Frequencies --	305.7046	308.4617	316.9631
Frequencies --	319.3570	320.5168	329.2813
Frequencies --	332.5205	345.4519	371.6722
Frequencies --	375.2416	381.8388	382.6941
Frequencies --	386.2384	404.7731	408.9562
Frequencies --	422.6656	425.0963	431.4770
Frequencies --	434.1563	441.4117	450.0580
Frequencies --	452.5026	454.7770	485.0869
Frequencies --	492.6782	496.8574	527.2374
Frequencies --	534.7242	539.8310	540.5460
Frequencies --	542.5619	551.4030	552.9974
Frequencies --	570.5966	581.1323	591.3134
Frequencies --	592.9670	601.0169	619.9452
Frequencies --	629.1368	630.2418	637.2898
Frequencies --	641.9497	643.6830	647.9928
Frequencies --	670.6319	673.4086	692.1213
Frequencies --	701.2070	710.1201	713.4676
Frequencies --	716.7984	719.4376	737.1828
Frequencies --	749.0187	765.7669	781.5884
Frequencies --	800.9865	806.7383	827.9828
Frequencies --	868.2822	891.1070	898.0958
Frequencies --	907.5306	917.1927	920.8150
Frequencies --	959.4987	968.0893	971.8072
Frequencies --	985.4729	990.6343	993.5216
Frequencies --	995.2322	1029.5304	1037.7111
Frequencies --	1038.4727	1040.2776	1042.3348
Frequencies --	1042.9289	1045.5907	1048.4407
Frequencies --	1055.6369	1057.4946	1059.0470
Frequencies --	1084.3831	1087.9170	1089.0962
Frequencies --	1126.0359	1134.6876	1171.9763
Frequencies --	1174.4517	1174.6468	1184.7859
Frequencies --	1187.6878	1213.5348	1221.7239
Frequencies --	1241.6903	1248.5846	1275.2758
Frequencies --	1310.3540	1327.4422	1335.7104
Frequencies --	1341.8371	1356.4046	1356.5220
Frequencies --	1368.2205	1378.9898	1411.9014
Frequencies --	1413.8828	1415.8430	1423.0026

Frequencies --	1424.0737	1426.0260	1429.7629
Frequencies --	1430.5570	1434.0230	1434.9949
Frequencies --	1436.2766	1447.2283	1450.3449
Frequencies --	1456.1344	1456.9714	1463.2999
Frequencies --	1468.5372	1471.3549	1472.9793
Frequencies --	1482.3184	1493.5380	1495.3971
Frequencies --	1497.1822	1500.4184	1502.3358
Frequencies --	1503.9129	1506.2432	1508.9509
Frequencies --	1513.5102	1515.9668	1518.3001
Frequencies --	1573.6390	1579.4216	1584.1667
Frequencies --	1596.1461	1596.7268	1598.0479
Frequencies --	1620.1563	1622.1770	3010.3486
Frequencies --	3011.0131	3011.3674	3012.8579
Frequencies --	3013.7086	3017.8384	3036.2990
Frequencies --	3101.9987	3105.0754	3109.2507
Frequencies --	3111.1067	3116.2428	3118.6724
Frequencies --	3143.9353	3146.4648	3150.5660
Frequencies --	3158.1679	3162.6919	3170.1130
Frequencies --	3174.3760	3176.4972	3191.5379
Frequencies --	3203.0408	3208.0592	3225.4710

proximal conformation



vacuum	toluene-like solvent	D3 dispersion
-3054.8998125	-3054.9102367	-0.57243288

Imaginary frequency corresponding to vibration along the reaction coordinate: -230 cm^{-1} .

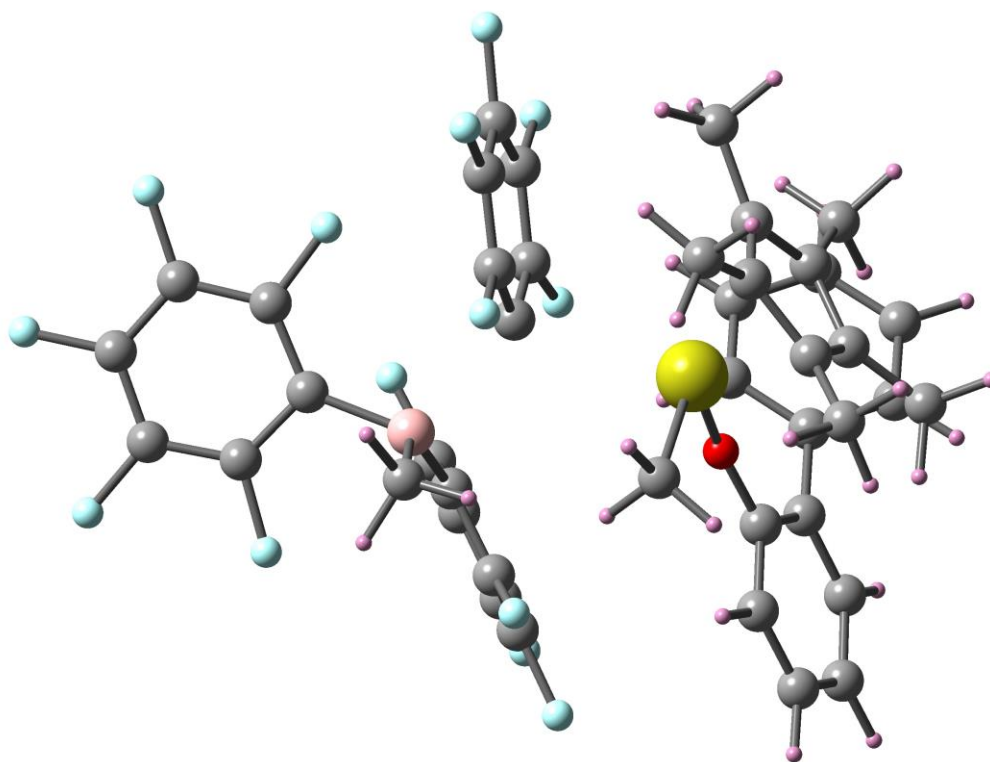
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C	-2.01520400	0.88973500	-2.47803000
H	-1.40683900	-0.02514400	-2.52449500

H	-3.00107500	0.67139200	-2.90006100
H	-1.53426800	1.70940400	-3.03493400
O	-2.35994300	-0.31513000	0.17403900
C	-2.89051300	-1.37436100	0.88147200
C	-2.53438700	-1.53630000	2.24698500
C	-3.75778500	-2.32982300	0.28228600
C	-3.02817100	-2.61871500	2.99561000
C	-4.25054300	-3.41562200	1.03551500
C	-3.88911100	-3.56111200	2.39127500
H	-2.73067500	-2.73133300	4.03957200
H	-4.90352400	-4.14747700	0.56025800
C	-2.30799400	3.57729400	0.54128200
C	-2.59548800	3.69386900	-0.86785900
C	-3.19778500	2.58483400	1.10576000
C	-3.70401200	2.81677700	-1.17001000
C	-4.07966600	2.13162000	0.05254500
F	7.74720500	-0.75315200	-0.57977600
C	6.36647800	-0.63119500	-0.63122400
C	5.72514200	0.50489000	-0.11719000
C	5.57598000	-1.64389300	-1.19938300
C	4.31976400	0.60394700	-0.18267400
F	6.47679300	1.52305200	0.45887900
C	4.17814900	-1.49037400	-1.23925100
F	6.17965400	-2.78492900	-1.71444700
C	3.46508300	-0.36756100	-0.73726900
F	3.79490000	1.77307100	0.38410300
F	3.48090000	-2.56035000	-1.82306400
B	1.81529300	-0.39253100	-1.01205400
C	0.78281900	1.31654800	-0.11258900
C	1.16302100	2.54688400	-0.71540500
C	0.83323300	1.37863400	1.30631700
C	1.65566400	3.66712200	-0.02531300
F	1.05429000	2.70448700	-2.10742400
C	1.33145100	2.45588100	2.05721600
F	0.32440000	0.30629600	2.06166600
C	1.76722100	3.60640700	1.37499200
F	2.00287700	4.84151500	-0.68789100
F	1.35536900	2.43492000	3.44843300
F	2.22962700	4.69929100	2.08277700
C	1.17468000	-1.70088800	-0.26871900
C	0.25890200	-2.58534300	-0.88542200
C	1.63224800	-2.15958800	0.99303800
C	-0.16536500	-3.80604400	-0.32597900
C	1.22498700	-3.36029800	1.60162700
C	0.31921100	-4.19855000	0.93132800
F	2.55570300	-1.40202800	1.72203200
F	1.70712300	-3.72653800	2.85377900
F	-0.10453400	-5.38550800	1.51121900
F	-1.06414400	-4.62433500	-1.00152200
F	-0.28782500	-2.28667800	-2.13808000
C	1.61638300	-0.17776000	-2.59900300
H	0.59133200	-0.00038200	-2.92559800
H	2.23619000	0.65355000	-2.96217900
H	1.96190300	-1.08751100	-3.11567000
C	-1.48753600	4.54704800	1.35846200
H	-2.16164700	5.34451200	1.71893600
H	-1.03850600	4.09383200	2.24957400

H	-0.70103900	5.04109900	0.77955300
C	-1.97370000	4.67845900	-1.83212100
H	-2.59499100	5.58947100	-1.89207600
H	-0.96785200	4.99063100	-1.52736900
H	-1.89937500	4.27356000	-2.85049200
C	-3.32069500	2.26700200	2.57949500
H	-2.34421300	2.19967300	3.08032400
H	-3.88815000	3.06620500	3.08781800
H	-3.85430800	1.32651300	2.76014400
C	-4.50516400	2.83329300	-2.44923100
H	-5.24751100	3.64954700	-2.40292800
H	-3.88169600	3.01231000	-3.33435000
H	-5.05930700	1.89961200	-2.60974800
C	-5.31827200	1.28704000	0.23539900
H	-5.23314300	0.58917900	1.07657800
H	-6.17873200	1.94664700	0.44528800
H	-5.56561400	0.70176600	-0.65795800
H	-1.85112300	-0.81773000	2.69420400
H	-4.26926400	-4.41075600	2.96031900
Br	-4.28335100	-2.19868300	-1.59866600

Frequencies --	-229.6961	9.8480	13.8684
Frequencies --	16.6797	27.1455	31.7061
Frequencies --	33.7510	37.2446	39.3968
Frequencies --	44.6303	47.9761	54.7046
Frequencies --	58.1872	60.5036	63.0704
Frequencies --	68.0229	88.6760	93.3890
Frequencies --	104.6124	110.1399	115.5506
Frequencies --	116.3500	120.6475	122.3451
Frequencies --	125.7676	132.6149	135.6839
Frequencies --	139.0820	143.3954	150.6090
Frequencies --	151.4088	156.1430	157.3707
Frequencies --	164.2892	164.8188	170.3722
Frequencies --	171.5451	178.8045	185.5209
Frequencies --	189.1885	192.2245	200.3567
Frequencies --	205.0344	220.2179	222.1672
Frequencies --	230.2687	236.0962	245.5839
Frequencies --	263.0734	264.1709	265.7601
Frequencies --	266.7901	271.4200	272.3827
Frequencies --	275.6649	278.4581	280.8016
Frequencies --	284.4262	288.1938	294.8323
Frequencies --	298.1683	299.0827	300.2973
Frequencies --	303.3867	307.1700	316.7246
Frequencies --	317.9188	328.4177	328.9215
Frequencies --	333.1635	345.8622	371.2437
Frequencies --	374.9811	381.6630	383.6247
Frequencies --	389.8809	407.2873	410.3092
Frequencies --	422.1929	424.6336	431.0503
Frequencies --	434.1353	440.9844	450.4585
Frequencies --	450.5564	454.8587	485.4846
Frequencies --	493.7296	511.8561	528.0697
Frequencies --	535.1565	539.9900	542.0668
Frequencies --	542.4697	551.4126	551.7383
Frequencies --	571.3471	584.5965	592.3167
Frequencies --	592.6785	604.3548	623.0319
Frequencies --	628.4981	630.7945	637.1818
Frequencies --	641.7244	643.8004	649.3082
Frequencies --	669.1893	671.8752	690.2215
Frequencies --	702.4019	709.3299	715.0108
Frequencies --	716.7818	719.9215	737.5972

Frequencies --	750.5535	768.0092	782.1794
Frequencies --	799.8024	805.4945	830.7809
Frequencies --	869.5814	888.7407	897.8463
Frequencies --	908.0368	917.5826	924.3491
Frequencies --	960.0074	965.8491	970.0084
Frequencies --	985.3487	990.6641	994.8218
Frequencies --	997.0924	1027.5656	1033.9966
Frequencies --	1036.6404	1041.4590	1042.7508
Frequencies --	1045.1754	1047.1891	1047.8092
Frequencies --	1052.8374	1057.9388	1059.6076
Frequencies --	1085.3320	1085.8923	1089.1885
Frequencies --	1124.3412	1134.0546	1171.7676
Frequencies --	1173.9114	1175.3239	1185.3820
Frequencies --	1190.8211	1213.8280	1222.6057
Frequencies --	1242.5657	1247.5154	1275.3049
Frequencies --	1310.0985	1327.4373	1334.6368
Frequencies --	1342.1253	1354.8163	1357.0555
Frequencies --	1370.2146	1378.8754	1411.9895
Frequencies --	1413.2746	1414.3251	1416.9549
Frequencies --	1423.0196	1424.1882	1428.2345
Frequencies --	1429.6120	1431.2437	1434.8542
Frequencies --	1435.4071	1447.3697	1448.3753
Frequencies --	1450.1611	1457.1984	1461.1865
Frequencies --	1466.3942	1469.9408	1472.9114
Frequencies --	1482.2831	1491.2572	1492.8604
Frequencies --	1493.9026	1498.6836	1500.7252
Frequencies --	1501.6541	1506.5796	1507.0000
Frequencies --	1510.3815	1515.6273	1518.1707
Frequencies --	1573.8333	1577.8620	1585.6343
Frequencies --	1595.3977	1596.8807	1597.6894
Frequencies --	1618.9858	1622.3670	3009.2539
Frequencies --	3010.2978	3011.1190	3013.4527
Frequencies --	3014.1097	3015.5062	3036.0904
Frequencies --	3096.9776	3103.2883	3105.6993
Frequencies --	3113.7796	3115.7154	3118.8799
Frequencies --	3142.3961	3146.1436	3149.8596
Frequencies --	3155.6669	3163.3124	3174.0285
Frequencies --	3176.9196	3177.0074	3192.3443
Frequencies --	3205.0451	3209.3313	3231.9412

Catalyst 21:**distal conformation**

vacuum	toluene-like solvent	D3 dispersion
-3273.2853126	-3273.2962492	-0.63909546

Imaginary frequency corresponding to vibration along the reaction coordinate: -240 cm^{-1} .

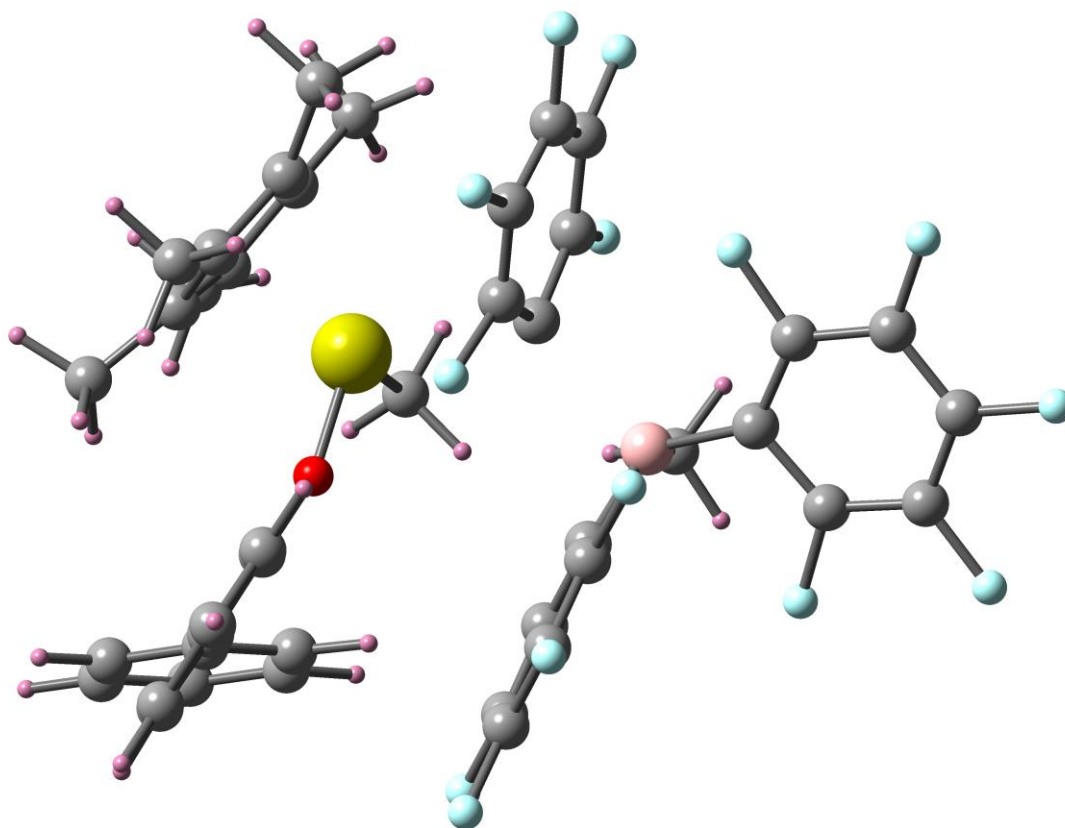
Ti	1.87311500	-1.20994900	-0.95021800
C	1.51660500	-0.91551500	-2.96992000
H	0.82276500	-0.06386800	-2.94050500
H	2.37753700	-0.65454400	-3.59596400
H	1.01321000	-1.80110400	-3.38633800
O	2.42588300	0.45716100	-0.60826800
C	3.12566600	1.65868900	-0.75097000
C	3.76831500	2.31872300	0.34427800
C	3.19495300	2.19613400	-2.06239200
C	4.48778900	3.50868800	0.04044200
C	3.90783700	3.37776400	-2.32176200
C	4.56692200	4.03644700	-1.26163400
H	4.96495700	4.04371400	0.86245500
H	3.93457300	3.78351900	-3.33471000
C	2.50490400	-3.49368500	-0.05054300
C	2.54485100	-3.61751000	-1.48416400
C	3.44076800	-2.45988000	0.34393500
C	3.54246300	-2.69585600	-1.98225400
C	4.10238700	-1.98163100	-0.85206000
F	-7.88309700	0.36968300	0.40969000

C	-6.52922900	0.31798800	0.11243100
C	-5.72738800	-0.72762200	0.59281200
C	-5.92924400	1.31097400	-0.67992900
C	-4.35364700	-0.75903300	0.27465800
F	-6.28966700	-1.72404700	1.38267400
C	-4.55442100	1.22882600	-0.96605300
F	-6.69564900	2.36053100	-1.17241100
C	-3.68624900	0.20078800	-0.50976600
F	-3.65412700	-1.84112600	0.82272800
F	-4.04772200	2.26691800	-1.76506300
B	-2.12577400	0.28073600	-1.09075600
C	-0.79398600	-1.31590400	-0.20273600
C	-1.16999400	-2.61475500	-0.63358400
C	-0.63436000	-1.24186700	1.20493500
C	-1.46643900	-3.69294600	0.21714300
F	-1.27392400	-2.89381100	-2.00850500
C	-0.91583700	-2.27629100	2.11412700
F	-0.13889800	-0.05755900	1.77640800
C	-1.35693200	-3.51211100	1.60737000
F	-1.82749000	-4.94306200	-0.28185200
F	-0.74058200	-2.12042500	3.48646700
F	-1.61819600	-4.56313900	2.46722500
C	-1.43315300	1.67856800	-0.61090000
C	-0.68974800	2.52354900	-1.46814900
C	-1.68744900	2.25789000	0.65926400
C	-0.24291300	3.81390000	-1.12396900
C	-1.24132200	3.53065300	1.05982600
C	-0.51426800	4.32310900	0.15563100
F	-2.43566400	1.56038300	1.61236500
F	-1.51835200	4.01501500	2.33290600
F	-0.06677600	5.58278000	0.52290000
F	0.46151800	4.58908100	-2.03844000
F	-0.36024200	2.11235100	-2.76604000
C	-2.18526000	-0.12495000	-2.64770500
H	-1.22183000	-0.29583800	-3.12956200
H	-2.80060600	-1.02341800	-2.79244200
H	-2.67709300	0.69586300	-3.19566100
C	1.86225200	-4.46719900	0.90936700
H	2.62039900	-5.21709800	1.19718500
H	1.52285400	-3.99673800	1.83944300
H	1.02598600	-5.01890200	0.46817000
C	1.80861300	-4.63882800	-2.32035400
H	2.46238600	-5.50811500	-2.51136500
H	0.90318000	-5.01360900	-1.82899900
H	1.51193600	-4.23985300	-3.30001500
C	3.81011400	-2.13041000	1.77142700
H	4.26762600	-1.14187800	1.87096300
H	2.94518400	-2.15975800	2.44867500
H	4.53809700	-2.87191000	2.14619600
C	4.10223000	-2.69338100	-3.38410700
H	4.86884300	-3.48372600	-3.46969500
H	3.33908200	-2.90027500	-4.14509000
H	4.58878500	-1.74311700	-3.63973300
C	5.31655900	-1.08428700	-0.90266600
H	5.39680000	-0.44502100	-0.01711200
H	6.22880500	-1.70476500	-0.94514900
H	5.32540000	-0.43234000	-1.78632200

H	2.67548500	1.68567800	-2.86868200
H	5.11698200	4.96184700	-1.44082300
C	3.73058500	1.87209700	1.77406500
C	2.50701800	1.61831200	2.44489400
C	4.93588500	1.79063100	2.52526900
C	2.48528300	1.29323400	3.81716200
H	1.56909800	1.69866900	1.90246200
C	4.91753400	1.46098500	3.89650200
H	5.89225600	1.97956500	2.03282000
C	3.68974300	1.21235400	4.54997000
H	1.52750400	1.11472100	4.31015700
H	5.85671100	1.40271400	4.45172900
H	3.67154600	0.96549800	5.61383300

Frequencies --	-240.3196	8.0306	12.4892
Frequencies --	23.5079	24.5708	28.7365
Frequencies --	31.4891	35.2706	37.3561
Frequencies --	39.8990	43.8227	49.4670
Frequencies --	52.4551	57.3918	58.9423
Frequencies --	64.6134	75.7637	78.3592
Frequencies --	88.1733	93.0158	95.5314
Frequencies --	110.7040	112.8336	114.5441
Frequencies --	120.8580	122.3931	125.9714
Frequencies --	127.1892	134.1883	141.7123
Frequencies --	143.4149	147.8719	149.5659
Frequencies --	154.8881	157.5079	161.5032
Frequencies --	162.1357	165.0088	172.7245
Frequencies --	179.7017	190.6954	191.1781
Frequencies --	194.5474	204.4696	207.3463
Frequencies --	220.3870	230.3429	231.2003
Frequencies --	246.0324	260.4558	263.7682
Frequencies --	265.1879	266.5423	268.6160
Frequencies --	272.0114	275.0471	276.4751
Frequencies --	282.6087	287.9898	290.7444
Frequencies --	294.5538	296.6975	299.4458
Frequencies --	300.2320	302.8153	303.6708
Frequencies --	306.5925	310.4871	316.8099
Frequencies --	320.4224	329.9129	332.9751
Frequencies --	334.2519	354.3015	369.1513
Frequencies --	376.0944	380.4327	380.8153
Frequencies --	389.2709	406.4868	408.6536
Frequencies --	409.4644	423.0879	425.4907
Frequencies --	431.0631	433.3742	439.2158
Frequencies --	450.0425	454.5372	474.3541
Frequencies --	484.3845	502.4499	508.8981
Frequencies --	527.8600	535.8363	539.4106
Frequencies --	540.2320	542.9316	550.9603
Frequencies --	552.3347	562.0923	566.9504
Frequencies --	580.1652	587.5493	593.3361
Frequencies --	603.0030	613.7619	614.2205
Frequencies --	621.4067	629.2045	637.6462
Frequencies --	642.3677	643.8751	645.3237
Frequencies --	649.2949	669.3316	688.1536
Frequencies --	691.7762	711.1522	711.6360
Frequencies --	717.3920	719.6851	736.6278
Frequencies --	739.0003	742.5580	751.1970
Frequencies --	768.2059	781.8324	783.0919
Frequencies --	800.6313	807.1765	835.1082
Frequencies --	864.3260	880.0437	888.3463
Frequencies --	897.0978	908.1005	910.9804
Frequencies --	916.7949	935.6183	966.4860

Frequencies --	967.4209	971.2983	984.2222
Frequencies --	989.4376	991.7746	995.3270
Frequencies --	998.9214	1001.1414	1009.7537
Frequencies --	1032.4699	1037.5114	1038.0900
Frequencies --	1041.0898	1043.4336	1044.5941
Frequencies --	1047.1902	1047.4649	1047.7735
Frequencies --	1058.3406	1061.1959	1065.2385
Frequencies --	1087.6932	1088.2353	1090.6883
Frequencies --	1092.8734	1124.8422	1125.3114
Frequencies --	1171.3783	1172.2578	1175.2124
Frequencies --	1185.2673	1186.0726	1189.2669
Frequencies --	1203.0299	1211.4784	1215.5808
Frequencies --	1224.9662	1245.5026	1266.1951
Frequencies --	1296.9517	1312.5390	1327.7616
Frequencies --	1338.8745	1339.9079	1342.1326
Frequencies --	1356.4814	1357.8890	1370.7104
Frequencies --	1372.0467	1377.3429	1411.1292
Frequencies --	1414.7638	1415.9602	1422.4405
Frequencies --	1424.1191	1426.9233	1429.0896
Frequencies --	1431.2707	1433.0439	1434.0741
Frequencies --	1438.6829	1446.1532	1449.9915
Frequencies --	1452.6570	1455.7371	1458.7960
Frequencies --	1462.8471	1470.2696	1473.0976
Frequencies --	1480.2775	1482.2946	1491.9382
Frequencies --	1493.7654	1494.7703	1499.9955
Frequencies --	1501.5285	1504.9899	1506.8332
Frequencies --	1507.8173	1508.2291	1509.5560
Frequencies --	1518.1561	1520.4400	1575.1844
Frequencies --	1577.4182	1584.3754	1595.5665
Frequencies --	1596.3975	1597.5260	1612.0397
Frequencies --	1618.4527	1622.7147	1623.1566
Frequencies --	3009.2761	3010.0178	3010.9643
Frequencies --	3014.4033	3015.3915	3018.4328
Frequencies --	3031.3220	3102.2402	3103.4045
Frequencies --	3104.5186	3109.8028	3115.1410
Frequencies --	3117.6888	3145.1660	3147.0975
Frequencies --	3154.9278	3156.8053	3163.5205
Frequencies --	3164.5247	3167.1544	3170.1248
Frequencies --	3172.6394	3176.3081	3179.2145
Frequencies --	3183.4638	3193.1903	3200.0563
Frequencies --	3202.3733	3242.3815	3242.9348

proximal conformation

vacuum	toluene-like solvent	D3 dispersion
-3273.2886275	-3273.2994946	-0.64076409

Imaginary frequency corresponding to vibration along the reaction coordinate: -236 cm^{-1} .

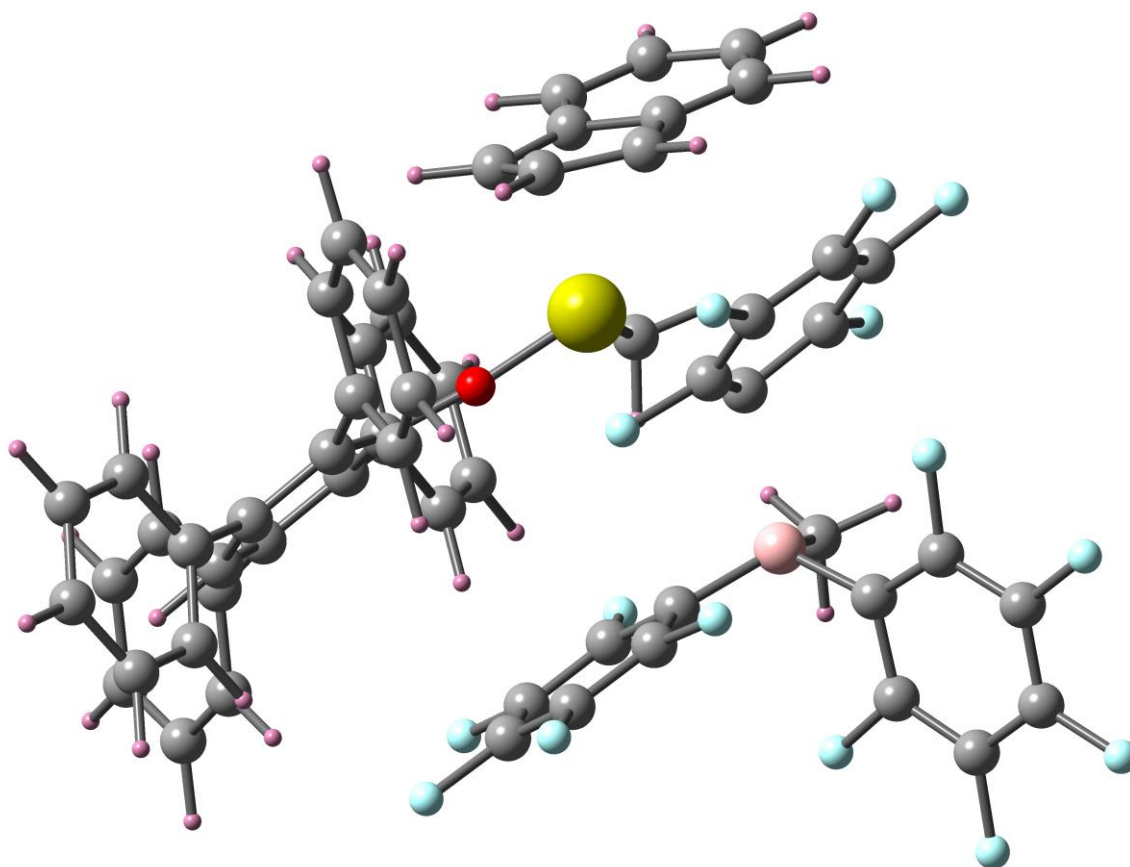
Ti	-1.76387000	1.40844900	-0.30954700
C	-1.97372400	1.07820300	-2.33442000
H	-1.33765600	0.18608300	-2.44276700
H	-2.98319400	0.82843300	-2.67852700
H	-1.56433200	1.91398800	-2.91993400
O	-2.29972200	-0.18274900	0.29488700
C	-2.83916100	-1.18995000	1.09578800
C	-2.25734400	-1.36353200	2.37809600
C	-3.92918200	-2.01134700	0.66485500
C	-2.74085700	-2.34474500	3.26001700
C	-4.39624400	-2.98605700	1.59012600
C	-3.82268200	-3.16068400	2.86365700
H	-2.27136100	-2.47496500	4.23694000
H	-5.21015500	-3.64150000	1.27763100
C	-1.90534100	3.75422000	0.63680400
C	-2.38971000	3.83249500	-0.71835700
C	-2.74221600	2.82361000	1.36656900

C	-3.56145200	2.99279300	-0.82191700
C	-3.78706600	2.37695900	0.47339100
F	7.83083900	-1.18629800	-0.94389600
C	6.45666000	-1.00008300	-0.91311700
C	5.90331400	0.19195500	-0.42390500
C	5.58531300	-2.00160500	-1.37278500
C	4.50267400	0.35693300	-0.40581700
F	6.73697900	1.20104000	0.04484200
C	4.19648200	-1.78162400	-1.33252900
F	6.10102700	-3.19586800	-1.86200000
C	3.57091700	-0.60001300	-0.85028400
F	4.06870900	1.57833900	0.12426400
F	3.41236400	-2.84308300	-1.81323400
B	1.91096600	-0.55521100	-1.02427300
C	0.99744300	1.27780000	-0.14952700
C	1.39535100	2.44838100	-0.84919300
C	1.16144900	1.41053600	1.25352300
C	1.99824300	3.57378600	-0.26225700
F	1.19760600	2.53614100	-2.23862000
C	1.77296800	2.49454100	1.90420500
F	0.65887400	0.40503100	2.10282000
C	2.21429600	3.58096900	1.12705700
F	2.35492400	4.69069300	-1.01437400
F	1.90596700	2.54453200	3.28920300
F	2.78694000	4.68222800	1.73543200
C	1.24512900	-1.77725500	-0.17111100
C	0.23454900	-2.62503400	-0.67813900
C	1.75452000	-2.20335000	1.08225100
C	-0.23628100	-3.78153100	-0.02866500
C	1.30916400	-3.34207000	1.77759300
C	0.30473700	-4.14599400	1.21372700
F	2.77137700	-1.47689100	1.70967600
F	1.84869800	-3.68034500	3.01368700
F	-0.15887600	-5.26775900	1.88379300
F	-1.23920800	-4.55832300	-0.60044300
F	-0.37202900	-2.34925900	-1.91141500
C	1.61592100	-0.39743700	-2.60039400
H	0.57770100	-0.19503800	-2.86685400
H	2.23863500	0.39492700	-3.03742200
H	1.89565000	-1.34019100	-3.09805400
C	-0.95005900	4.73022400	1.28283800
H	-1.54399600	5.57650600	1.67245300
H	-0.41165100	4.30977600	2.13891700
H	-0.22430900	5.15531800	0.58171900
C	-1.85959000	4.75052000	-1.79601300
H	-2.34666000	5.73903900	-1.72291300
H	-0.77762900	4.91598700	-1.71334300
H	-2.06060200	4.36706200	-2.80467000
C	-2.65940000	2.55911400	2.85392500
H	-3.13249800	1.61116400	3.13697700
H	-1.62315500	2.53685600	3.22020200
H	-3.17911300	3.36098200	3.40750100
C	-4.53207000	2.97593500	-1.97838800
H	-5.25262000	3.80477700	-1.86176600
H	-4.03499100	3.11271300	-2.94688800
H	-5.11179400	2.04519100	-2.02496400
C	-5.02858800	1.61854000	0.87540700

H	-4.85732700	0.95602700	1.73158900
H	-5.81039100	2.34026800	1.17145500
H	-5.43519700	1.01262000	0.05860900
H	-1.42082200	-0.73073700	2.66364300
H	-4.20369100	-3.93641800	3.52999800
C	-4.61592100	-1.92286600	-0.66627500
C	-6.03426900	-1.82485600	-0.71893500
C	-3.90855200	-2.02805200	-1.89157700
C	-6.72102300	-1.81978400	-1.95072200
H	-6.60170700	-1.74265800	0.21061300
C	-4.59466100	-2.03258200	-3.12439700
H	-2.82811400	-2.14134500	-1.88414400
C	-6.00211000	-1.92494800	-3.16231500
H	-7.81067700	-1.74023000	-1.96307500
H	-4.02731800	-2.13373500	-4.05258100
H	-6.53042100	-1.93303700	-4.11839300

Frequencies --	-235.9041	8.1831	16.1379
Frequencies --	18.8376	26.5287	29.0291
Frequencies --	32.0492	34.2647	36.9672
Frequencies --	38.6587	43.0194	49.7586
Frequencies --	51.6246	56.8355	60.8996
Frequencies --	63.4621	65.5831	85.5412
Frequencies --	90.7143	94.4617	100.9207
Frequencies --	110.3627	114.5477	120.7419
Frequencies --	121.1937	124.0284	125.6755
Frequencies --	131.5544	134.2817	140.4883
Frequencies --	143.2311	151.2527	152.3515
Frequencies --	156.3029	157.5960	160.9445
Frequencies --	164.9713	169.4361	175.6295
Frequencies --	179.7137	189.4159	193.9113
Frequencies --	198.9656	204.7387	211.1271
Frequencies --	217.3868	220.1673	235.5659
Frequencies --	240.3521	253.0097	263.4558
Frequencies --	264.7817	265.8491	266.7520
Frequencies --	269.8683	273.9630	277.2358
Frequencies --	279.2265	283.4453	287.4256
Frequencies --	290.9699	295.5998	297.4843
Frequencies --	300.0578	302.2734	304.3234
Frequencies --	305.8080	306.2661	316.7456
Frequencies --	317.3563	328.1903	333.2414
Frequencies --	334.3383	348.4371	370.2641
Frequencies --	374.8823	381.5240	382.1943
Frequencies --	392.1474	404.2514	409.6850
Frequencies --	410.1619	422.2970	424.7709
Frequencies --	430.8810	433.7705	440.1309
Frequencies --	450.5486	454.9063	472.3984
Frequencies --	484.9233	508.2354	512.7521
Frequencies --	529.8107	535.6800	539.7978
Frequencies --	542.0078	543.2172	551.2129
Frequencies --	554.0126	563.3612	571.2129
Frequencies --	580.8880	590.2839	593.4584
Frequencies --	604.2454	612.7140	615.4292
Frequencies --	622.0360	628.4233	637.6917
Frequencies --	641.4755	643.3669	646.7221
Frequencies --	648.0509	671.1143	688.6017
Frequencies --	690.5194	712.4812	714.3266
Frequencies --	716.9324	719.8305	737.3609
Frequencies --	738.1546	741.9551	750.6195
Frequencies --	768.7017	782.6647	783.5714
Frequencies --	803.2753	806.6023	832.6426

Frequencies --	866.8221	882.8204	887.0304
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Frequencies --	917.2406	940.0265	967.5477
Frequencies --	968.6709	974.2119	983.7898
Frequencies --	990.5447	992.4596	996.7051
Frequencies --	997.9007	1000.9943	1009.7183
Frequencies --	1031.2608	1037.5970	1038.5393
Frequencies --	1042.2527	1043.2668	1045.1404
Frequencies --	1047.0657	1047.5175	1048.4994
Frequencies --	1057.2329	1060.0420	1063.3283
Frequencies --	1088.8789	1089.2030	1089.8668
Frequencies --	1092.4672	1125.8097	1127.1835
Frequencies --	1172.1552	1172.4123	1176.0722
Frequencies --	1183.8784	1186.9568	1187.5788
Frequencies --	1209.1907	1211.0393	1214.4673
Frequencies --	1223.5943	1243.2417	1264.9828
Frequencies --	1295.8362	1311.4000	1328.0652
Frequencies --	1337.6533	1338.0237	1343.6572
Frequencies --	1354.7050	1357.8716	1370.1047
Frequencies --	1371.2471	1378.1354	1412.8133
Frequencies --	1414.7285	1415.4025	1421.5352
Frequencies --	1423.3599	1426.0550	1428.5178
Frequencies --	1430.4157	1430.9113	1432.9900
Frequencies --	1434.7078	1444.6838	1446.6707
Frequencies --	1450.7182	1451.8481	1456.0019
Frequencies --	1463.4470	1470.7517	1473.0159
Frequencies --	1480.0910	1483.1339	1493.5276
Frequencies --	1494.6686	1496.1671	1498.7022
Frequencies --	1500.9044	1503.8155	1508.0575
Frequencies --	1508.7268	1509.0498	1512.5250
Frequencies --	1517.8700	1521.2853	1574.1995
Frequencies --	1577.5735	1585.5001	1595.2858
Frequencies --	1597.0964	1597.9377	1611.5543
Frequencies --	1619.5774	1622.4588	1623.5732
Frequencies --	3007.8162	3009.7052	3010.6597
Frequencies --	3012.5386	3013.2534	3015.9145
Frequencies --	3034.3912	3098.1154	3105.2672
Frequencies --	3106.9766	3116.3114	3118.1675
Frequencies --	3119.8233	3139.8740	3146.9975
Frequencies --	3147.9006	3152.3781	3153.4808
Frequencies --	3162.7886	3168.7985	3170.5292
Frequencies --	3171.7901	3174.5565	3175.1332
Frequencies --	3183.1313	3190.4614	3200.0969
Frequencies --	3201.7633	3239.0916	3249.1629

Catalyst 22:

vacuum	toluene-like solvent	D3 dispersion
-3923.215211	-3923.2300953	-0.84743460

Imaginary frequency corresponding to vibration along the reaction coordinate: -229 cm^{-1} .

Ti	0.08926600	2.20969700	0.26826000
C	0.06351600	2.89763000	-1.65898100
H	-0.00685100	1.97268000	-2.24801000
H	-0.78954900	3.54045000	-1.89317100
H	1.00739100	3.42645300	-1.85649200
O	-1.35528900	1.16918500	0.30797600
C	-2.56122800	0.46008100	0.38056400
C	-2.81651500	-0.38527900	1.51143700
C	-3.46572800	0.54882900	-0.72906300
C	-3.90645800	-1.30353000	1.42247200
C	-4.54922700	-0.37609600	-0.78405500
C	-4.71079300	-1.31078900	0.26167900
C	1.30642200	3.69617700	1.96506500
C	1.12230900	4.72562200	0.96593700
C	0.02575900	3.21189200	2.36164300
C	-0.30486100	4.82666200	0.70411300
C	-0.97409900	3.82469000	1.52183900
F	7.55438000	-3.80318100	-2.06317200
C	6.40686400	-3.05167300	-1.85859500

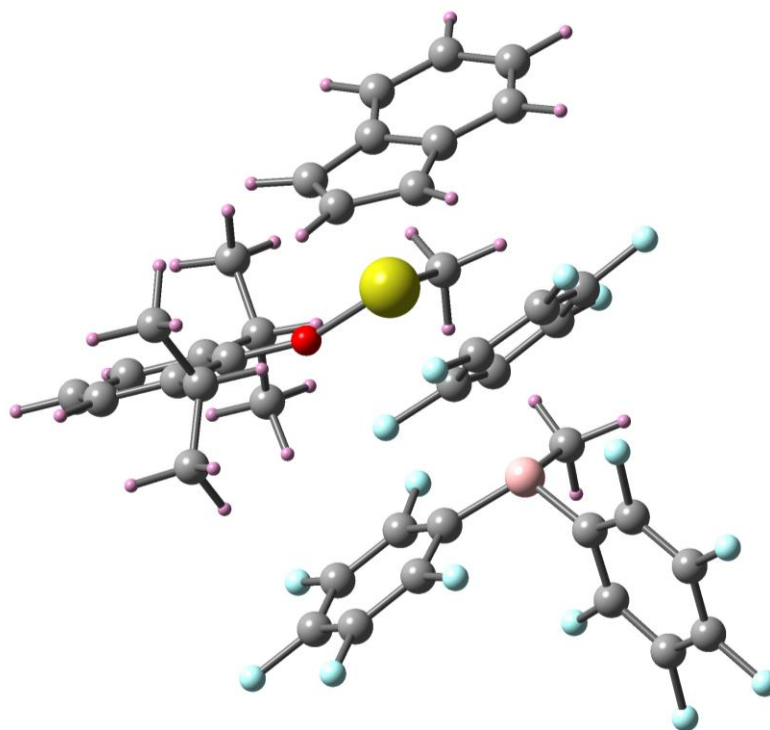
C	6.36385200	-2.06121400	-0.86638400
C	5.25906600	-3.26607300	-2.63993500
C	5.18529400	-1.30923200	-0.67902000
F	7.47939800	-1.83144600	-0.06964100
C	4.11227700	-2.48440600	-2.41091300
F	5.26644900	-4.24399100	-3.62733600
C	4.00353200	-1.46357000	-1.42839800
F	5.25238900	-0.37097500	0.35814600
F	3.01464100	-2.77836500	-3.23732600
B	2.56954200	-0.61388700	-1.44991600
C	2.43438300	0.92075300	0.17587800
C	3.42049000	1.93323800	0.01304900
C	2.43084100	0.38251100	1.48998500
C	4.35252800	2.31524800	0.99311900
F	3.50978800	2.63729800	-1.19607500
C	3.34087400	0.70526900	2.51142900
F	1.42241800	-0.52732500	1.83742200
C	4.32255200	1.67939000	2.24861200
F	5.28677100	3.32101500	0.75965800
F	3.28002400	0.11340600	3.76772400
F	5.22672300	2.03793100	3.23059700
C	1.33167400	-1.62848400	-1.12592700
C	0.12540600	-1.65055600	-1.86361700
C	1.43858100	-2.69427400	-0.19578900
C	-0.87765800	-2.62712600	-1.71665800
C	0.45494800	-3.67986300	0.00368800
C	-0.71546100	-3.65140100	-0.77216500
F	2.57809300	-2.81581000	0.60356200
F	0.62419800	-4.67593700	0.95885000
F	-1.70569800	-4.60836100	-0.59241800
F	-2.03071200	-2.58426200	-2.49692000
F	-0.14125900	-0.66885400	-2.82467100
C	2.56789900	0.28283700	-2.78642900
H	1.76743400	1.02003000	-2.85114400
H	3.52508800	0.80776600	-2.90777100
H	2.45759900	-0.38959700	-3.65284600
H	-5.53826200	-2.01690600	0.20593000
C	-4.27235300	-2.27581700	2.51652800
C	-4.13570300	-3.67055000	2.29329400
C	-4.83089400	-1.84129200	3.74548100
C	-4.52968000	-4.60329300	3.27653900
H	-3.71128500	-4.02893300	1.35363200
C	-5.23125300	-2.77216700	4.72698800
H	-4.96166700	-0.77486800	3.93400500
C	-5.07874900	-4.15764000	4.49863400
H	-4.40592800	-5.67210700	3.08703100
H	-5.66237300	-2.41557100	5.66555400
H	-5.38562900	-4.87844400	5.26005900
C	-5.55433400	-0.41890700	-1.90787800
C	-6.53892600	0.58865600	-2.06855300
C	-5.57790700	-1.53312500	-2.78593100
C	-7.51461900	0.48995800	-3.08311300
H	-6.54943500	1.44737900	-1.39549100
C	-6.54868400	-1.63032900	-3.80557300
H	-4.82764500	-2.31845800	-2.67885200
C	-7.52182800	-0.61860200	-3.95826200
H	-8.26747300	1.27510700	-3.18685300

H	-6.54342300	-2.49273300	-4.47638300
H	-8.27624400	-0.69393600	-4.74489900
C	-2.03627000	-0.29770300	2.79704400
C	-1.18805200	-1.34382100	3.23481100
C	-2.25525100	0.79870700	3.67195400
C	-0.56702300	-1.29334300	4.49932200
H	-1.01391100	-2.20445000	2.58963700
C	-1.64520100	0.84838000	4.94371500
H	-2.93695500	1.59801000	3.37193800
C	-0.79351400	-0.19838700	5.36094800
H	0.09112700	-2.10759400	4.80896300
H	-1.84355700	1.69308500	5.60811900
H	-0.31916100	-0.16442700	6.34411600
C	-3.34819000	1.60762900	-1.79376600
C	-3.74202300	2.93888600	-1.49988100
C	-2.97304100	1.29485000	-3.12361100
C	-3.76770700	3.92788700	-2.50582300
H	-4.06450800	3.19350500	-0.48712200
C	-2.98830300	2.28350500	-4.12921500
H	-2.67433300	0.27810100	-3.37507500
C	-3.38953400	3.60306400	-3.82722100
H	-4.09789900	4.94123500	-2.26330700
H	-2.69491900	2.01972300	-5.14771200
H	-3.41383600	4.36406300	-4.61045000
H	2.24537300	3.43306700	2.43247800
H	-0.16286100	2.49669300	3.15362500
H	-2.04786400	3.71376100	1.63058500
C	2.04101800	5.59232200	0.30251700
H	3.11350600	5.51689400	0.48589500
C	1.53236300	6.56127600	-0.56678000
H	2.21397200	7.24941300	-1.07108700
C	0.12160400	6.67880400	-0.80535700
H	-0.23564700	7.46089300	-1.47898300
C	-0.79522700	5.82114700	-0.19060700
H	-1.86451200	5.91795100	-0.38217500

Frequencies --	-229.4374	9.1301	12.3008
Frequencies --	18.5013	21.4723	24.4719
Frequencies --	27.3643	30.2563	33.0735
Frequencies --	33.6550	35.7267	38.2517
Frequencies --	41.1255	42.2048	44.5384
Frequencies --	45.7058	53.2986	54.5825
Frequencies --	56.5581	60.6254	62.2876
Frequencies --	69.0469	69.7679	71.3434
Frequencies --	75.1688	79.8727	87.5714
Frequencies --	94.0615	96.5257	99.6371
Frequencies --	109.8803	115.2666	116.9601
Frequencies --	121.4287	126.1149	130.2513
Frequencies --	134.5203	136.1083	143.9378
Frequencies --	150.3685	153.8526	157.8540
Frequencies --	166.1521	179.8270	192.3781
Frequencies --	193.4483	199.2058	204.0537
Frequencies --	210.5558	212.3159	221.0765
Frequencies --	226.2148	228.8947	234.4219
Frequencies --	238.4351	250.0937	253.4336
Frequencies --	254.7137	261.2875	263.7044
Frequencies --	265.2962	265.5811	266.9760
Frequencies --	270.8685	274.2042	276.2469
Frequencies --	277.2754	290.4513	294.7201

Frequencies --	300.0698	303.9533	305.9397
Frequencies --	317.0287	318.4168	327.1818
Frequencies --	327.4313	330.5478	333.5323
Frequencies --	359.7380	368.8851	376.4624
Frequencies --	380.6782	391.4655	404.2456
Frequencies --	404.8879	405.1177	405.8220
Frequencies --	409.9793	410.5303	411.2130
Frequencies --	422.8070	424.7536	431.7519
Frequencies --	433.3557	434.4640	439.9271
Frequencies --	441.8169	450.7183	454.4756
Frequencies --	484.4910	493.5080	520.0372
Frequencies --	522.1301	525.1239	539.6490
Frequencies --	539.8753	542.0938	544.2362
Frequencies --	545.9315	550.1832	551.0425
Frequencies --	564.3802	570.3515	590.1318
Frequencies --	593.0660	600.0519	611.6089
Frequencies --	615.6614	617.1716	619.1980
Frequencies --	623.7505	629.7743	633.4703
Frequencies --	636.4852	639.1826	642.4059
Frequencies --	643.6744	649.1498	651.3510
Frequencies --	663.0836	670.7453	688.1286
Frequencies --	691.7444	702.1683	711.2867
Frequencies --	711.8987	712.4695	715.0730
Frequencies --	716.5981	717.7318	719.5027
Frequencies --	737.5076	738.4348	741.6849
Frequencies --	744.2236	745.4638	750.6208
Frequencies --	766.0611	767.6929	773.6339
Frequencies --	782.3755	782.9955	794.6596
Frequencies --	805.9506	806.8058	820.7421
Frequencies --	830.3692	857.5955	861.7113
Frequencies --	862.5946	865.5951	868.0775
Frequencies --	871.3097	873.5588	880.3673
Frequencies --	887.2646	892.8048	898.4954
Frequencies --	907.8122	916.2054	918.2265
Frequencies --	936.9464	937.5252	943.0160
Frequencies --	945.7687	963.6828	975.7230
Frequencies --	986.6099	987.4207	987.8880
Frequencies --	990.6303	993.6646	995.9957
Frequencies --	996.7735	997.8784	1004.6150
Frequencies --	1005.9575	1006.3484	1009.7966
Frequencies --	1010.9488	1015.0844	1015.7810
Frequencies --	1019.9431	1025.3412	1038.5327
Frequencies --	1038.9139	1044.5175	1045.5266
Frequencies --	1051.0326	1053.9085	1054.9011
Frequencies --	1058.1738	1059.0329	1060.8432
Frequencies --	1074.6198	1086.5108	1089.9758
Frequencies --	1091.2360	1092.0462	1092.2371
Frequencies --	1119.1542	1127.3769	1141.2903
Frequencies --	1174.9623	1182.8840	1183.3562
Frequencies --	1183.3868	1184.4516	1184.6112
Frequencies --	1186.8780	1205.1156	1206.3944
Frequencies --	1207.4678	1207.7677	1209.2488
Frequencies --	1215.5270	1221.9869	1228.2113
Frequencies --	1244.9233	1248.9194	1251.9310
Frequencies --	1269.9651	1277.2270	1300.5814
Frequencies --	1311.2143	1315.7288	1328.4613
Frequencies --	1329.3486	1331.5240	1334.4091
Frequencies --	1335.6415	1338.6502	1344.1165
Frequencies --	1357.7232	1361.8930	1366.0114
Frequencies --	1368.3965	1368.7875	1370.0143
Frequencies --	1370.7949	1375.9730	1376.9969
Frequencies --	1378.0698	1414.8630	1421.6450
Frequencies --	1422.7023	1424.7443	1427.4468

Frequencies --	1439.5369	1440.8272	1443.4559
Frequencies --	1444.6635	1445.5908	1446.2543
Frequencies --	1452.8700	1469.6614	1470.1724
Frequencies --	1473.0879	1489.7308	1496.6529
Frequencies --	1496.8942	1497.2701	1499.8778
Frequencies --	1502.5791	1507.9660	1524.4292
Frequencies --	1564.8831	1570.9624	1583.0762
Frequencies --	1587.6535	1594.2242	1595.1589
Frequencies --	1596.4713	1597.1918	1598.1977
Frequencies --	1599.7751	1619.9831	1622.7096
Frequencies --	1623.0478	1624.2057	1624.4214
Frequencies --	1625.0077	1628.3785	3026.2883
Frequencies --	3034.1907	3118.6312	3146.3782
Frequencies --	3150.3708	3153.6825	3154.3099
Frequencies --	3155.1544	3160.7190	3162.9545
Frequencies --	3163.6727	3164.8644	3165.9553
Frequencies --	3170.6696	3174.8140	3177.7145
Frequencies --	3178.1786	3178.5879	3186.1269
Frequencies --	3187.0428	3187.5402	3189.4363
Frequencies --	3189.8278	3193.0082	3193.1510
Frequencies --	3195.7866	3196.4741	3202.0638
Frequencies --	3207.2517	3210.1140	3213.7012
Frequencies --	3250.8880	3273.2026	3296.6682

Catalyst 23:

vacuum	toluene-like solvent	D3 dispersion
-3235.1834396	-3235.1935063	-0.63293598

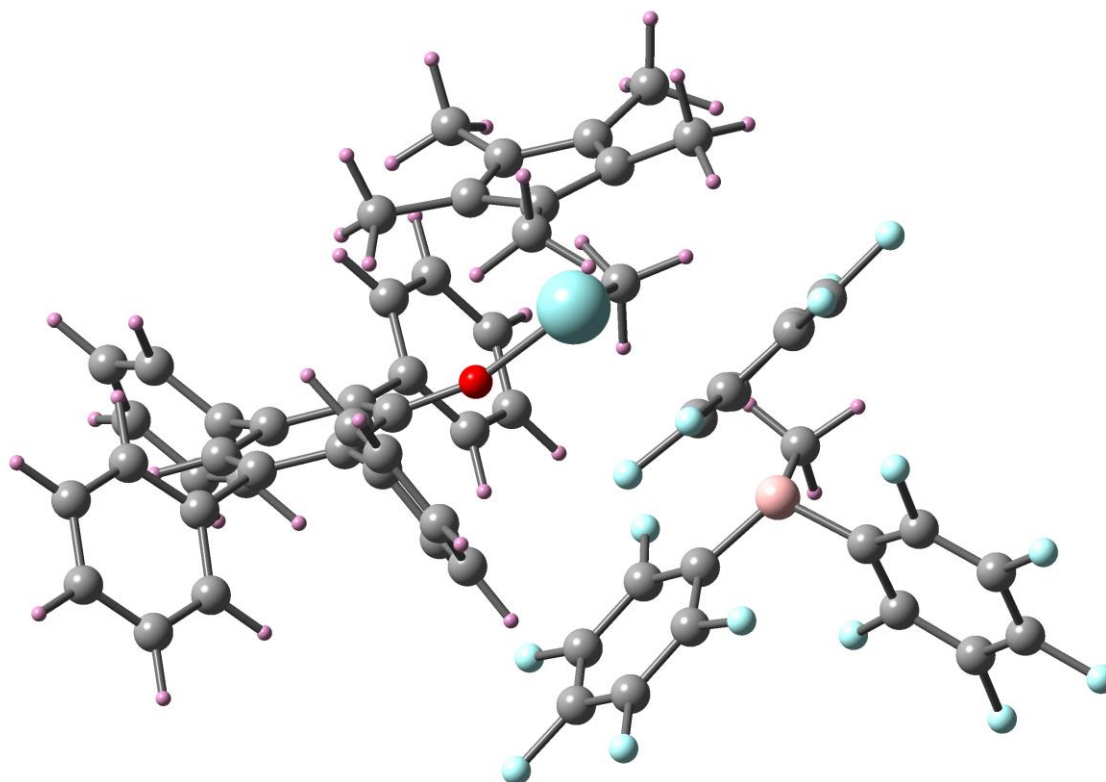
Imaginary frequency corresponding to vibration along the reaction coordinate: -217 cm^{-1} .

Ti	-1.83855300	1.22195500	-0.26279100
C	-1.97612100	1.39433800	-2.31315700
H	-1.46539700	0.48853200	-2.67119700
H	-2.99435600	1.43829100	-2.71287900
H	-1.42566100	2.29770400	-2.61440100
O	-2.54915800	-0.38376800	0.02565500
C	-3.45713000	-1.40159300	0.38086200
C	-3.53528900	-1.83661600	1.74547800
C	-4.28007800	-1.97337700	-0.64582100
C	-4.46112800	-2.86205500	2.05150200
C	-5.18691000	-2.99018300	-0.26535700
C	-5.28148000	-3.43533600	1.06452100
H	-4.53674100	-3.21710800	3.07926500
H	-5.82203300	-3.44327800	-1.02667500
C	-1.85191800	3.37464800	1.00787700
C	-2.41975300	3.87640600	-0.22335500
C	-2.73886900	2.39027900	1.54380000
C	-3.64951400	3.13633800	-0.47084100
C	-3.80023500	2.16577100	0.59946700
F	7.78851600	-0.45822000	-0.77916300
C	6.40390500	-0.38336900	-0.78737600
C	5.73398500	0.62301300	-0.07656100
C	5.63818200	-1.31619100	-1.50657200
C	4.32489700	0.67713400	-0.10192000
F	6.46086000	1.55551800	0.65438000

C	4.23533900	-1.21230800	-1.49818500
F	6.27031000	-2.33013300	-2.21576900
C	3.49488000	-0.21675000	-0.80483200
F	3.76999500	1.70593300	0.67080200
F	3.56116700	-2.19982500	-2.23509000
B	1.84456400	-0.26138100	-1.05059700
C	0.77238800	1.28812200	0.09958100
C	1.13500100	2.60184800	-0.31315300
C	0.83715500	1.13416300	1.51124500
C	1.58551600	3.62243600	0.54164300
F	1.04437500	2.95828600	-1.66648000
C	1.28420500	2.10750600	2.42147300
F	0.39872000	-0.06957300	2.08428300
C	1.67674100	3.36413400	1.92230400
F	1.91645900	4.88471700	0.05916400
F	1.32278800	1.86970700	3.79007500
F	2.11160400	4.34989700	2.78635000
C	-2.67474500	-1.25598900	2.87776300
H	-2.00874300	-0.49998400	2.45015800
C	-4.22520700	-1.54002800	-2.11870200
H	-3.44359500	-0.78380700	-2.22073100
C	1.24982200	-1.67353500	-0.48251500
C	0.30700900	-2.46483900	-1.17974200
C	1.77756000	-2.31647500	0.66694400
C	-0.06664600	-3.77059900	-0.80711100
C	1.42616300	-3.61144300	1.08854100
C	0.49845300	-4.35315000	0.33815700
F	2.71305000	-1.65899200	1.47136000
F	1.98194800	-4.16335600	2.23641900
F	0.13531400	-5.63172600	0.73145400
F	-0.98737200	-4.49171500	-1.56227700
F	-0.32432500	-1.97280500	-2.32979900
C	1.59048400	0.16686600	-2.58378200
H	0.55078900	0.35053000	-2.85281200
H	2.17171800	1.06212500	-2.84301700
H	1.94833600	-0.64859700	-3.23250000
H	-5.98537500	-4.22678700	1.32916600
C	-3.54568300	-0.56105700	3.96686700
H	-4.20945200	0.20418300	3.53528400
H	-4.18106600	-1.28423500	4.49962700
H	-2.89859100	-0.07668700	4.71618100
C	-1.75914200	-2.33686400	3.52360000
H	-2.34348100	-3.11642700	4.03493900
H	-1.13093800	-2.82819700	2.76870900
H	-1.09278500	-1.87229200	4.26659100
C	-3.82322100	-2.72075400	-3.05140200
H	-2.86386200	-3.14344300	-2.72996600
H	-4.57519600	-3.52403400	-3.05056700
H	-3.71331300	-2.36332700	-4.08771000
C	-5.56540700	-0.89122300	-2.57568800
H	-5.84051100	-0.03752500	-1.93555300
H	-5.47536100	-0.52828700	-3.61239800
H	-6.39773300	-1.61076400	-2.54635300
H	-0.98958500	3.78324600	1.51599100
H	-2.63125800	1.90202200	2.50554100
H	-4.64900000	1.50461600	0.74215000
C	-2.00619900	4.90753500	-1.12069700

H	-1.08194400	5.46068100	-0.94852500
C	-2.82826200	5.21151300	-2.20750800
H	-2.54427200	6.01004100	-2.89599900
C	-4.05763400	4.50165900	-2.43489500
H	-4.68083000	4.78734000	-3.28512900
C	-4.47016200	3.46989500	-1.58921600
H	-5.40754000	2.94086300	-1.76884700
Frequencies --	-217.0368	11.8037	14.8913
Frequencies --	21.5470	23.1880	30.3277
Frequencies --	32.2720	34.0849	38.2996
Frequencies --	40.9882	46.3186	48.3243
Frequencies --	54.8098	57.2629	62.3880
Frequencies --	71.0269	74.5043	81.0537
Frequencies --	84.0804	91.8384	93.6813
Frequencies --	97.1747	106.3109	109.7217
Frequencies --	116.0038	120.6207	121.8058
Frequencies --	126.8477	134.0629	140.0108
Frequencies --	143.2989	151.1649	155.7433
Frequencies --	157.1870	164.5604	166.3460
Frequencies --	186.5913	197.4520	199.4162
Frequencies --	201.6786	210.8432	215.7529
Frequencies --	220.0110	221.7737	225.5761
Frequencies --	237.0223	242.3255	243.5449
Frequencies --	249.9112	261.7073	264.1163
Frequencies --	265.7532	266.4773	267.7760
Frequencies --	271.1642	272.5805	275.0239
Frequencies --	276.9947	277.3648	292.8964
Frequencies --	298.5430	301.9381	303.6972
Frequencies --	306.1124	312.1151	313.5914
Frequencies --	317.4718	319.8751	328.2344
Frequencies --	331.5180	334.4756	368.8596
Frequencies --	371.7900	375.4103	380.5380
Frequencies --	393.0697	412.0918	421.8063
Frequencies --	423.4893	425.3205	431.3902
Frequencies --	432.2365	433.4728	433.5705
Frequencies --	440.9182	441.2755	450.8755
Frequencies --	454.3469	485.3867	516.5494
Frequencies --	535.2383	538.1192	540.0424
Frequencies --	542.5850	544.0665	545.9415
Frequencies --	551.2070	564.1279	571.2849
Frequencies --	590.9725	591.5702	599.3777
Frequencies --	604.8684	608.1502	628.3940
Frequencies --	629.4957	637.6050	641.9897
Frequencies --	643.8468	649.1673	669.3208
Frequencies --	673.0781	692.8818	714.4206
Frequencies --	717.7029	720.1608	725.6240
Frequencies --	737.3509	737.5529	740.6756
Frequencies --	749.7955	761.6242	768.9800
Frequencies --	783.4264	796.3478	815.4720
Frequencies --	818.1023	820.8039	830.6004
Frequencies --	863.1066	875.6174	876.0406
Frequencies --	880.8068	886.9184	893.0292
Frequencies --	898.8695	907.6196	919.3633
Frequencies --	922.0688	925.8868	931.2201
Frequencies --	932.4447	939.2944	963.5177
Frequencies --	965.4694	977.9022	987.2728
Frequencies --	991.6768	993.7551	997.7869
Frequencies --	1007.5920	1011.9284	1039.0304
Frequencies --	1043.8795	1055.0834	1057.6794
Frequencies --	1060.2827	1065.0308	1068.7383
Frequencies --	1072.8848	1086.8559	1112.2261

Frequencies --	1113.8795	1117.3044	1141.0557
Frequencies --	1166.6413	1167.9475	1177.1207
Frequencies --	1181.6942	1183.7440	1186.3586
Frequencies --	1205.4709	1211.3304	1214.9615
Frequencies --	1223.0177	1243.0779	1248.1009
Frequencies --	1250.3257	1273.0045	1275.3620
Frequencies --	1305.6204	1311.1206	1326.8119
Frequencies --	1327.9027	1332.3871	1336.2883
Frequencies --	1338.4490	1341.7920	1357.4054
Frequencies --	1363.7342	1370.0392	1376.9655
Frequencies --	1377.3220	1383.8580	1400.8747
Frequencies --	1401.2682	1414.8921	1419.1041
Frequencies --	1419.5549	1421.0724	1423.0936
Frequencies --	1425.8849	1430.2008	1434.3955
Frequencies --	1443.1985	1446.6380	1469.2861
Frequencies --	1470.3856	1473.2399	1473.4448
Frequencies --	1486.8943	1488.8154	1489.3465
Frequencies --	1491.0103	1492.5999	1498.8743
Frequencies --	1499.8654	1501.9656	1502.4265
Frequencies --	1506.4223	1510.2454	1561.7523
Frequencies --	1570.3042	1582.2081	1594.3659
Frequencies --	1596.2391	1597.0182	1605.2506
Frequencies --	1619.1492	1622.7622	1629.2470
Frequencies --	3005.0362	3008.6617	3020.0205
Frequencies --	3023.0517	3024.6520	3038.3212
Frequencies --	3103.7411	3106.7898	3109.6385
Frequencies --	3111.1595	3113.6100	3117.3050
Frequencies --	3121.5439	3136.1981	3147.3893
Frequencies --	3147.9200	3158.8064	3166.0992
Frequencies --	3166.2428	3170.0486	3175.9196
Frequencies --	3178.1833	3188.4988	3188.9460
Frequencies --	3200.6144	3201.4676	3216.7767
Frequencies --	3249.1172	3276.3131	3300.1212

Catalyst 24:

vacuum	toluene-like solvent	D3 dispersion
-3954.5930776	-3954.6059203	-0.88028237

Imaginary frequency corresponding to vibration along the reaction coordinate: -234 cm^{-1} .

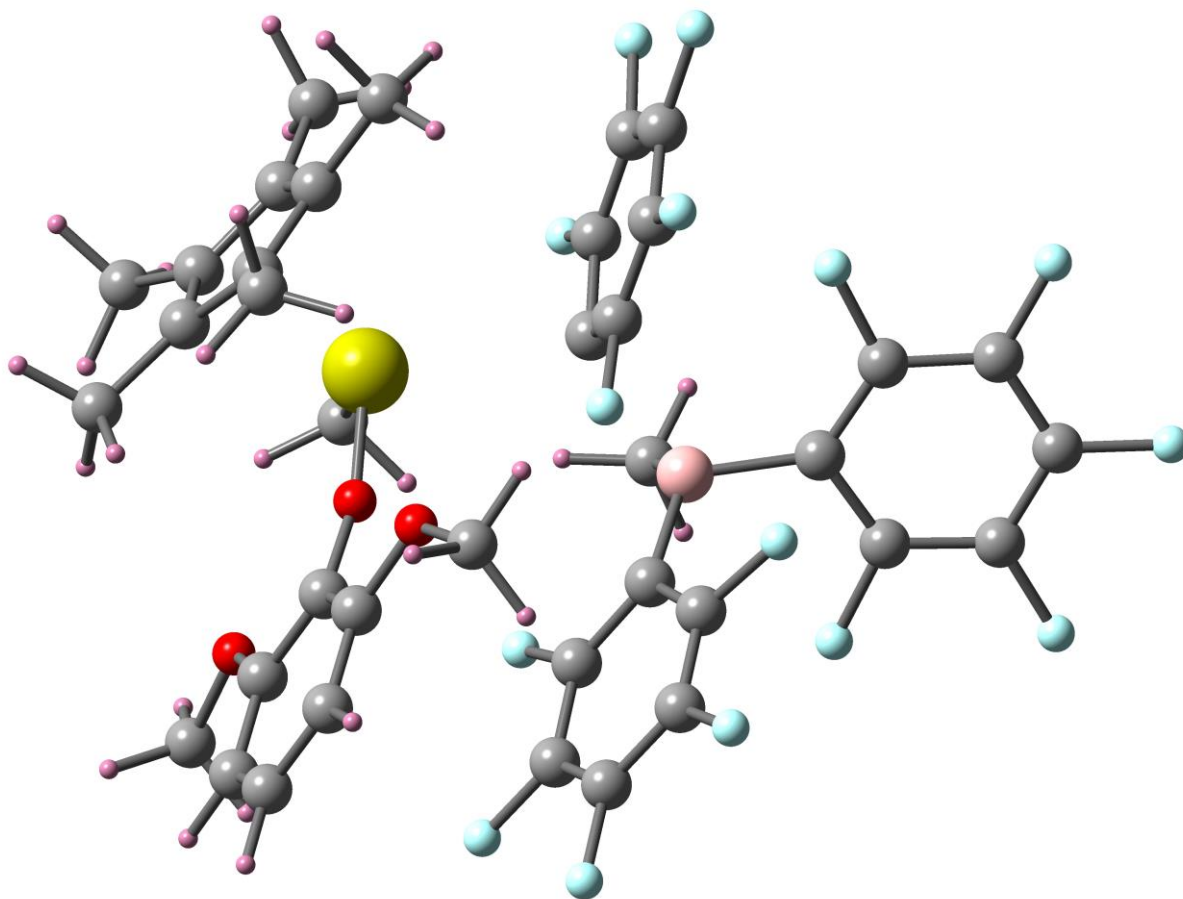
Zr	-0.18640900	1.90787600	-0.65455000
C	-0.04350900	1.66417200	-2.84186500
H	0.01914100	0.57507000	-2.99284500
H	-0.87500600	2.03858300	-3.45054900
H	0.89268000	2.13616500	-3.18531000
O	-1.59607500	0.59339400	-0.26089200
C	-2.83645500	-0.00693500	0.02768600
C	-3.20489800	-0.25283700	1.39396000
C	-3.72048100	-0.32098200	-1.06066300
C	-4.53082400	-0.71230100	1.66487000
C	-5.03630400	-0.78594600	-0.75476500
C	-5.42243100	-0.93163100	0.59423700
H	-6.42255800	-1.30226300	0.81512800
C	-0.43820800	3.99357600	0.79535000
C	0.45758700	4.44565500	-0.25410300
C	-1.73118300	3.74316300	0.19332900
C	-0.26097900	4.42072700	-1.50219800
C	-1.61490100	3.98866400	-1.22887200
F	8.73520200	-2.89664000	-0.53847100
C	7.44454500	-2.39642800	-0.62482400
C	7.09137400	-1.20328600	0.02264000
C	6.45804800	-3.07847100	-1.35646700

C	5.77209100	-0.71509700	-0.08122500
F	8.03945700	-0.51594500	0.77148000
C	5.15904000	-2.54319800	-1.42988900
F	6.77146800	-4.27229700	-1.99526000
C	4.74058500	-1.33309500	-0.81360700
F	5.52612900	0.45672300	0.64208300
F	4.23810700	-3.31042000	-2.16220200
B	3.16677600	-0.88933800	-1.13759800
C	2.58435700	1.06397600	-0.16639800
C	3.43542700	2.11583600	-0.59416000
C	2.44959500	1.02535800	1.24226600
C	4.16331000	2.95876600	0.26267100
F	3.59649000	2.37632000	-1.96665400
C	3.13765300	1.83736100	2.15982100
F	1.51602600	0.12941600	1.79712800
C	4.01915700	2.80922500	1.65451500
F	4.98985500	3.96455000	-0.22858600
F	2.94243000	1.73398600	3.53357900
F	4.69543100	3.65181200	2.52009700
C	2.16034900	-1.97331300	-0.44633100
C	1.07217200	-2.57218900	-1.12128100
C	2.40561000	-2.53929100	0.83060800
C	0.29371500	-3.62393400	-0.59940800
C	1.65257900	-3.58192600	1.39891200
C	0.58570000	-4.13825100	0.67348200
F	3.44625900	-2.04901300	1.62366300
F	1.93948600	-4.05550500	2.67456600
F	-0.17808200	-5.16159800	1.21420700
F	-0.76384100	-4.15585600	-1.33312500
F	0.70271000	-2.13784800	-2.39793800
C	3.05658100	-0.52426900	-2.69822700
H	2.11212300	-0.06979200	-2.99844000
H	3.87072200	0.14869600	-2.99881400
H	3.16986100	-1.44918100	-3.28568100
C	-0.13341400	4.02357400	2.28018900
H	-0.21749200	5.05779600	2.65745200
H	-0.82639000	3.40274900	2.85863800
H	0.88299100	3.67819600	2.51097100
C	1.76005800	5.18288300	-0.03301200
H	1.52496300	6.22814300	0.23558300
H	2.35468100	4.77730600	0.78915000
H	2.39077200	5.21076800	-0.92924500
C	-3.02177700	3.50458500	0.94575500
H	-2.84342900	3.00550200	1.90137000
H	-3.50888300	4.47222900	1.15582800
H	-3.73273000	2.89520300	0.37526400
C	0.24960600	4.97474100	-2.81352100
H	0.20806000	6.07779600	-2.79350700
H	1.29371000	4.69442900	-3.01052700
H	-0.35190200	4.63974600	-3.66670800
C	-2.76759600	4.05396300	-2.20532600
H	-3.60213100	3.41025800	-1.90759600
H	-3.14878200	5.08976600	-2.24612700
H	-2.47649500	3.77328100	-3.22444600
C	-5.04900100	-1.01824200	3.04923900
C	-4.58429500	-2.13602300	3.78831400
C	-6.09352400	-0.23358500	3.60299000

C	-5.13797800	-2.45144800	5.04696300
H	-3.79497600	-2.76615900	3.37630200
C	-6.64513100	-0.54246900	4.86490100
H	-6.47383300	0.62560400	3.04539300
C	-6.16787500	-1.65395900	5.59335600
H	-4.76734700	-3.31989800	5.59666600
H	-7.44485900	0.07954800	5.27445300
H	-6.59494200	-1.89823200	6.56885800
C	-6.05289500	-1.17846500	-1.79802900
C	-5.86971100	-2.31937900	-2.62102200
C	-7.27041800	-0.45831300	-1.90969700
C	-6.86718000	-2.72003900	-3.53423200
H	-4.95152100	-2.90233300	-2.54040400
C	-8.26779400	-0.85278900	-2.82725800
H	-7.43597800	0.41803300	-1.27855800
C	-8.06939100	-1.98680600	-3.64489400
H	-6.70640200	-3.60529500	-4.15413300
H	-9.19483900	-0.27888000	-2.90079900
H	-8.84092300	-2.29733100	-4.35340900
C	-2.25741000	-0.09924200	2.55726100
C	-1.21527200	-1.04044100	2.74795600
C	-2.47685900	0.86586300	3.57429500
C	-0.42125900	-1.02491500	3.91337700
H	-1.04573000	-1.80616300	1.99110300
C	-1.67468400	0.89680700	4.73350700
H	-3.30205000	1.57273200	3.48066700
C	-0.64400900	-0.05162200	4.90996100
H	0.36969500	-1.76603700	4.04143500
H	-1.86920200	1.64517900	5.50568900
H	-0.02756000	-0.03664400	5.81135900
C	-3.31552700	-0.22628800	-2.50978600
C	-2.41046600	-1.16892400	-3.05755000
C	-3.93121100	0.69905700	-3.39008000
C	-2.12662400	-1.18716200	-4.43894100
H	-1.94571500	-1.90966100	-2.41027700
C	-3.64622700	0.68987500	-4.77126400
H	-4.65862200	1.41221400	-2.99924600
C	-2.74295200	-0.25653100	-5.30322900
H	-1.43102800	-1.93027000	-4.83473600
H	-4.14261000	1.40574700	-5.43114000
H	-2.52942500	-0.27406400	-6.37450500
Frequencies --	-234.0445	-16.5406	-6.8353
Frequencies --	10.5579	12.0115	17.6694
Frequencies --	18.6654	23.5220	26.6967
Frequencies --	30.9126	33.9535	34.5775
Frequencies --	37.3834	39.9496	41.6702
Frequencies --	45.9862	47.2302	49.7266
Frequencies --	54.4877	57.1239	60.3818
Frequencies --	61.4715	68.1459	70.6533
Frequencies --	78.4027	83.6843	86.3813
Frequencies --	89.2985	96.2520	101.7389
Frequencies --	108.5961	112.1883	116.4504
Frequencies --	120.3692	120.9140	122.5918
Frequencies --	123.9787	127.2147	132.2696
Frequencies --	133.0300	136.2626	142.2467
Frequencies --	143.0995	148.6222	150.7919
Frequencies --	152.4206	156.4913	163.7086

Frequencies --	165.2974	175.2394	179.6397
Frequencies --	189.4383	192.9036	201.8490
Frequencies --	202.4544	211.5470	212.6602
Frequencies --	213.8706	218.1949	223.1546
Frequencies --	227.5196	232.5113	241.1179
Frequencies --	253.6001	257.4236	258.7774
Frequencies --	263.9097	265.1129	265.7302
Frequencies --	268.0604	275.7963	276.0358
Frequencies --	276.4385	278.8780	282.4488
Frequencies --	287.7188	292.5754	297.7766
Frequencies --	301.5130	301.6549	303.5643
Frequencies --	305.6598	317.0700	318.0485
Frequencies --	321.6553	326.5617	327.2299
Frequencies --	333.7995	336.0061	366.8915
Frequencies --	375.1398	376.9070	379.9380
Frequencies --	386.8313	393.5996	402.7329
Frequencies --	404.4124	405.9872	410.2556
Frequencies --	412.9701	414.4956	420.5631
Frequencies --	426.2379	431.1996	433.6409
Frequencies --	440.0472	441.5589	450.5749
Frequencies --	454.4281	483.3684	485.2823
Frequencies --	493.4624	520.3451	527.9981
Frequencies --	535.8326	539.0232	540.4239
Frequencies --	542.2013	542.6300	546.4788
Frequencies --	550.3054	551.5666	566.7191
Frequencies --	572.2666	583.0224	589.3758
Frequencies --	593.0268	603.8847	614.6638
Frequencies --	616.6750	617.8555	621.2347
Frequencies --	624.5645	629.2586	631.7645
Frequencies --	637.3833	640.1550	642.2279
Frequencies --	644.1350	647.9607	653.1107
Frequencies --	662.0532	669.8464	687.0671
Frequencies --	689.5894	698.2610	703.9598
Frequencies --	708.6874	710.2692	711.0335
Frequencies --	717.1922	717.4650	718.4244
Frequencies --	720.2688	738.4241	746.6742
Frequencies --	755.8438	766.4609	771.7213
Frequencies --	782.8095	783.2564	794.8644
Frequencies --	798.1901	804.2052	805.2708
Frequencies --	832.4131	857.5594	859.9690
Frequencies --	861.2792	869.6585	870.6487
Frequencies --	888.2079	899.2058	907.6507
Frequencies --	914.3402	920.9618	930.7267
Frequencies --	934.8604	941.4196	943.8122
Frequencies --	946.2128	968.8329	971.0055
Frequencies --	983.6710	985.9406	987.2201
Frequencies --	992.6334	994.9632	996.4820
Frequencies --	999.0584	1002.3112	1004.5883
Frequencies --	1005.8154	1009.2486	1011.9609
Frequencies --	1016.3563	1020.6572	1021.3384
Frequencies --	1034.1254	1037.3638	1040.7652
Frequencies --	1042.9884	1044.8169	1046.2087
Frequencies --	1047.0877	1047.9391	1051.7599
Frequencies --	1053.3053	1054.9844	1055.4108
Frequencies --	1059.2500	1062.2218	1085.3596
Frequencies --	1086.7068	1089.0856	1089.8017
Frequencies --	1090.1541	1090.9573	1091.5183
Frequencies --	1114.4729	1123.6988	1129.3990
Frequencies --	1172.7072	1173.7939	1175.4462
Frequencies --	1182.1733	1182.7898	1182.8850
Frequencies --	1185.4436	1196.2870	1203.6510
Frequencies --	1205.1792	1206.6718	1207.4535
Frequencies --	1216.1409	1223.7220	1224.3219

Frequencies --	1248.4737	1257.4286	1277.4986
Frequencies --	1299.0585	1311.9346	1318.4277
Frequencies --	1327.6819	1329.5833	1330.2109
Frequencies --	1331.3022	1333.2434	1343.4219
Frequencies --	1344.8417	1358.2095	1366.1306
Frequencies --	1368.8878	1370.0850	1370.3720
Frequencies --	1371.9492	1377.9664	1379.5208
Frequencies --	1413.4655	1414.8321	1415.1335
Frequencies --	1422.7555	1423.4100	1426.0744
Frequencies --	1427.1816	1429.1293	1432.5367
Frequencies --	1435.0589	1438.4454	1442.3525
Frequencies --	1444.6070	1444.8754	1446.5516
Frequencies --	1446.9927	1451.6140	1454.7670
Frequencies --	1461.0049	1462.4616	1469.3748
Frequencies --	1472.9378	1483.3927	1492.9754
Frequencies --	1496.2197	1497.1190	1497.2253
Frequencies --	1497.7136	1499.6441	1502.0554
Frequencies --	1503.5341	1505.1845	1506.8510
Frequencies --	1507.3588	1508.2378	1512.9912
Frequencies --	1518.9294	1521.6006	1524.4626
Frequencies --	1576.4736	1585.9024	1590.0173
Frequencies --	1595.2973	1596.3342	1596.4946
Frequencies --	1596.8394	1597.3242	1600.0667
Frequencies --	1618.7398	1621.8704	1623.5043
Frequencies --	1623.7647	1624.0828	1624.7105
Frequencies --	3005.1504	3011.9354	3012.8268
Frequencies --	3013.4708	3014.4458	3019.8194
Frequencies --	3040.2432	3101.8340	3112.9264
Frequencies --	3115.2911	3121.2169	3122.0602
Frequencies --	3124.0553	3124.3979	3149.7502
Frequencies --	3150.0236	3150.7232	3152.0643
Frequencies --	3154.8327	3158.2928	3158.4180
Frequencies --	3158.5956	3163.0449	3165.4134
Frequencies --	3168.6126	3170.5525	3170.8083
Frequencies --	3171.8290	3180.6267	3183.1309
Frequencies --	3184.1643	3184.2054	3186.5159
Frequencies --	3188.7387	3190.2664	3191.7546
Frequencies --	3193.2664	3195.3055	3196.5193
Frequencies --	3206.4416	3209.8317	3223.3072

Catalyst 30:

vacuum	toluene-like solvent	D3 dispersion
-3271.2843549	-3271.2941904	-0.60057760

Imaginary frequency corresponding to vibration along the reaction coordinate: -241 cm^{-1} .

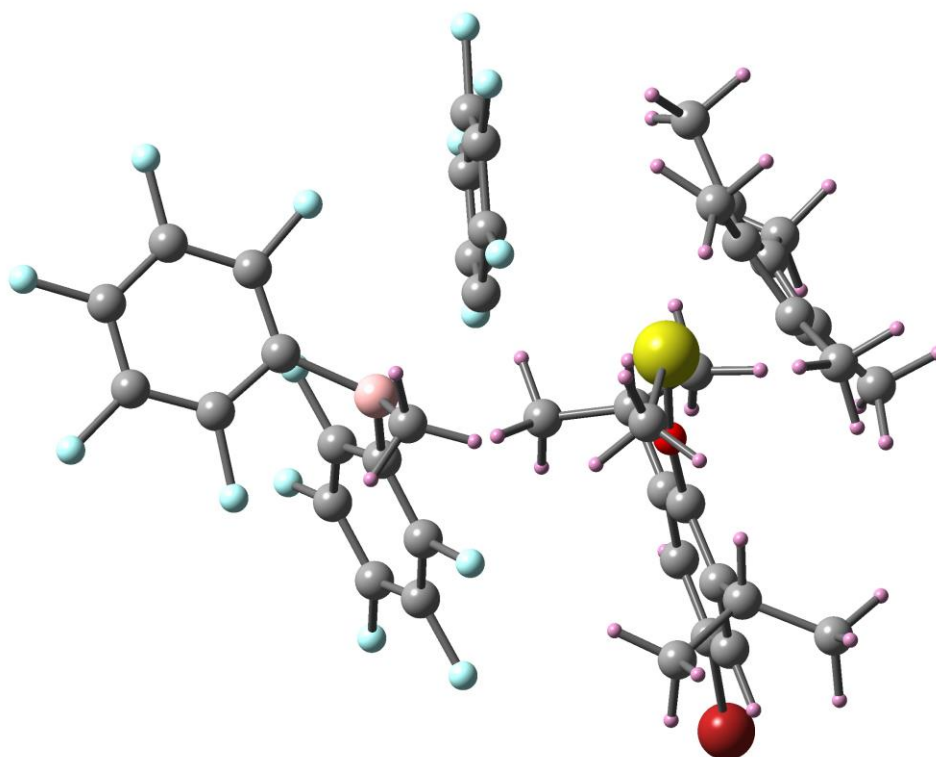
Ti	-2.06833500	1.18136300	-0.58038000
C	-1.98958100	0.78168800	-2.60289700
H	-1.26574700	-0.04513300	-2.61452100
H	-2.93104500	0.42136200	-3.03197500
H	-1.60819900	1.64514500	-3.16805500
O	-2.46923800	-0.45237300	0.00032700
C	-3.05976500	-1.60125300	0.47058400
C	-2.96129600	-1.95642700	1.85232700
C	-3.73566100	-2.47875400	-0.43309300
C	-3.52779600	-3.16884200	2.31195100
C	-4.29916200	-3.68581000	0.04223900
C	-4.18842700	-4.01897400	1.40527600
H	-3.44981900	-3.45385600	3.35870900
H	-4.80511200	-4.36666100	-0.63829400
C	-2.66669700	3.39290200	0.41869000
C	-2.81618400	3.55965400	-1.00668300
C	-3.58425000	2.36379700	0.85738600
C	-3.84176400	2.64723500	-1.45378100

C	-4.31364500	1.89966400	-0.30110700
F	7.75916100	-0.50901000	-0.16103400
C	6.38582000	-0.43149300	-0.34218100
C	5.66714400	0.69436900	0.08604200
C	5.68375400	-1.47663700	-0.96542000
C	4.27138700	0.74993300	-0.11002700
F	6.33417600	1.74744200	0.70194300
C	4.29141900	-1.36855500	-1.13330200
F	6.36819700	-2.60205600	-1.40974800
C	3.50252400	-0.26565400	-0.71031600
F	3.66262900	1.92086600	0.35639500
F	3.68009300	-2.45665400	-1.77855700
B	1.89482100	-0.33348500	-1.13330000
C	0.68675800	1.37064200	-0.18180500
C	0.99045700	2.62484800	-0.77035700
C	0.73871400	1.41386800	1.23543600
C	1.40129700	3.77129700	-0.06794600
F	0.88661300	2.78755800	-2.16525400
C	1.15026700	2.52035200	1.99940500
F	0.33884200	0.29189300	1.97577300
C	1.50336700	3.70684600	1.33309700
F	1.67661200	4.97554900	-0.71646200
F	1.18028900	2.48185000	3.39245900
F	1.88822800	4.82318800	2.05465000
C	1.20275900	-1.67342300	-0.51372400
C	0.34927500	-2.52985300	-1.24958700
C	1.54053200	-2.18705000	0.76512800
C	-0.13451300	-3.76517100	-0.77907700
C	1.05651400	-3.39916400	1.28942100
C	0.21481900	-4.20505200	0.50607300
F	2.41893900	-1.48744100	1.59646300
F	1.39949500	-3.80898100	2.57531700
F	-0.27473400	-5.40544700	1.00116500
F	-0.96191600	-4.55356100	-1.57628900
F	-0.06320900	-2.19517400	-2.54394000
C	1.80207500	-0.00031400	-2.70354700
H	0.79515300	0.14940700	-3.09664900
H	2.40007400	0.88721400	-2.95179700
H	2.24105900	-0.84954000	-3.25508900
C	-1.93208600	4.32399200	1.35483200
H	-2.65504400	5.05496200	1.75912300
H	-1.49356700	3.80701100	2.21738200
H	-1.14761200	4.90092300	0.85418700
C	-2.13425900	4.61102700	-1.85371300
H	-2.59945500	5.59695400	-1.68043500
H	-1.06703900	4.70778900	-1.62354500
H	-2.21929200	4.39373300	-2.92595900
C	-3.84410800	2.00659700	2.30326200
H	-2.95838000	1.59838400	2.80850500
H	-4.15842500	2.90663700	2.85782100
H	-4.64265700	1.26208000	2.40180200
C	-4.50081200	2.66104100	-2.81194000
H	-5.25603800	3.46604500	-2.84266900
H	-3.79089300	2.85009500	-3.62716000
H	-5.01980500	1.71924500	-3.03119700
C	-5.49845100	0.96164600	-0.30020900
H	-5.50561000	0.30027200	0.57412600

H	-6.43451700	1.54674400	-0.27875900
H	-5.52710400	0.32495600	-1.19375900
H	-4.61698700	-4.95605500	1.76437300
O	-2.28636800	-1.04433300	2.66002900
O	-3.78889700	-2.04996100	-1.76059600
C	-1.89134300	-1.45244000	4.01582000
H	-1.26730100	-0.63009500	4.38271400
H	-2.77136600	-1.57726400	4.66786800
H	-1.30083300	-2.38151400	3.99400800
C	-4.22415200	-3.00602900	-2.78864400
H	-3.60513000	-3.91535200	-2.76600200
H	-5.28924300	-3.26485300	-2.67010700
H	-4.07507300	-2.48107200	-3.73946600

Frequencies --	-240.6620	10.3121	15.2544
Frequencies --	18.6293	24.1220	29.5079
Frequencies --	32.2824	37.2440	40.5948
Frequencies --	43.6224	44.1626	52.5723
Frequencies --	53.2720	60.4756	61.6733
Frequencies --	66.7052	74.1417	78.7517
Frequencies --	81.5026	89.9992	95.0505
Frequencies --	103.7981	107.2503	110.5338
Frequencies --	112.0913	115.3487	120.6750
Frequencies --	124.9798	128.0364	136.0482
Frequencies --	139.1107	145.4840	148.2854
Frequencies --	151.5589	157.1441	165.9866
Frequencies --	168.4799	172.5221	177.3727
Frequencies --	180.7786	183.7515	185.9849
Frequencies --	191.4102	198.1878	200.4106
Frequencies --	208.7426	213.6189	221.5103
Frequencies --	222.9148	226.2575	241.2431
Frequencies --	256.5877	260.9258	263.9219
Frequencies --	264.8075	265.2985	266.7117
Frequencies --	267.9137	274.0541	275.2408
Frequencies --	275.7362	276.9651	283.7841
Frequencies --	285.1072	290.5831	297.4050
Frequencies --	298.1765	302.6415	303.7271
Frequencies --	305.3954	315.7310	317.2461
Frequencies --	323.4212	327.4560	332.6493
Frequencies --	340.2647	357.1677	366.0651
Frequencies --	374.7115	375.3014	379.6984
Frequencies --	383.2362	397.5143	404.6630
Frequencies --	407.7879	422.0329	424.4467
Frequencies --	431.7072	433.0411	438.0782
Frequencies --	449.7889	453.1373	484.0191
Frequencies --	511.8293	520.5341	530.5867
Frequencies --	536.2806	539.8625	541.7129
Frequencies --	542.6384	550.9823	555.3504
Frequencies --	566.5852	577.6188	581.5504
Frequencies --	587.9938	590.4026	595.0408
Frequencies --	601.9602	608.7262	616.7284
Frequencies --	628.9881	635.9849	640.0709
Frequencies --	643.1581	648.0185	665.8648
Frequencies --	686.9515	690.4082	711.5950
Frequencies --	716.8976	719.3838	725.0326
Frequencies --	728.1787	738.1064	751.0974
Frequencies --	759.9102	782.5119	801.5004
Frequencies --	808.6536	831.8907	846.1554
Frequencies --	853.3319	887.2971	894.3488
Frequencies --	907.7916	913.6204	916.8706
Frequencies --	952.3760	967.0794	974.2593

Frequencies --	982.9986	983.7357	989.7519
Frequencies --	999.6355	1031.3509	1040.3470
Frequencies --	1044.9754	1045.9392	1048.5599
Frequencies --	1049.1666	1056.4954	1056.8609
Frequencies --	1061.2065	1082.5072	1088.6591
Frequencies --	1088.8359	1090.7641	1102.1074
Frequencies --	1124.3852	1127.4428	1128.0201
Frequencies --	1167.4548	1168.8162	1171.4926
Frequencies --	1176.0914	1177.1574	1181.9938
Frequencies --	1209.2543	1215.2699	1221.5665
Frequencies --	1227.1251	1247.0477	1256.7375
Frequencies --	1291.1567	1313.0225	1329.6297
Frequencies --	1338.8886	1342.1280	1357.5288
Frequencies --	1364.9870	1369.4604	1374.4069
Frequencies --	1411.4654	1415.1817	1415.8544
Frequencies --	1419.6163	1423.7757	1425.4817
Frequencies --	1428.8581	1430.0422	1431.9096
Frequencies --	1437.6315	1443.5521	1445.0977
Frequencies --	1446.8392	1449.9874	1453.9217
Frequencies --	1457.7614	1461.9569	1468.0560
Frequencies --	1470.8227	1472.6408	1477.2275
Frequencies --	1482.6113	1486.5397	1487.0864
Frequencies --	1488.1614	1490.5365	1492.0121
Frequencies --	1493.3963	1493.7115	1494.8250
Frequencies --	1499.2905	1501.6900	1504.1376
Frequencies --	1506.2837	1511.2173	1517.6480
Frequencies --	1522.4748	1576.3755	1583.6069
Frequencies --	1591.4162	1596.9707	1598.6579
Frequencies --	1603.8749	1620.6197	1622.4107
Frequencies --	3007.5461	3009.4810	3010.8116
Frequencies --	3011.3223	3013.2457	3015.6856
Frequencies --	3020.0273	3021.7528	3024.1327
Frequencies --	3104.7912	3107.7468	3108.6495
Frequencies --	3110.7423	3111.5655	3113.6395
Frequencies --	3115.1057	3116.6910	3146.2052
Frequencies --	3149.4046	3152.7472	3157.9401
Frequencies --	3159.1199	3164.7634	3168.0227
Frequencies --	3171.1196	3171.8771	3181.2320
Frequencies --	3197.1528	3217.8669	3225.8439

Catalyst 31:

vacuum	toluene-like solvent	D3 dispersion
-3290.6268308	-3290.6369593	-0.67063835

Imaginary frequency corresponding to vibration along the reaction coordinate: -232 cm^{-1} .

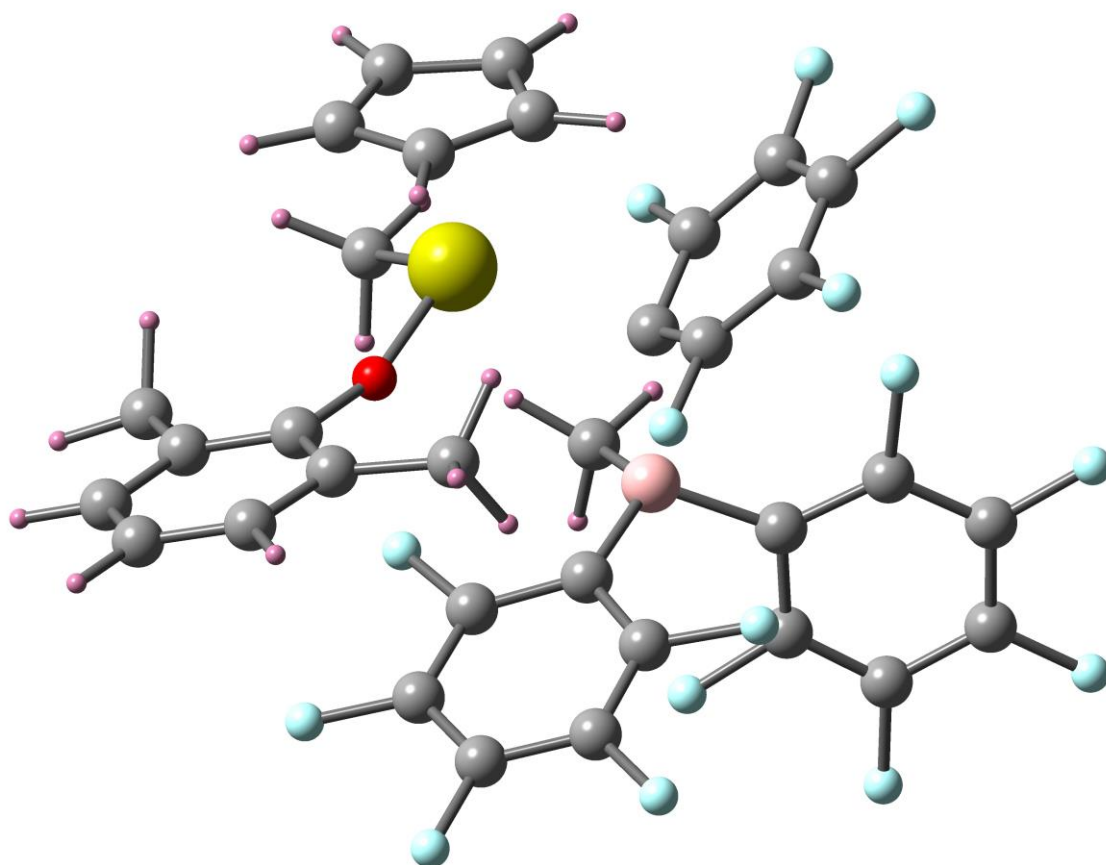
Ti	-1.03675600	2.20409400	-0.57707100
C	-0.68210100	1.84651000	-2.57850800
H	-0.50072100	0.76139900	-2.55876400
H	-1.45317300	2.07135200	-3.32196000
H	0.24524100	2.38256800	-2.83421400
O	-2.20987600	0.89682000	-0.22887400
C	-3.27584400	0.01535100	0.01553700
C	-3.48182300	-0.49897300	1.33913200
C	-4.12213600	-0.37591800	-1.07785100
C	-4.52485200	-1.43590600	1.53317600
C	-5.14353600	-1.31969100	-0.82372300
C	-5.33518500	-1.84082900	0.46382600
H	-4.69379300	-1.84657900	2.52611100
H	-5.78551300	-1.64424300	-1.63946800
C	-0.57129400	4.47516700	0.41386900
C	-0.53168000	4.66566300	-1.01394900
C	-1.88367800	3.97961400	0.76996000
C	-1.82939700	4.31196000	-1.54655900
C	-2.67089700	3.89106500	-0.43987400
F	8.04588500	-2.77214200	-0.32014300
C	6.74957300	-2.29670100	-0.45289600
C	6.34170800	-1.13067000	0.21273300

C	5.81572500	-2.97580900	-1.25366100
C	5.01881000	-0.66495400	0.06209100
F	7.24067700	-0.44771300	1.02349900
C	4.51034700	-2.46516000	-1.37080200
F	6.18721900	-4.13935700	-1.91650100
C	4.03862600	-1.28803000	-0.73308800
F	4.71168500	0.48328300	0.79890500
F	3.63681900	-3.21399100	-2.17732000
B	2.48619900	-0.86166700	-1.12003500
C	1.80292900	1.13047800	0.01116800
C	2.61218800	2.22614400	-0.36000600
C	1.65171900	1.00984200	1.40774400
C	3.29366200	3.06330000	0.54030900
F	2.79201300	2.54032900	-1.72558700
C	2.30295000	1.80373200	2.36931100
F	0.77292700	0.03029300	1.92192600
C	3.15209400	2.83237900	1.92083700
F	4.07705100	4.13364200	0.10362800
F	2.10656100	1.62378200	3.73870200
F	3.79066900	3.65662800	2.83350800
C	-2.64348500	-0.10585500	2.56642600
H	-1.90220100	0.64038500	2.25375800
C	-3.98082200	0.16417500	-2.51085100
H	-3.27349300	0.99938200	-2.48152200
C	1.42234100	-1.93956700	-0.53838700
C	0.30241200	-2.40520300	-1.26637100
C	1.61996200	-2.62751800	0.68681600
C	-0.54253900	-3.44975000	-0.84533500
C	0.80470300	-3.67525200	1.15127100
C	-0.28835900	-4.09578400	0.37481500
F	2.67015300	-2.26285300	1.53220300
F	1.05624600	-4.28723400	2.37312800
F	-1.11487500	-5.11658000	0.81718800
F	-1.62649600	-3.84423500	-1.62314200
F	-0.03269400	-1.83198000	-2.49951800
C	2.44541400	-0.36272000	-2.64142300
H	1.51512300	0.11895400	-2.94379800
H	3.27464100	0.32590200	-2.85078300
H	2.58057900	-1.24203800	-3.29413700
C	0.44489200	4.97160500	1.41486600
H	0.09533800	5.94000000	1.81466800
H	0.56604800	4.30352500	2.27661500
H	1.42850100	5.14931400	0.97043200
C	0.60160300	5.27985600	-1.80262700
H	0.46165600	6.37381000	-1.86101400
H	1.58171700	5.10126300	-1.34650300
H	0.64457700	4.90528500	-2.83374900
C	-2.40173900	3.84179400	2.18219300
H	-3.31255700	3.23703800	2.23499100
H	-1.66282600	3.39868300	2.86467800
H	-2.64984200	4.84023200	2.58251200
C	-2.30145800	4.60410500	-2.95081000
H	-2.63840100	5.65391800	-3.01036100
H	-1.50628600	4.47748300	-3.69611000
H	-3.14981500	3.97526800	-3.25079600
C	-4.16234200	3.65896500	-0.49856500
H	-4.50428200	2.91710700	0.23402400

H	-4.68832800	4.60428000	-0.27776000
H	-4.49349700	3.32788800	-1.48873400
C	-3.52284300	0.52971000	3.68603700
H	-4.19426500	1.30930100	3.29682100
H	-4.14827100	-0.22585200	4.18482200
H	-2.87836000	0.98090500	4.45682700
C	-1.85494000	-1.31995300	3.13735000
H	-1.13855400	-1.70549200	2.40430600
H	-1.28777800	-1.01608400	4.03033500
H	-2.52679000	-2.14158700	3.42666900
C	-3.39204500	-0.91179600	-3.47129400
H	-3.36198400	-0.52316800	-4.50192500
H	-2.37250400	-1.18831400	-3.18067400
H	-4.00285900	-1.82677400	-3.47312600
C	-5.32386300	0.71665400	-3.07378800
H	-5.77818700	1.45892400	-2.40047700
H	-5.14638200	1.19741300	-4.04939100
H	-6.06392100	-0.08032500	-3.23732800
Br	-6.76673000	-3.15218500	0.77493900

Frequencies --	-231.6162	-5.0141	9.9553
Frequencies --	13.3910	17.4303	25.9553
Frequencies --	27.2775	28.4199	33.0321
Frequencies --	35.2197	40.2906	42.2948
Frequencies --	46.0031	50.0829	55.8426
Frequencies --	65.4610	71.4681	80.2747
Frequencies --	81.9106	84.5402	88.8038
Frequencies --	95.0024	99.6249	107.4231
Frequencies --	109.4450	113.4551	116.6279
Frequencies --	118.6813	120.2562	124.0330
Frequencies --	127.1977	128.5592	131.5763
Frequencies --	137.9513	146.1599	150.2213
Frequencies --	151.5844	155.1228	158.6091
Frequencies --	162.8614	166.3721	168.3113
Frequencies --	176.4355	180.0226	190.1998
Frequencies --	196.8784	200.2188	203.3665
Frequencies --	204.2034	207.1332	218.7952
Frequencies --	222.8399	228.1904	229.7335
Frequencies --	239.2320	242.2302	245.8705
Frequencies --	250.0725	255.0346	262.0722
Frequencies --	263.6452	265.2930	265.6128
Frequencies --	268.9911	272.4836	274.7062
Frequencies --	276.5594	285.7998	286.2575
Frequencies --	295.8787	296.4056	298.9462
Frequencies --	301.6894	303.3516	304.0756
Frequencies --	308.8667	311.2045	315.8772
Frequencies --	316.8587	324.1816	325.9163
Frequencies --	332.7846	333.3100	352.5237
Frequencies --	364.4722	376.3652	382.2337
Frequencies --	382.9340	385.4847	408.1122
Frequencies --	416.5174	421.5912	424.2960
Frequencies --	427.2414	431.4298	432.0502
Frequencies --	437.1219	437.6577	449.1045
Frequencies --	453.0942	463.0323	483.1959
Frequencies --	508.7068	527.8738	535.8300
Frequencies --	539.2346	540.4293	540.9401
Frequencies --	550.5722	552.7551	559.5843
Frequencies --	566.9028	581.8386	588.4332
Frequencies --	590.8798	602.1727	608.2703
Frequencies --	610.0001	622.7879	625.7218
Frequencies --	629.3672	637.1091	641.1854

Frequencies --	642.7358	644.3686	661.6714
Frequencies --	682.8596	706.4283	706.6944
Frequencies --	717.8765	720.0429	741.1181
Frequencies --	754.6896	768.0322	778.6736
Frequencies --	785.5121	801.6189	806.0409
Frequencies --	806.7976	838.4239	877.3233
Frequencies --	879.6734	894.6588	895.8527
Frequencies --	907.9762	908.8191	915.4179
Frequencies --	921.2483	933.6080	936.9327
Frequencies --	945.2795	962.7798	965.1908
Frequencies --	966.5976	973.1799	974.4210
Frequencies --	992.1955	1003.9244	1020.7052
Frequencies --	1038.8889	1040.2421	1043.0063
Frequencies --	1044.6213	1046.0153	1051.2758
Frequencies --	1060.2299	1066.7366	1070.1639
Frequencies --	1084.3400	1088.4019	1088.9274
Frequencies --	1101.6613	1111.7060	1116.1598
Frequencies --	1121.5503	1125.0555	1164.4961
Frequencies --	1171.6111	1171.9389	1176.1066
Frequencies --	1180.0416	1183.1239	1197.7686
Frequencies --	1218.2806	1229.4398	1239.5598
Frequencies --	1250.1762	1268.4991	1297.1065
Frequencies --	1315.3666	1316.9957	1319.4804
Frequencies --	1331.5686	1332.8196	1344.8118
Frequencies --	1353.6797	1360.0515	1366.9340
Frequencies --	1372.2209	1372.3370	1403.9610
Frequencies --	1404.1031	1409.9859	1415.5968
Frequencies --	1417.5904	1421.0839	1423.1494
Frequencies --	1424.1297	1424.4549	1426.2803
Frequencies --	1426.5742	1426.9831	1431.1970
Frequencies --	1433.9742	1434.5434	1438.6367
Frequencies --	1441.4606	1448.9415	1456.4659
Frequencies --	1458.5438	1463.6322	1471.7088
Frequencies --	1472.6642	1480.8896	1486.4902
Frequencies --	1486.7384	1488.1024	1489.4024
Frequencies --	1491.7550	1493.8522	1496.5571
Frequencies --	1498.1130	1498.4713	1501.4298
Frequencies --	1502.1192	1503.5463	1506.5556
Frequencies --	1507.3664	1509.4613	1511.7535
Frequencies --	1513.0147	1517.3652	1521.1101
Frequencies --	1573.6127	1577.7569	1582.4827
Frequencies --	1587.2086	1597.3584	1597.9540
Frequencies --	1619.7441	1622.5597	3011.3562
Frequencies --	3011.9977	3012.5891	3014.0382
Frequencies --	3014.6476	3014.8979	3015.6543
Frequencies --	3016.2986	3024.3874	3028.3723
Frequencies --	3031.8384	3088.4631	3098.8631
Frequencies --	3105.1142	3108.5677	3110.5803
Frequencies --	3110.9131	3111.5585	3113.7958
Frequencies --	3115.3592	3120.3393	3121.9218
Frequencies --	3122.4806	3129.5607	3137.4820
Frequencies --	3139.3681	3147.7891	3163.6325
Frequencies --	3165.0655	3169.8459	3172.0465
Frequencies --	3172.2716	3174.8179	3176.7957
Frequencies --	3207.9963	3215.0631	3217.3868

Catalyst 33:

vacuum	toluene-like solvent	D3 dispersion
-2924.4670496	-2924.4769852	-0.50699176

Imaginary frequency corresponding to vibration along the reaction coordinate: -202 cm^{-1} .

Ti	-1.95516400	1.67602400	-0.76127700
C	-2.04655700	1.50851300	-2.83122800
H	-1.76443900	0.45798700	-2.99442300
H	-3.01258100	1.69921700	-3.31330200
H	-1.28617900	2.18473500	-3.25292400
O	-2.90561300	0.25256500	-0.27544300
C	-3.99351100	-0.51012500	0.17822500
C	-4.13295600	-0.78343900	1.57401600
C	-4.91859500	-1.01242800	-0.78933300
C	-5.25255100	-1.54709100	1.98248600
C	-6.01389000	-1.77363600	-0.32013500
C	-6.18943800	-2.03649500	1.05241300
H	-5.37720500	-1.76743100	3.04421300
H	-6.72747500	-2.16987900	-1.04459100
H	-7.04146700	-2.62766700	1.39296800
H	-1.37031200	3.86094700	1.48274900
C	-2.03306000	3.70198100	0.64039300
C	-1.82715600	4.16574100	-0.70572600
C	-3.30541900	3.04655100	0.69655900

H	-0.97419600	4.72665300	-1.07249500
C	-2.96908200	3.78957300	-1.47970500
H	-3.76201500	2.60530300	1.57514900
C	-3.87985600	3.08474000	-0.61779600
H	-3.12427000	4.01057800	-2.52922300
H	-4.84130700	2.66889800	-0.90359400
F	7.07503000	-1.69524200	-0.11971600
C	5.73665600	-1.36937500	-0.27827900
C	5.24310600	-0.12926400	0.15171700
C	4.84264700	-2.27285200	-0.87702800
C	3.87782500	0.17828600	-0.02297500
F	6.09937900	0.78776900	0.74998200
C	3.49114900	-1.91244300	-1.02539500
F	5.29928500	-3.50953200	-1.31537500
C	2.92488400	-0.67774200	-0.60737400
F	3.50341200	1.44181500	0.45692300
F	2.67895000	-2.88320200	-1.63374600
B	1.32099000	-0.45312100	-1.00947600
C	0.52517600	1.39628600	-0.19679800
C	1.08880500	2.56593000	-0.78535100
C	0.53012800	1.46333300	1.22612300
C	1.64540300	3.64420900	-0.07688400
F	1.08771300	2.71314300	-2.17969800
C	1.09070500	2.49821700	1.99436400
F	-0.10076500	0.45276500	1.95845800
C	1.66092300	3.59968100	1.32948400
F	2.15323000	4.75938200	-0.73215300
F	1.05719100	2.47800300	3.38255800
F	2.19751200	4.64534100	2.05231900
C	-3.11690000	-0.34918300	2.61468300
H	-2.20892300	-0.96659900	2.55876500
H	-2.79280500	0.69073600	2.49620200
H	-3.53001900	-0.46205200	3.62621800
C	-4.75264200	-0.77443300	-2.27886100
H	-4.83577400	0.29237600	-2.53515000
H	-3.77349600	-1.12152000	-2.63471200
H	-5.52680200	-1.31275900	-2.84172200
C	0.40604600	-1.62994300	-0.33013600
C	-0.65611100	-2.28380800	-0.99592900
C	0.70911400	-2.20917400	0.92972500
C	-1.36247600	-3.38941800	-0.48553100
C	0.03346600	-3.31113400	1.48566400
C	-1.01431100	-3.91371400	0.76892400
F	1.74160100	-1.68739300	1.71483100
F	0.39035100	-3.80969900	2.73297100
F	-1.69999200	-4.99604600	1.29757300
F	-2.40382500	-3.95974700	-1.20988200
F	-1.08840900	-1.84213100	-2.25355200
C	1.28621600	-0.23145200	-2.60913300
H	0.33444400	0.09980900	-3.02507400
H	2.05925600	0.48460700	-2.92048300
H	1.52672100	-1.19375900	-3.09005600

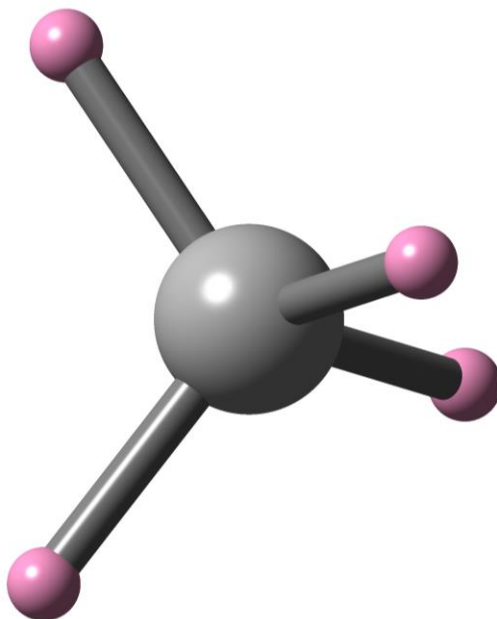
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Frequencies --	50.8576	54.4365	56.9947

Frequencies --	61.2759	68.5757	82.6612
Frequencies --	91.4189	99.1993	103.0578
Frequencies --	103.7286	110.5020	119.4030
Frequencies --	121.2104	128.3128	135.5473
Frequencies --	138.2971	143.1620	144.5303
Frequencies --	151.6122	156.8648	163.4780
Frequencies --	165.6302	185.5898	199.1606
Frequencies --	201.9781	206.8973	218.9718
Frequencies --	221.1878	230.1751	233.2761
Frequencies --	240.2445	248.9630	250.0575
Frequencies --	263.9222	265.3856	267.0391
Frequencies --	270.1456	271.9034	272.7811
Frequencies --	275.9955	277.3304	290.3549
Frequencies --	300.0535	301.8620	305.3723
Frequencies --	309.1342	317.5668	320.2825
Frequencies --	323.3290	330.6407	333.1756
Frequencies --	349.8462	357.3480	373.2747
Frequencies --	376.0667	380.2211	403.0210
Frequencies --	408.8579	423.7234	426.1767
Frequencies --	431.8881	433.7356	442.6045
Frequencies --	451.3631	454.9533	486.1253
Frequencies --	494.5851	502.6483	514.9423
Frequencies --	541.1153	544.5309	548.1301
Frequencies --	551.4543	552.0089	563.7912
Frequencies --	566.0422	571.7843	575.9299
Frequencies --	595.1293	629.3055	630.6308
Frequencies --	638.3829	642.1749	643.8873
Frequencies --	648.6617	676.7275	689.1466
Frequencies --	694.9928	716.2157	717.8827
Frequencies --	722.1373	734.9431	739.2499
Frequencies --	744.9671	751.9618	783.4732
Frequencies --	787.6778	803.0889	811.7128
Frequencies --	824.3601	834.0789	841.0864
Frequencies --	843.5560	880.1145	895.7750
Frequencies --	899.1540	908.4093	909.4168
Frequencies --	909.7636	918.3695	919.2514
Frequencies --	923.8126	989.7319	991.0109
Frequencies --	995.0905	996.8492	1007.2037
Frequencies --	1031.0610	1040.8527	1043.2285
Frequencies --	1044.7171	1051.3411	1056.0917
Frequencies --	1057.2296	1059.9093	1062.5957
Frequencies --	1084.0080	1095.3123	1095.7386
Frequencies --	1110.9477	1133.2198	1177.1757
Frequencies --	1181.2283	1190.8319	1194.7378
Frequencies --	1214.8600	1223.0989	1252.4567
Frequencies --	1279.3252	1279.6220	1290.5045
Frequencies --	1311.8040	1327.1001	1333.6768
Frequencies --	1340.9365	1355.8805	1356.6005
Frequencies --	1372.2243	1379.6796	1395.9025
Frequencies --	1402.5087	1415.1138	1420.1921
Frequencies --	1420.9726	1424.1185	1428.8885
Frequencies --	1435.2827	1446.9389	1449.8040
Frequencies --	1453.4279	1455.7050	1470.8297
Frequencies --	1473.3164	1473.6124	1490.8227
Frequencies --	1491.8109	1496.7959	1502.6706
Frequencies --	1506.2660	1509.8430	1571.5924
Frequencies --	1583.9691	1595.6048	1597.1281
Frequencies --	1601.7756	1605.4989	1619.2343
Frequencies --	1623.1526	3012.3741	3030.2138
Frequencies --	3033.1205	3043.9303	3116.8904
Frequencies --	3120.7112	3132.5396	3139.6138
Frequencies --	3145.2006	3154.2554	3160.2505
Frequencies --	3166.5329	3177.5838	3197.6039

Frequencies --	3209.1581	3250.6247	3257.3182
Frequencies --	3273.6920	3277.2025	3293.9997

6. Product for Transfer of H from Counterion to Cation
[\(return to table of contents\)](#)

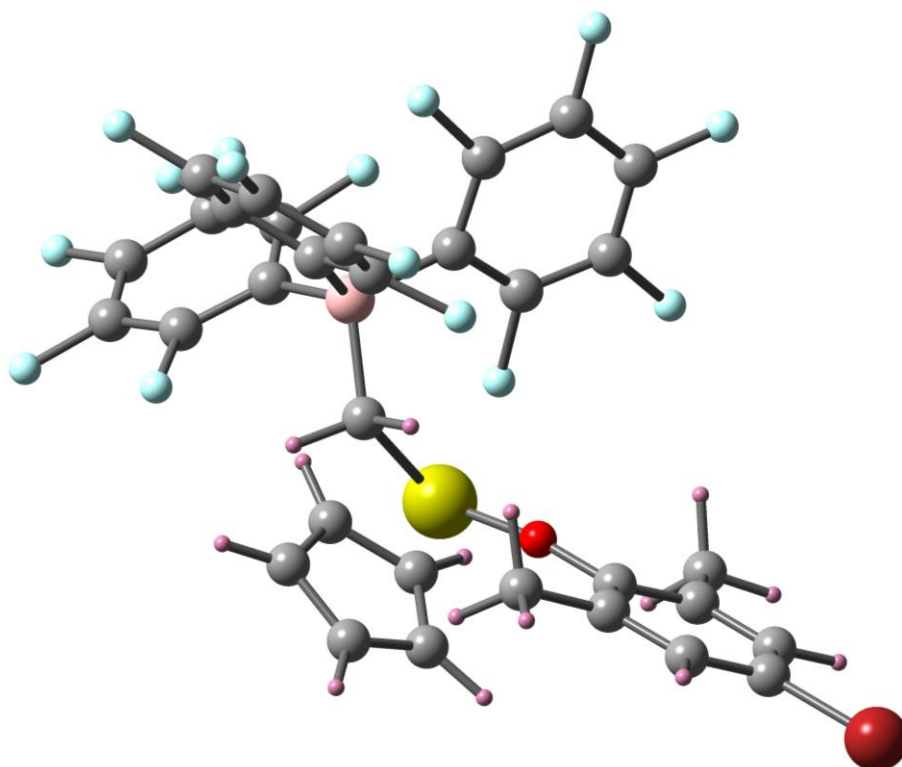
Methane



vacuum	toluene-like solvent	D3 dispersion
-40.4927543	-40.4928808	-0.00899984

C	0.00000000	0.00000000	0.00000000
H	0.63476900	0.63476900	0.63476900
H	-0.63476900	-0.63476900	0.63476900
H	-0.63476900	0.63476900	-0.63476900
H	0.63476900	-0.63476900	-0.63476900

Frequencies --	1351.0512	1351.0512	1351.0512
Frequencies --	1553.8481	1553.8481	2993.0697
Frequencies --	3152.6002	3152.6002	3152.6002

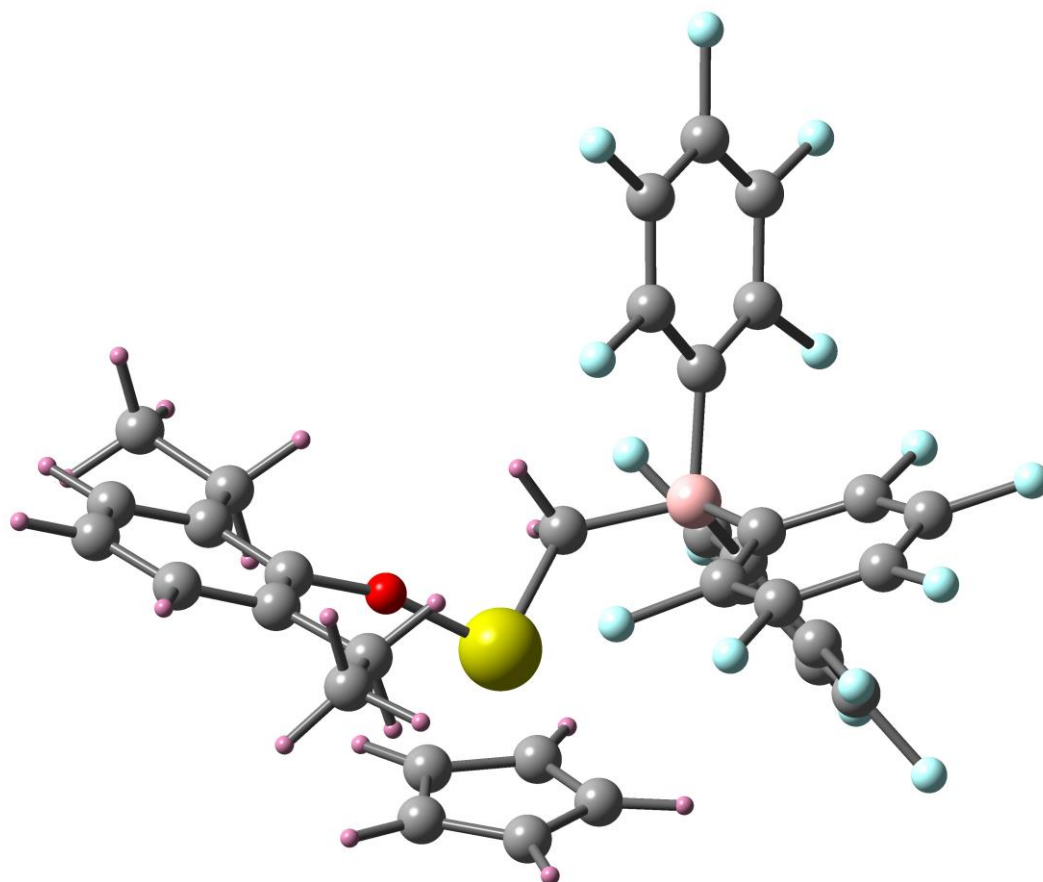
Catalyst 1:

vacuum	toluene-like solvent	D3 dispersion	
-2896.5919646	-2896.6038821	-0.47667860	
Ti	-0.79608400	-1.65907100	-0.82316100
O	-2.39227700	-0.87813700	-0.64761500
C	-3.73723300	-0.52987800	-0.59756000
C	-4.18493500	0.56050800	-1.40126300
C	-4.61452100	-1.25195500	0.26505800
C	-5.55362100	0.90876200	-1.34119200
C	-5.97420700	-0.86651800	0.30035800
C	-6.43030200	0.19867100	-0.49914500
H	-5.92083200	1.73591400	-1.94737400
H	-6.66362000	-1.39884600	0.95460400
H	-1.39440400	-2.36724200	-3.73682800
C	-0.94579200	-2.84599300	-2.86992500
C	0.45666500	-2.84938900	-2.53710900
C	-1.64370200	-3.63111900	-1.88726300
H	1.24586000	-2.37497100	-3.10650600
C	0.61491700	-3.60565800	-1.33270400
H	-2.71273400	-3.81961100	-1.86857900
C	-0.68168300	-4.08107100	-0.92500100
H	1.54681900	-3.78441500	-0.80579100
H	-0.88822900	-4.68659700	-0.04582000
F	-0.49856100	0.37636400	5.51130100
C	0.03005800	0.34931300	4.23281300
C	0.96940000	1.31112300	3.81760100
C	-0.35411500	-0.64854600	3.32261100

C	1.49330300	1.27216900	2.50899400
F	1.38018700	2.28754100	4.71056600
C	0.20618900	-0.60443400	2.03856600
F	-1.25982100	-1.63717800	3.68891300
C	1.12179300	0.31770300	1.52653100
F	2.46880400	2.22812600	2.23336600
F	-0.19320300	-1.74153600	1.20525200
B	1.71623000	0.27710800	-0.04295500
C	2.13066500	1.83591000	-0.49484400
C	2.98139600	-0.80352300	-0.18397200
C	0.48002800	-0.13660200	-1.16151300
C	3.42332700	2.28550200	-0.85606400
C	1.15654100	2.86276300	-0.55977600
C	3.61632200	-1.47697000	0.88660500
C	3.53962600	-1.14404800	-1.44198100
H	-0.28332300	0.65804700	-1.13141000
H	0.94986300	-0.12552400	-2.15114900
C	3.71760700	3.59210800	-1.29775000
F	4.53515000	1.44201100	-0.75114100
C	1.39648900	4.18046800	-0.98627000
F	-0.16517500	2.60778100	-0.13477900
C	4.67334600	-2.40152000	0.74292400
F	3.22874400	-1.25058900	2.21638400
C	4.59011400	-2.05637200	-1.64329300
F	3.07035200	-0.52418500	-2.61396700
C	2.69511200	4.55078100	-1.37311800
F	5.01607800	3.94430500	-1.64467300
F	0.36807000	5.11682800	-1.01964900
C	5.16806800	-2.69942600	-0.53560100
F	5.22794000	-3.01782000	1.85812600
F	5.06349000	-2.32387900	-2.92297200
F	2.96245300	5.84046400	-1.80647700
F	6.20285800	-3.60610400	-0.70368100
C	-3.23432700	1.34385800	-2.28842700
H	-2.49536400	1.89535500	-1.68743700
H	-2.67445100	0.68369100	-2.96886600
H	-3.78011300	2.07361700	-2.90109600
C	-4.12405800	-2.38577300	1.14916100
H	-3.64730300	-3.18543700	0.56228300
H	-3.38570000	-2.03358900	1.88547400
H	-4.95711100	-2.83469600	1.70589600
Br	-8.32655900	0.70626200	-0.43302900

Frequencies --	7.7738	12.3405	19.2616
Frequencies --	25.2082	29.5039	30.6825
Frequencies --	34.6492	40.9696	41.5569
Frequencies --	48.5821	50.0762	59.5035
Frequencies --	72.4172	78.2582	88.3009
Frequencies --	100.9422	103.6037	107.5229
Frequencies --	113.0716	117.8298	121.0805
Frequencies --	126.9215	129.4949	137.2030
Frequencies --	145.3475	151.1001	151.8939
Frequencies --	155.4428	157.5049	160.2512
Frequencies --	163.1334	182.0957	191.8216
Frequencies --	199.6670	218.3881	220.7322
Frequencies --	222.0055	223.5102	227.1348
Frequencies --	246.5418	249.1103	262.7270
Frequencies --	264.5474	264.9231	265.4436

Frequencies --	273.5987	276.9259	282.0399
Frequencies --	292.1794	302.5995	306.0665
Frequencies --	316.9656	320.6332	332.1676
Frequencies --	334.1771	337.7123	346.9113
Frequencies --	356.0488	376.3524	378.3761
Frequencies --	379.9021	380.4416	384.0132
Frequencies --	391.9525	408.9374	431.6307
Frequencies --	432.0781	433.8444	443.1424
Frequencies --	453.1756	457.1368	466.7334
Frequencies --	500.8577	509.7932	532.0073
Frequencies --	538.0855	545.3976	551.1308
Frequencies --	561.8100	564.3761	568.0041
Frequencies --	570.1604	576.7889	580.4869
Frequencies --	590.0465	619.9733	626.4255
Frequencies --	635.2783	639.7933	642.4862
Frequencies --	657.5206	675.1430	694.1999
Frequencies --	721.6213	730.6497	731.7318
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Frequencies --	862.9030	863.5304	879.2224
Frequencies --	885.6516	889.9835	890.6453
Frequencies --	907.8643	910.8606	929.3773
Frequencies --	949.1318	978.1927	1009.5503
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Frequencies --	1031.4738	1032.8200	1047.4048
Frequencies --	1047.9282	1051.1067	1055.6235
Frequencies --	1056.8900	1057.9202	1074.6334
Frequencies --	1090.0634	1096.0615	1122.8635
Frequencies --	1126.5795	1204.5145	1211.6053
Frequencies --	1212.5854	1215.6974	1265.3071
Frequencies --	1286.2655	1287.0250	1299.2449
Frequencies --	1315.4936	1320.0660	1336.4755
Frequencies --	1340.3565	1343.6288	1354.5610
Frequencies --	1383.7560	1391.2272	1395.4736
Frequencies --	1413.1241	1414.3305	1414.7349
Frequencies --	1419.8724	1424.0536	1427.6729
Frequencies --	1429.1181	1441.7345	1450.9800
Frequencies --	1468.6234	1470.3846	1474.6176
Frequencies --	1486.1718	1492.0985	1501.3535
Frequencies --	1504.2465	1586.3655	1586.6101
Frequencies --	1590.4236	1593.6437	1595.0762
Frequencies --	1618.0570	1619.7589	1633.0658
Frequencies --	3020.5297	3026.4061	3046.4250
Frequencies --	3107.9927	3112.0102	3137.9680
Frequencies --	3139.4037	3153.8662	3201.0258
Frequencies --	3203.6047	3233.8406	3238.6086
Frequencies --	3261.4518	3268.4152	3296.3710

Catalyst 2:

vacuum	toluene-like solvent	D3 dispersion
-2962.6086205	-2962.6202086	-0.50224128

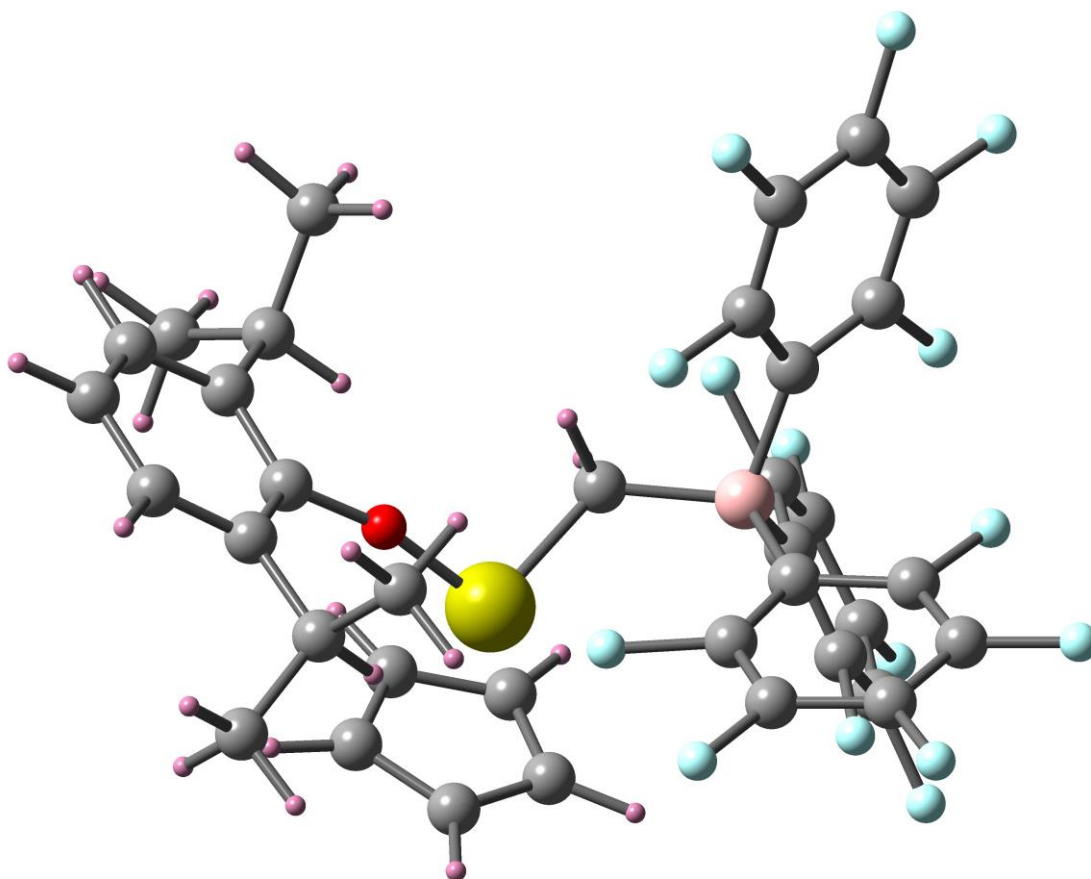
Ti	-1.77470800	-1.31174500	-0.08040700
O	-3.24917600	-0.40921100	-0.49835800
C	-4.55452400	0.00587200	-0.76127200
C	-4.89224600	0.35642300	-2.10291000
C	-5.47232600	0.09058000	0.32923900
C	-6.22055800	0.77883400	-2.33807900
C	-6.78393100	0.52434500	0.03051200
C	-7.15692800	0.85815600	-1.28728100
H	-6.52706300	1.05632200	-3.34523000
H	-7.51860800	0.60997500	0.82933400
H	-8.17630700	1.19021900	-1.49402500
H	-2.32516100	-3.20244500	-2.41328000
C	-1.99241800	-3.27658800	-1.38132000
C	-0.62359800	-3.27196300	-0.93045900
C	-2.84269400	-3.45171400	-0.23393300
H	0.25113200	-3.19159200	-1.56275900
C	-0.63260700	-3.41116500	0.49437700
H	-3.92781600	-3.49671200	-0.24622100
C	-2.00206800	-3.51539200	0.92464300
H	0.23830200	-3.42571000	1.14149100

H	-2.33667400	-3.63192300	1.95262000
F	0.98450300	0.83488100	5.81628600
C	1.01737000	0.63820900	4.44657000
C	2.18807600	0.89892200	3.70750500
C	-0.11641700	0.17101800	3.76485900
C	2.19865800	0.69446900	2.31562000
F	3.32192300	1.34831200	4.36569400
C	-0.01566300	-0.00484700	2.37451400
F	-1.29435300	-0.10612600	4.44722600
C	1.08992700	0.22896900	1.55800800
F	3.40654500	0.95097600	1.67127600
F	-1.26195600	-0.49853300	1.79279400
B	1.17454700	0.10852400	-0.12028000
C	1.57043700	1.68269000	-0.57032900
C	2.26988900	-1.04336500	-0.61446800
C	-0.27589600	-0.25181500	-0.92319200
C	2.79188500	2.13045500	-1.13046200
C	0.64543700	2.73515600	-0.35727900
C	2.86713900	-2.03223600	0.19838000
C	2.63245900	-1.16908100	-1.97990100
H	-0.89166900	0.65913100	-1.04154300
H	-0.01203400	-0.59368100	-1.93358300
C	3.05093500	3.46524700	-1.50562200
F	3.86308000	1.25389900	-1.31662900
C	0.85547800	4.08117400	-0.70782900
F	-0.58440800	2.47108600	0.28140600
C	3.77234800	-3.01276300	-0.25893500
F	2.55036600	-2.12665200	1.56740300
C	3.52907500	-2.12405900	-2.49121800
F	2.08488900	-0.29230000	-2.92921600
C	2.07245800	4.45169600	-1.30330900
F	4.27425800	3.81782400	-2.06234700
F	-0.12093600	5.04221600	-0.46520200
C	4.11734900	-3.05594800	-1.61832500
F	4.31054100	-3.94468300	0.62178500
F	3.83775700	-2.15733800	-3.84582400
F	2.30815400	5.76908700	-1.66732200
F	5.00340100	-4.01022700	-2.09488200
C	-3.83604700	0.27479100	-3.20697900
H	-2.96382700	0.87432200	-2.89643100
H	-3.47014400	-0.76533900	-3.27076400
C	-5.01005900	-0.24851700	1.74822900
H	-4.62792300	-1.28485900	1.76100400
H	-4.14470600	0.39190200	1.99291500
C	-6.05618800	-0.10544200	2.87460500
H	-6.42608900	0.92782200	2.96063400
H	-6.92163600	-0.76931700	2.72238800
H	-5.59658100	-0.37241800	3.83893800
C	-4.26972200	0.72723100	-4.61785400
H	-5.09082800	0.11097000	-5.01658400
H	-4.59280400	1.77963200	-4.62887500
H	-3.41936900	0.63530600	-5.31143200

Frequencies --	10.2976	13.7503	17.2337
Frequencies --	24.7358	28.4726	31.9317
Frequencies --	34.0389	39.7159	42.3914
Frequencies --	43.6433	46.4888	52.9447

Frequencies --	61.5498	63.8336	74.9832
Frequencies --	85.8954	95.1079	107.9576
Frequencies --	111.1859	114.9357	121.3548
Frequencies --	124.7939	134.5166	138.0113
Frequencies --	142.9348	147.8675	155.5103
Frequencies --	157.5625	162.6333	165.5283
Frequencies --	171.9444	177.3111	187.7328
Frequencies --	202.9050	214.1706	216.7168
Frequencies --	220.2997	223.7709	243.3415
Frequencies --	257.2522	263.8583	264.2953
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Frequencies --	275.8026	278.2293	283.8497
Frequencies --	292.0987	301.7651	305.7495
Frequencies --	306.2036	313.4239	321.8374
Frequencies --	325.3925	331.4740	335.3884
Frequencies --	338.9866	346.4028	360.6723
Frequencies --	367.3784	373.5639	376.4986
Frequencies --	378.1627	380.2520	394.9035
Frequencies --	428.0609	431.1343	432.0221
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Frequencies --	469.1001	505.8436	523.6116
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Frequencies --	547.8919	550.2973	562.2955
Frequencies --	567.9246	576.8581	577.5756
Frequencies --	587.1785	603.6273	613.8303
Frequencies --	624.9929	635.3222	637.1665
Frequencies --	642.4869	652.3567	676.1084
Frequencies --	704.6118	711.3135	716.8831
Frequencies --	729.0540	730.6858	738.5825
Frequencies --	745.3142	749.4571	766.1152
Frequencies --	773.0526	789.2374	793.1618
Frequencies --	793.9533	806.6383	823.3701
Frequencies --	829.3582	838.7599	840.1390
Frequencies --	841.5930	852.3881	867.6367
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Frequencies --	907.2010	912.7694	924.2074
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Frequencies --	996.5149	1007.2089	1023.7873
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Frequencies --	1034.5311	1045.6254	1049.5609
Frequencies --	1056.9945	1058.1429	1079.4892
Frequencies --	1089.4163	1094.2306	1096.2167
Frequencies --	1097.3192	1100.3023	1120.7854
Frequencies --	1126.1262	1195.7511	1202.9437
Frequencies --	1204.4564	1210.9332	1215.8252
Frequencies --	1262.9979	1277.0806	1287.2416
Frequencies --	1287.9001	1292.7245	1295.6769
Frequencies --	1314.8395	1319.9078	1328.2142
Frequencies --	1337.6555	1343.2034	1344.4154
Frequencies --	1348.5430	1382.1326	1390.7252
Frequencies --	1393.8787	1398.9015	1412.5843
Frequencies --	1414.9780	1417.4851	1417.6727
Frequencies --	1421.5012	1434.8074	1441.8017
Frequencies --	1451.7095	1466.7693	1466.8823
Frequencies --	1469.1720	1472.2557	1478.8167
Frequencies --	1492.9788	1499.8711	1503.0789
Frequencies --	1504.7459	1505.8420	1589.6530
Frequencies --	1593.0671	1595.5479	1599.7980
Frequencies --	1606.9249	1616.4526	1619.6546
Frequencies --	1630.8620	3002.5696	3007.3389
Frequencies --	3011.9543	3014.3889	3015.0458
Frequencies --	3049.4875	3058.2356	3115.7530
Frequencies --	3116.1611	3117.3019	3120.8520

Frequencies --	3121.2269	3171.0678	3204.4418
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Catalyst 3:

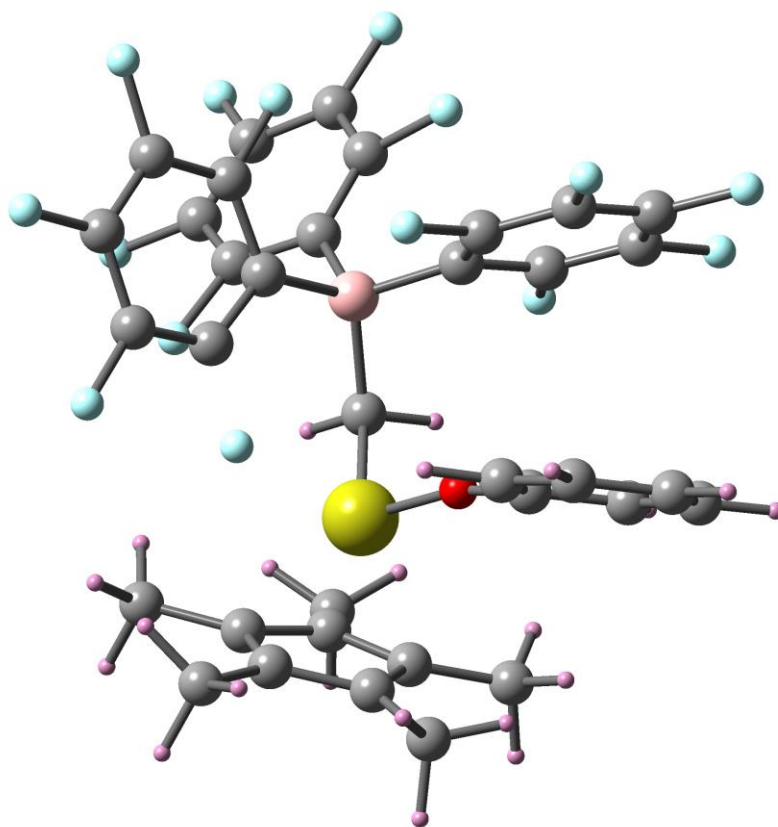
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C	-4.70005800	1.47839400	-1.44665000
C	-5.29501600	-0.19847100	0.32794400
C	-6.01451100	1.99284200	-1.35068200
C	-6.58956900	0.36794600	0.37880700
C	-6.94987900	1.44786400	-0.45098400
H	-6.30657800	2.83253700	-1.98213300
H	-7.32390200	-0.03534700	1.07601700
H	-7.95674200	1.86601400	-0.39226200
H	-2.09626200	-1.19928400	-3.85117200
C	-1.77774400	-1.88168800	-3.06740000
C	-0.41561700	-2.15590200	-2.68542700
C	-2.64336600	-2.70261500	-2.26312900
H	0.46852700	-1.71705100	-3.12948600
C	-0.44390000	-3.11898000	-1.62607200
H	-3.72809300	-2.72500000	-2.31312000
C	-1.81906600	-3.45165900	-1.36163500
H	0.41894400	-3.52478800	-1.10742200

H	-2.16953600	-4.15565900	-0.61071600
F	1.20225800	-2.80714300	5.17377400
C	1.22023200	-2.15163400	3.95474800
C	2.37487100	-1.47373000	3.51652700
C	0.08737000	-2.15095200	3.12714300
C	2.37029000	-0.81064800	2.27578400
F	3.50811900	-1.47499500	4.31434400
C	0.17254000	-1.46395500	1.90456300
F	-1.07540700	-2.80788900	3.51026800
C	1.26123400	-0.76287200	1.38799000
F	3.56308900	-0.18977100	1.91240000
F	-1.06947300	-1.54544200	1.14090300
B	1.32946100	0.14035700	-0.03333500
C	1.66808700	1.68313100	0.55037600
C	2.45608000	-0.46254600	-1.09976300
C	-0.11176400	0.29070500	-0.92204900
C	2.86908200	2.41699600	0.39091100
C	0.70701900	2.36757700	1.33557600
C	3.07176300	-1.73230300	-1.03262600
C	2.82826400	0.26248900	-2.26063500
H	-0.73996100	1.10107100	-0.50862100
H	0.17273800	0.59285700	-1.93867100
C	3.07655900	3.71838900	0.89402200
F	3.97043800	1.86221900	-0.26398200
C	0.86462700	3.66177300	1.86342700
F	-0.50820400	1.73275900	1.66904800
C	4.00664100	-2.22488800	-1.96697100
F	2.74423800	-2.63794600	-0.00489000
C	3.75467000	-0.17743600	-3.22273900
F	2.25724800	1.52028000	-2.50842700
C	2.06355400	4.35484700	1.62916100
F	4.28323900	4.37370000	0.68131300
F	-0.14567300	4.25335400	2.61531900
C	4.36328000	-1.43565100	-3.07096500
F	4.56299300	-3.48994300	-1.81173900
F	4.07243400	0.61490300	-4.31935400
F	2.24863300	5.63492700	2.12997100
F	5.28003600	-1.89514800	-4.00433200
C	-3.68421000	2.10560400	-2.41366700
H	-2.76121300	1.51223400	-2.36931700
C	-4.89097800	-1.33404700	1.28150800
H	-3.98066700	-1.80614700	0.88295500
C	-5.95643700	-2.46001300	1.38865500
H	-6.88114700	-2.11378600	1.87399700
H	-6.22340300	-2.85764300	0.39654900
H	-5.56096300	-3.28983800	1.99577400
C	-4.52888500	-0.76713400	2.68808800
H	-5.40679700	-0.30667100	3.16694200
H	-4.16329500	-1.57281400	3.34448700
H	-3.74262500	-0.00015700	2.61906500
C	-4.17610900	2.07100300	-3.88977100
H	-4.42642900	1.04502800	-4.20452800
H	-5.07044500	2.69423700	-4.04107800
H	-3.38891500	2.45344100	-4.55928900
C	-3.30656100	3.55236400	-1.97773400
H	-2.52452500	3.95697400	-2.64005200
H	-4.17231000	4.23069300	-2.02458900

H	-2.92180000	3.56825100	-0.94632800
Frequencies --	8.9473	12.4309	15.6490
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Frequencies --	32.2248	33.6327	38.6564
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Frequencies --	224.1173	233.0161	245.4255
Frequencies --	247.7834	255.1660	263.9999
Frequencies --	264.4186	264.7494	268.5755
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Frequencies --	302.1654	306.6092	310.7813
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Frequencies --	604.8032	616.0951	625.3937
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Frequencies --	963.5788	968.2691	979.4873
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Frequencies --	1332.7021	1337.6251	1338.2164
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Frequencies --	1450.9367	1467.2374	1469.0758
Frequencies --	1472.2531	1473.9346	1484.8814
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Catalyst 4:

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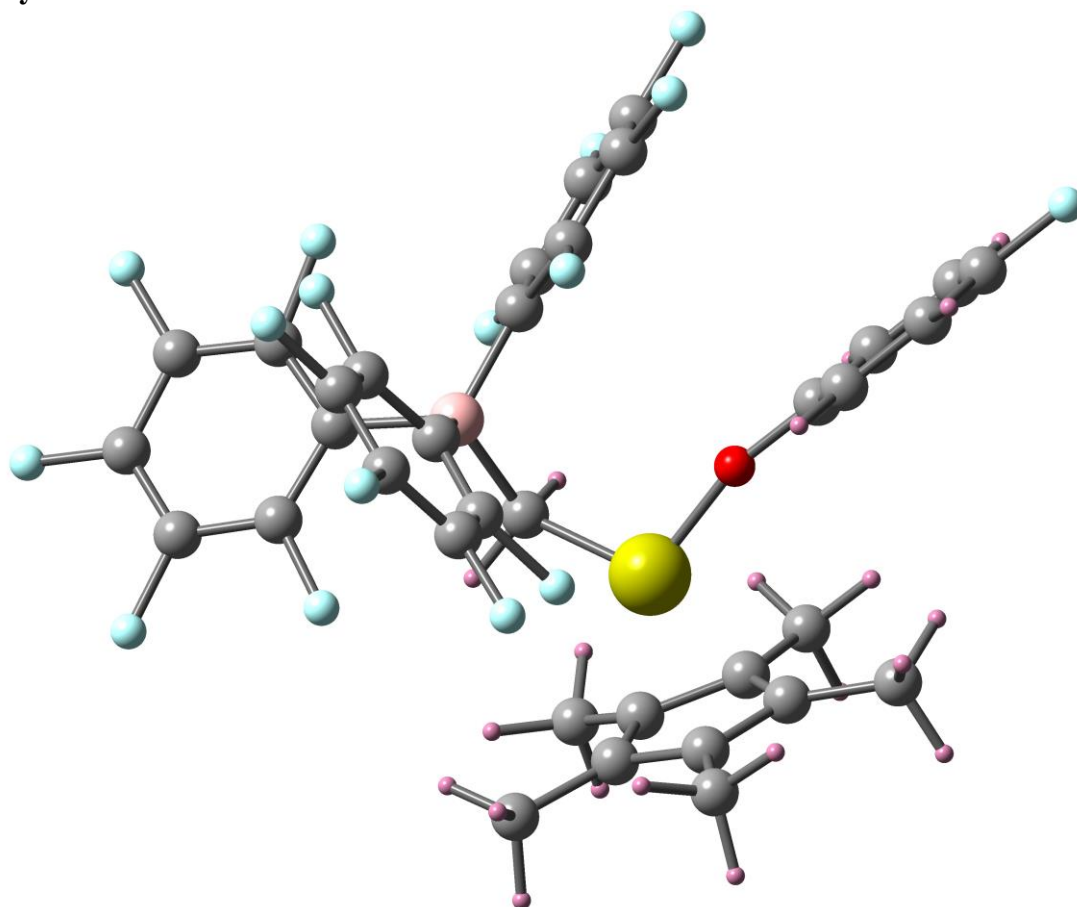
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C	4.13831500	0.84792700	1.54300700
C	4.13206400	1.83953800	-0.70827500
C	5.15459100	1.74526800	1.92826200
C	5.15042400	2.72986700	-0.31070300
C	5.66656600	2.68463400	1.00432400
H	5.53749100	1.71612400	2.95050000
H	5.53041300	3.46388100	-1.02441300
H	6.44893100	3.38169000	1.30937100
C	1.46193700	-2.88382500	-2.55261200
C	2.74416500	-2.19523300	-2.55796100
C	1.42111400	-3.72044700	-1.38308300
C	3.51512500	-2.66080900	-1.42217000
C	2.68363900	-3.57372700	-0.67615500
F	-1.67660000	-2.16367300	5.32166300
C	-1.50178000	-1.59874700	4.06930800
C	-2.30344800	-0.52167900	3.64379500
C	-0.51483100	-2.08413100	3.19858200
C	-2.11039100	0.03461500	2.36571900

F	-3.26984500	-0.01420500	4.49886300
C	-0.39235800	-1.47119200	1.94083300
F	0.31114400	-3.13828500	3.57465800
C	-1.14439300	-0.41539000	1.42655200
F	-2.91646600	1.12726100	2.05290500
F	0.68968000	-2.05423400	1.15143100
B	-1.02680800	0.25668400	-0.11261600
C	-2.61148100	0.22508400	-0.68299500
C	-0.34654600	1.77527500	-0.07430800
C	-0.14623700	-0.66372100	-1.23607200
C	-3.43278000	1.34051200	-0.97767600
C	-3.26848100	-1.01034300	-0.90306900
C	0.24751700	2.39705700	1.04643800
C	-0.23921400	2.55991600	-1.25032300
H	-0.75176100	-1.49788900	-1.60700500
H	0.07424900	-0.01210100	-2.10036400
C	-4.73858500	1.25002400	-1.50273200
F	-2.99907700	2.64244100	-0.71560300
C	-4.56963400	-1.15710800	-1.41710200
F	-2.62350700	-2.22200500	-0.56868700
C	0.84888400	3.67236500	1.03484500
F	0.30679000	1.74194100	2.28950900
C	0.35301700	3.83262400	-1.32066800
F	-0.76824200	2.08189200	-2.46168700
C	-5.31369900	-0.00950600	-1.73552200
F	-5.47177300	2.39885800	-1.77676300
F	-5.12311300	-2.42075000	-1.60763100
C	0.90116000	4.40383400	-0.16017200
F	1.41424200	4.19831400	2.19181000
F	0.40634300	4.52888100	-2.52487400
F	-6.59622600	-0.11936300	-2.25385900
F	1.50345600	5.65394500	-0.20261200
C	4.95882300	-2.32500200	-1.12781400
H	5.17940400	-2.30897600	-0.05167400
H	5.61609100	-3.08635600	-1.58290600
H	5.25488200	-1.35209300	-1.53949300
C	3.24456200	-1.29741500	-3.66794900
H	4.01012700	-0.59027600	-3.32245600
H	3.70169000	-1.90657500	-4.46718200
H	2.43450200	-0.71661100	-4.13098500
C	0.44781600	-2.85848800	-3.67055600
H	0.30953600	-1.85462100	-4.09461400
H	0.78279000	-3.51741000	-4.49030300
H	-0.53547100	-3.22049800	-3.34488600
C	0.29606200	-4.65220600	-0.99405500
H	-0.69262400	-4.24295700	-1.24023300
H	0.39719000	-5.60963000	-1.53442100
H	0.30270500	-4.88570300	0.07868100
C	3.08912100	-4.33215100	0.56888500
H	2.26106500	-4.44915700	1.28150200
H	3.42689800	-5.34719800	0.29724400
H	3.91982600	-3.84657500	1.09893900
H	3.72422600	0.13372100	2.25587200
H	3.71456300	1.88075400	-1.71486100

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Frequencies --	25.6165	27.6431	31.2417

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Frequencies --	296.1526	302.6554	303.7070
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Frequencies --	374.6643	376.9123	379.4420
Frequencies --	379.5776	388.3597	397.6212
Frequencies --	408.0345	408.8823	419.2257
Frequencies --	431.2751	432.0371	438.3245
Frequencies --	445.1237	452.2028	458.5763
Frequencies --	467.6581	491.4438	515.2649
Frequencies --	534.4618	536.9311	539.3686
Frequencies --	542.0374	547.3525	556.6277
Frequencies --	567.3118	580.1965	588.8084
Frequencies --	600.5986	603.9356	609.8573
Frequencies --	614.4752	623.9361	634.2271
Frequencies --	636.3586	641.2173	653.0022
Frequencies --	664.6532	675.4904	690.1783
Frequencies --	704.9219	717.2774	729.9347
Frequencies --	736.0496	746.6400	747.9078
Frequencies --	758.6426	766.3345	801.0997
Frequencies --	804.7797	823.0027	832.9041
Frequencies --	842.6119	865.8111	872.9784
Frequencies --	906.6142	910.3720	913.0878
Frequencies --	921.8268	968.4663	970.8764
Frequencies --	972.3730	972.5711	996.2889
Frequencies --	1005.9617	1007.5763	1022.4314
Frequencies --	1029.4305	1030.9584	1040.9025
Frequencies --	1043.0590	1044.1622	1045.2978
Frequencies --	1047.5605	1048.8736	1049.5952
Frequencies --	1054.6201	1086.7278	1089.2629
Frequencies --	1089.8298	1099.2182	1125.7258
Frequencies --	1173.4467	1174.7428	1183.5501
Frequencies --	1189.3622	1202.5392	1209.0641
Frequencies --	1212.7410	1241.9773	1295.3789
Frequencies --	1313.9540	1319.7984	1323.3996
Frequencies --	1337.7775	1344.0079	1348.2507
Frequencies --	1375.3160	1386.7768	1410.5875
Frequencies --	1412.9047	1414.7742	1416.6790
Frequencies --	1420.8211	1424.5906	1426.0037
Frequencies --	1427.6881	1429.7997	1434.3051
Frequencies --	1448.4720	1451.9037	1455.4282
Frequencies --	1462.7638	1466.4466	1469.9981
Frequencies --	1471.8763	1480.4440	1484.0865
Frequencies --	1490.1392	1491.4036	1496.0892
Frequencies --	1497.9494	1504.5695	1506.1392
Frequencies --	1509.4968	1513.5718	1519.5672
Frequencies --	1590.9596	1593.6011	1597.3366
Frequencies --	1598.7746	1609.6216	1616.6871

Frequencies --	1621.7346	1630.4946	3009.0493
Frequencies --	3010.5643	3011.0935	3012.2054
Frequencies --	3013.5016	3028.1375	3098.0494
Frequencies --	3100.5787	3102.2409	3103.3737
Frequencies --	3104.6011	3135.2771	3137.1144
Frequencies --	3143.1241	3145.8797	3147.7403
Frequencies --	3148.8429	3166.9051	3174.1512
Frequencies --	3189.8647	3197.5742	3207.1118

Catalyst 5:

vacuum	toluene-like solvent	D3 dispersion
-3101.1486692	-3101.1606136	-0.52463612

Ti	1.28909500	-1.68140400	-0.64797100
O	2.45701200	-0.38815100	-0.23446300
C	3.58127800	0.35009000	0.09706100
C	4.09554200	0.28866600	1.41613400
C	4.19172900	1.17980500	-0.87540300
C	5.22905300	1.04844200	1.76244600
C	5.32704800	1.94052500	-0.53472900
C	5.82519700	1.85477100	0.77700500
H	5.63807200	1.02656200	2.77209400
H	5.81078700	2.59222400	-1.26175700
C	0.89751300	-3.17057200	-2.53177700
C	2.27299200	-2.69028600	-2.53253300
C	0.71438100	-3.96797900	-1.34863500
C	2.94811200	-3.24600600	-1.37689800
C	1.97522100	-4.00156300	-0.62547600
F	-1.63718600	-1.51867200	5.52293500
C	-1.48643500	-1.08905900	4.21523200
C	-2.13608600	0.07427000	3.75771900
C	-0.67730300	-1.80174100	3.31779400
C	-1.97170500	0.49077900	2.42397000

F	-2.92499700	0.80165300	4.63538900
C	-0.57005600	-1.31412600	2.00471900
F	-0.00660700	-2.95146500	3.72128900
C	-1.18003200	-0.18616500	1.45784000
F	-2.61849100	1.67306200	2.07179500
F	0.31758700	-2.13726600	1.18477300
B	-1.11243300	0.33972300	-0.14159800
C	-2.73851600	0.40365600	-0.57818300
C	-0.30400000	1.78592100	-0.28535900
C	-0.39178000	-0.72962300	-1.25119200
C	-3.50011500	1.56064200	-0.87353900
C	-3.50250100	-0.78674000	-0.65109700
C	0.46899200	2.41429800	0.71590300
C	-0.26172900	2.47819900	-1.52179600
H	-1.11801900	-1.47155500	-1.60020800
H	-0.08148500	-0.14091700	-2.13338800
C	-4.85466000	1.54103900	-1.26688100
F	-2.94726800	2.83679800	-0.74942500
C	-4.85452700	-0.86216900	-1.03124600
F	-2.91646400	-2.02151500	-0.29435800
C	1.17588200	3.62242700	0.54572900
F	0.61245800	1.83190700	1.98793400
C	0.42653000	3.68281900	-1.74814400
F	-0.95642300	1.96794100	-2.63114700
C	-5.54036000	0.31906300	-1.35757700
F	-5.52502400	2.72466500	-1.55195500
F	-5.51393800	-2.08762300	-1.08176400
C	1.15224500	4.27038300	-0.69792700
F	1.91595800	4.16259300	1.59232400
F	0.40001700	4.29558300	-2.99717600
F	-6.87196900	0.27928600	-1.74481100
F	1.84881700	5.45473600	-0.89487700
C	4.42079800	-3.13162800	-1.05839800
H	4.61822800	-3.09486200	0.02201900
H	4.95545600	-4.01208500	-1.45527800
H	4.88013000	-2.24300600	-1.50884000
C	2.91929600	-1.91086500	-3.65655300
H	3.81022100	-1.36090800	-3.32715500
H	3.24069600	-2.60180000	-4.45522800
H	2.22821000	-1.19015100	-4.11603200
C	-0.08584300	-3.00690900	-3.66575100
H	-0.02482500	-2.01677000	-4.13757900
H	0.12211400	-3.75688200	-4.44853100
H	-1.12357000	-3.15664200	-3.34186500
C	-0.53958500	-4.71486100	-0.95780300
H	-1.45187800	-4.21545800	-1.30614200
H	-0.52729600	-5.72530200	-1.40285000
H	-0.62606000	-4.84346000	0.12954600
C	2.24537500	-4.78693300	0.63895100
H	1.38581600	-4.79443500	1.32277800
H	2.46819500	-5.83835700	0.38768700
H	3.10976100	-4.39760200	1.19424100
H	3.60052500	-0.33151400	2.16347000
H	3.77154300	1.23709500	-1.87939700
F	6.95993400	2.60852400	1.11794600

Frequencies --

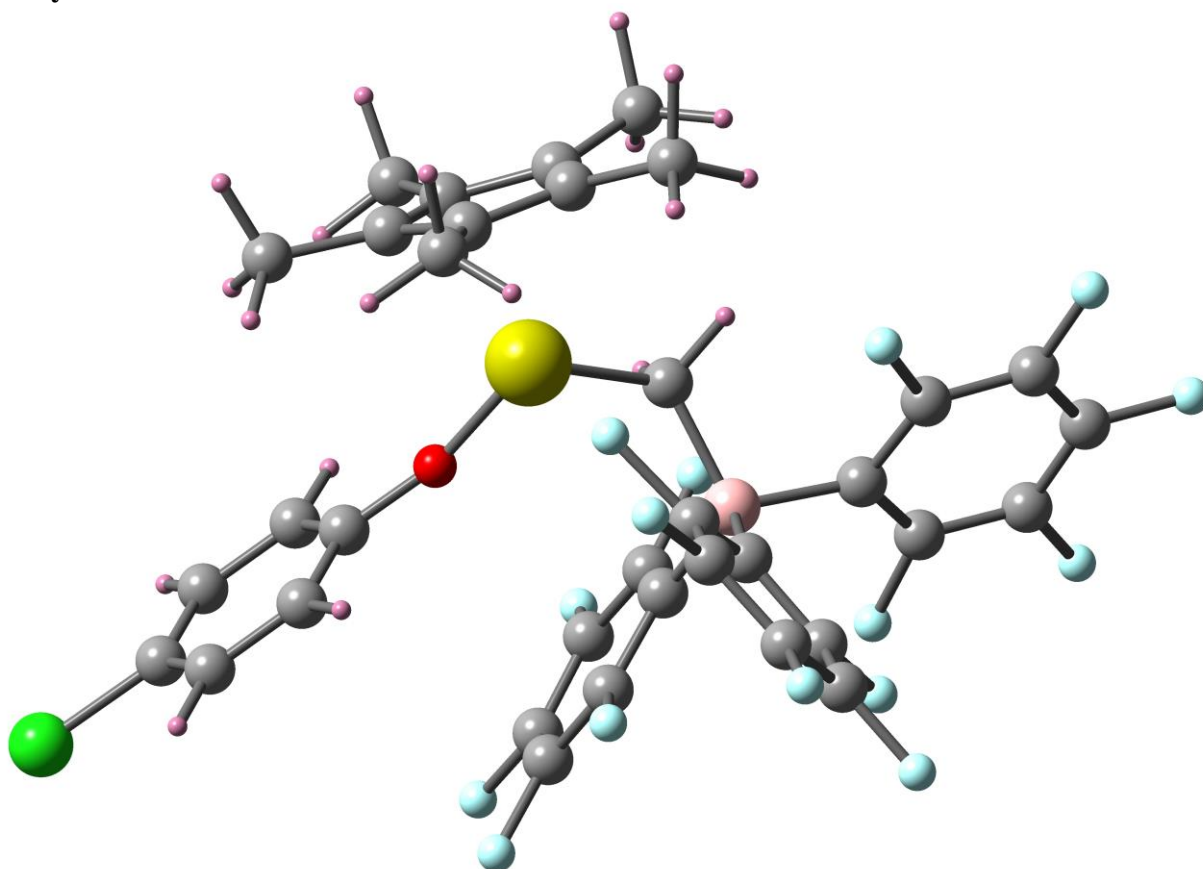
6.7060

13.2751

16.6856

Frequencies --	25.1773	25.7799	27.5020
Frequencies --	31.3395	32.1938	38.0130
Frequencies --	41.3852	48.5963	56.2601
Frequencies --	77.5032	79.3425	84.4099
Frequencies --	91.0920	94.4184	106.8732
Frequencies --	110.7804	111.6098	113.8894
Frequencies --	114.8911	118.5225	120.8219
Frequencies --	124.0017	128.8812	133.8114
Frequencies --	134.6201	138.4915	144.3067
Frequencies --	148.6228	156.9647	159.0709
Frequencies --	161.5201	166.1481	168.2470
Frequencies --	171.0382	191.9504	213.9870
Frequencies --	217.8146	219.5532	225.6653
Frequencies --	243.7829	255.8402	263.8569
Frequencies --	264.6113	264.8134	275.7345
Frequencies --	277.3506	278.6203	285.0862
Frequencies --	289.0979	297.0978	298.6203
Frequencies --	302.6877	304.5025	305.9553
Frequencies --	312.8248	324.6595	331.7702
Frequencies --	337.7783	353.7213	359.3397
Frequencies --	363.1423	373.7350	375.6442
Frequencies --	377.4300	379.9294	380.6381
Frequencies --	394.1889	399.0642	403.7300
Frequencies --	415.7280	417.6436	431.2612
Frequencies --	432.3651	443.0518	450.5736
Frequencies --	456.1220	458.7334	466.8984
Frequencies --	484.0805	513.9639	534.0229
Frequencies --	536.4336	539.2568	540.9781
Frequencies --	546.8875	554.5167	564.3079
Frequencies --	576.9797	580.8869	592.7101
Frequencies --	601.3314	603.4188	609.0207
Frequencies --	624.4954	633.0222	634.1064
Frequencies --	635.8878	641.7848	656.7429
Frequencies --	671.4695	702.4298	703.7524
Frequencies --	716.7941	729.5108	735.4130
Frequencies --	745.7917	746.8514	766.0831
Frequencies --	790.7587	799.1326	802.7188
Frequencies --	806.1500	822.1947	830.4840
Frequencies --	843.0854	863.4543	872.0679
Frequencies --	906.2305	911.2452	917.4994
Frequencies --	945.4605	958.3107	966.1726
Frequencies --	968.8163	972.0152	1004.2428
Frequencies --	1013.0054	1022.3070	1032.0845
Frequencies --	1039.8217	1043.5855	1044.1357
Frequencies --	1045.3866	1046.3574	1048.8666
Frequencies --	1049.8485	1056.1815	1085.4492
Frequencies --	1087.6586	1094.1175	1111.8540
Frequencies --	1124.4092	1168.5138	1173.3838
Frequencies --	1173.6633	1201.8561	1203.1570
Frequencies --	1209.4836	1213.8214	1254.8895
Frequencies --	1294.6720	1303.3776	1314.0964
Frequencies --	1321.5026	1338.1496	1344.5049
Frequencies --	1349.1527	1360.2781	1382.7565
Frequencies --	1409.2449	1412.1013	1413.3788
Frequencies --	1416.9190	1421.1805	1422.2156
Frequencies --	1423.4300	1427.0218	1427.0967
Frequencies --	1430.0011	1434.6697	1447.5876
Frequencies --	1451.5147	1462.0408	1466.4077
Frequencies --	1469.4784	1471.3343	1480.2242
Frequencies --	1488.0774	1490.0306	1495.3218
Frequencies --	1495.8637	1496.3587	1504.3971
Frequencies --	1505.5121	1508.9371	1512.1503
Frequencies --	1519.6033	1590.1040	1593.1900

Frequencies --	1597.0954	1600.8362	1616.7853
Frequencies --	1618.5062	1621.2304	1630.2789
Frequencies --	3010.1314	3010.7849	3011.7252
Frequencies --	3012.4993	3013.7305	3025.7729
Frequencies --	3099.1712	3099.9904	3101.8018
Frequencies --	3103.7066	3106.5557	3135.9238
Frequencies --	3138.5577	3140.6709	3143.7265
Frequencies --	3146.6075	3152.7792	3195.5686
Frequencies --	3198.1956	3215.6981	3219.3041

Catalyst 6:

vacuum	toluene-like solvent	D3 dispersion
-3016.2787222	-3016.290322	-0.53197437

Ti	-0.92507400	1.86345200	-0.64028300
O	-2.24586800	0.70172900	-0.29794800
C	-3.45962500	0.08270200	-0.05303000
C	-4.02675000	0.14001300	1.24352600
C	-4.11321800	-0.62443400	-1.09123800
C	-5.25624500	-0.49840100	1.49758600
C	-5.34461900	-1.26003000	-0.83742000
C	-5.90729200	-1.18778000	0.45363900
H	-5.69240600	-0.46738700	2.49574600
H	-5.84833700	-1.81311200	-1.62988100
C	-0.29111400	3.34385400	-2.46387500
C	-1.70859500	3.01951400	-2.53849900
C	-0.07625600	4.08444000	-1.24942400
C	-2.37192200	3.61806100	-1.39721600
C	-1.35862000	4.24326900	-0.58239300
F	2.16042200	1.50925000	5.48043900
C	1.92089300	1.06474900	4.19114700
C	2.46774700	-0.14945900	3.73222100
C	1.12016800	1.81234400	3.31479100
C	2.21487800	-0.58053400	2.41679300

F	3.24310200	-0.91297500	4.59110500
C	0.92159000	1.30806900	2.01901000
F	0.54523400	3.01166600	3.72181400
C	1.43069000	0.13180100	1.47040100
F	2.75511200	-1.81710500	2.07039700
F	0.04269800	2.16647700	1.22737400
B	1.23712100	-0.41812500	-0.10903000
C	2.81081200	-0.73927000	-0.61596300
C	0.21366100	-1.72784400	-0.18601000
C	0.65688500	0.74019700	-1.21185300
C	3.35948200	-2.00399200	-0.94023200
C	3.75203100	0.31192200	-0.73935400
C	-0.57356000	-2.23584100	0.87120400
C	-0.01183000	-2.41120400	-1.40765800
H	1.47004200	1.40054000	-1.53038200
H	0.30709800	0.19797600	-2.10922800
C	4.67534400	-2.20462700	-1.40659500
F	2.61769500	-3.17486400	-0.76764400
C	5.07614000	0.16673000	-1.19120700
F	3.39524600	1.62622100	-0.36362400
C	-1.46014300	-3.32696800	0.76244200
F	-0.54619500	-1.63836100	2.14440000
C	-0.88394200	-3.50075700	-1.57416300
F	0.67877600	-2.01754900	-2.56676500
C	5.54343100	-1.10963000	-1.54426000
F	5.12887200	-3.48171500	-1.71505300
F	5.92165900	1.26893700	-1.28740100
C	-1.61641800	-3.97325900	-0.47214900
F	-2.19958600	-3.74921100	1.86213000
F	-1.03294900	-4.11146300	-2.81576300
F	6.84117500	-1.28533800	-2.00251600
F	-2.49365900	-5.03961300	-0.61011500
C	-3.86223000	3.65664200	-1.15113200
H	-4.11614100	3.63513400	-0.08221500
H	-4.28248400	4.58933800	-1.56584700
H	-4.38786900	2.82227700	-1.63186800
C	-2.38469300	2.34192300	-3.71017000
H	-3.33474100	1.86917900	-3.42960000
H	-2.61114100	3.08516000	-4.49433100
H	-1.74825100	1.57351300	-4.17120100
C	0.72099000	3.10539700	-3.55821800
H	0.57331600	2.14328100	-4.06736000
H	0.63414800	3.89759100	-4.32203200
H	1.75206200	3.12879100	-3.18326300
C	1.23711300	4.66967000	-0.78418300
H	2.09320900	4.02599600	-1.02447400
H	1.41049900	5.64164700	-1.27828300
H	1.24967200	4.85243600	0.29829800
C	-1.59621700	5.02135400	0.69327100
H	-0.80459900	4.86317100	1.43855800
H	-1.62217800	6.10274500	0.47448900
H	-2.55445000	4.76418400	1.16450800
H	-3.50481400	0.66107400	2.04639200
H	-3.65754500	-0.68705000	-2.07937000
Cl	-7.50717300	-1.99803500	0.77756300

Frequencies --

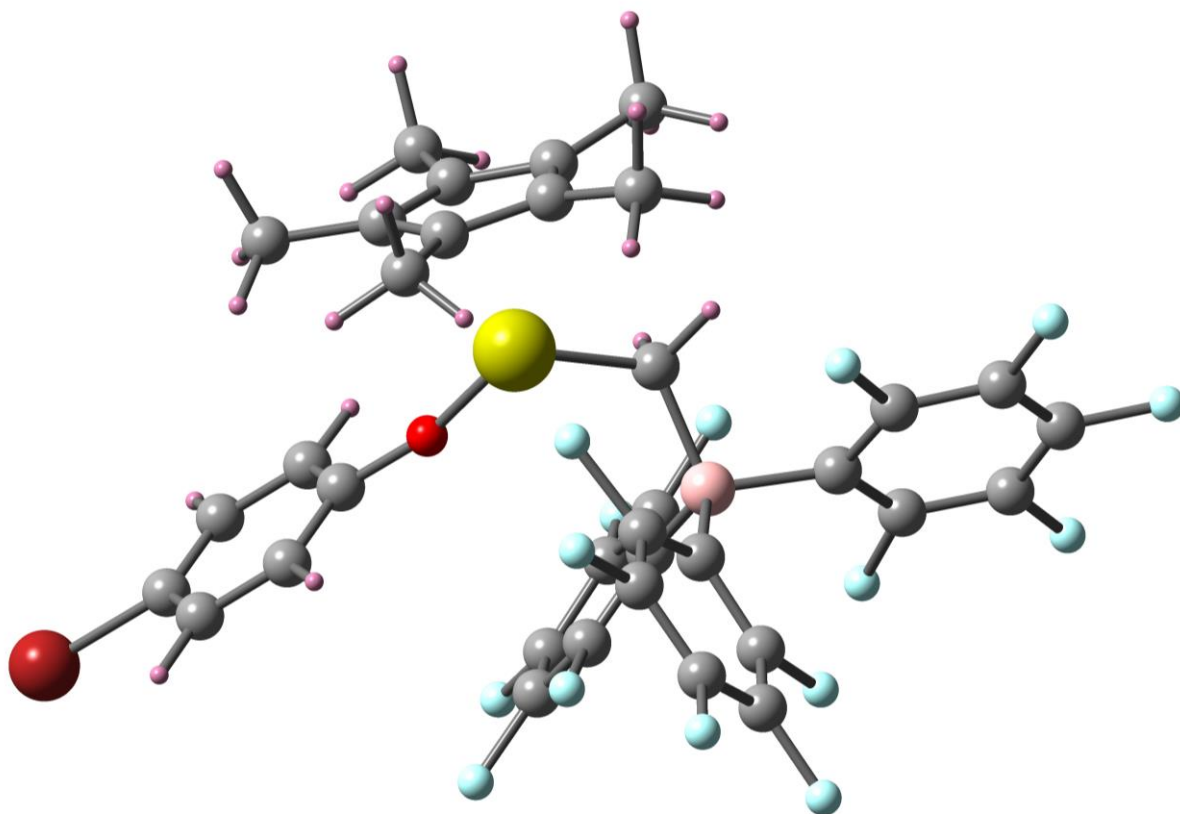
7.0078

16.2819

16.8661

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Frequencies --	40.7300	47.5068	56.1943
Frequencies --	74.2509	77.8219	85.6340
Frequencies --	91.8495	100.3199	101.8330
Frequencies --	103.2767	110.5162	111.6137
Frequencies --	116.1176	117.4915	120.8889
Frequencies --	123.5740	128.0172	131.0021
Frequencies --	135.2513	137.2077	144.7272
Frequencies --	149.2571	156.9731	158.5730
Frequencies --	161.5158	164.6978	168.2944
Frequencies --	173.0490	182.1036	210.2348
Frequencies --	217.1344	219.7725	224.5163
Frequencies --	233.3845	253.5122	264.1192
Frequencies --	264.4973	265.1686	265.8367
Frequencies --	273.5522	275.8349	278.8725
Frequencies --	280.1741	292.1257	295.7316
Frequencies --	299.4471	302.5614	303.0353
Frequencies --	306.4486	314.8477	324.0600
Frequencies --	331.9904	335.9559	338.6219
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Frequencies --	388.3357	397.3693	402.8148
Frequencies --	410.9182	416.9641	431.3448
Frequencies --	431.8925	441.7709	445.3057
Frequencies --	449.5555	458.5234	462.5679
Frequencies --	468.1329	484.5046	514.5500
Frequencies --	534.0150	536.9624	539.5426
Frequencies --	542.4573	547.5977	555.5573
Frequencies --	568.9603	580.6924	589.9019
Frequencies --	601.9644	604.6354	612.5412
Frequencies --	624.2969	628.6353	634.8113
Frequencies --	636.5719	641.5168	647.0874
Frequencies --	655.9223	671.9636	701.3686
Frequencies --	704.5660	717.6796	730.5103
Frequencies --	736.3069	746.9879	747.9178
Frequencies --	766.2039	778.8577	784.5717
Frequencies --	799.9168	803.3563	825.3756
Frequencies --	839.1485	867.8739	873.8970
Frequencies --	906.3782	911.1275	916.8261
Frequencies --	932.6410	946.6881	967.5276
Frequencies --	971.0957	978.4935	1006.8919
Frequencies --	1012.3488	1022.9150	1033.4240
Frequencies --	1041.1655	1043.3370	1044.2975
Frequencies --	1045.2987	1046.3392	1048.7466
Frequencies --	1050.1995	1056.3275	1075.9393
Frequencies --	1086.8846	1089.6346	1110.3501
Frequencies --	1115.4444	1125.0402	1173.5544
Frequencies --	1174.1408	1189.9433	1202.7073
Frequencies --	1209.6613	1213.5530	1250.3051
Frequencies --	1295.6030	1308.6659	1314.1534
Frequencies --	1320.3038	1337.9828	1344.3494
Frequencies --	1348.5087	1352.8720	1387.2207
Frequencies --	1409.3796	1412.5721	1414.0375
Frequencies --	1415.0000	1416.3786	1421.0200
Frequencies --	1423.8918	1425.6916	1427.1637
Frequencies --	1431.0380	1434.1464	1448.4017
Frequencies --	1451.6218	1463.1515	1466.8100
Frequencies --	1470.0403	1471.8592	1480.3629
Frequencies --	1485.6604	1489.3155	1493.0528
Frequencies --	1495.6550	1498.1950	1505.6082
Frequencies --	1505.9061	1510.0001	1514.0252
Frequencies --	1519.1872	1583.1525	1590.0688

Frequencies --	1593.4778	1597.0774	1605.4279
Frequencies --	1616.8865	1621.7252	1630.7113
Frequencies --	3010.7564	3011.5759	3012.7473
Frequencies --	3013.1382	3014.3441	3022.5516
Frequencies --	3099.9241	3100.5892	3102.8486
Frequencies --	3103.8271	3107.6747	3136.7132
Frequencies --	3139.5224	3143.7216	3146.8881
Frequencies --	3149.7120	3153.7476	3193.3484
Frequencies --	3195.9683	3212.2894	3216.2377

Catalyst 7:

vacuum	toluene-like solvent	D3 dispersion
-3014.482553	-3014.4940513	-0.53320764

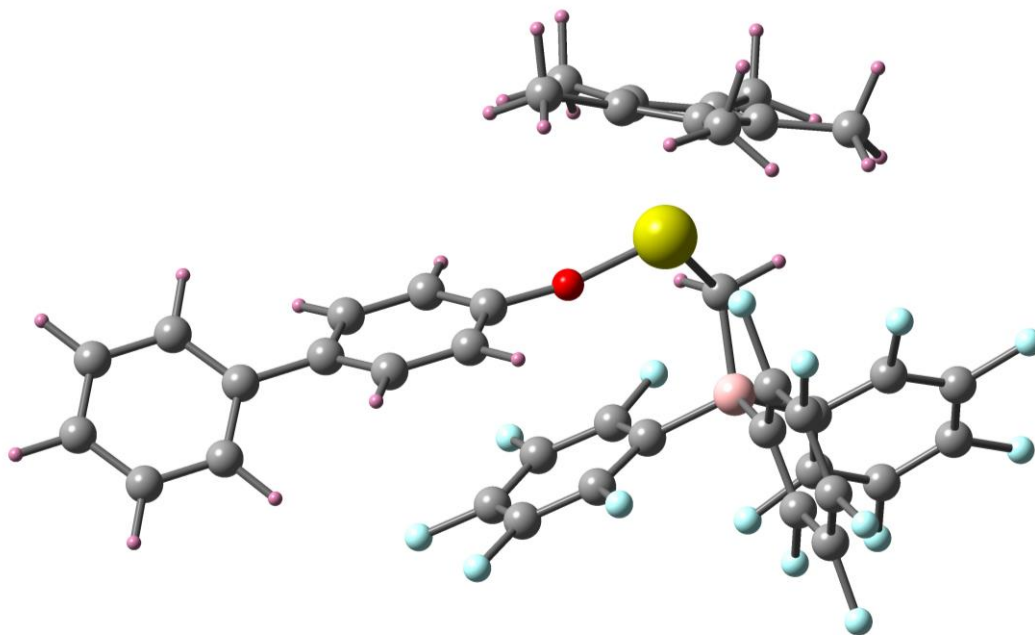
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O	-1.80974500	0.98892400	-0.35589800
C	-3.08495100	0.49015500	-0.15453900
C	-3.68393500	0.58412900	1.12490900
C	-3.77683400	-0.13511600	-1.21946900
C	-4.97666700	0.06577800	1.33596500
C	-5.07096300	-0.65184200	-1.01106300
C	-5.66505700	-0.54189400	0.26422600
H	-5.43104800	0.13147300	2.32446300
H	-5.59821000	-1.13809100	-1.83175000
C	0.44498000	3.48357100	-2.40958700
C	-0.99081500	3.28283300	-2.54227100
C	0.67618900	4.17487000	-1.16919200
C	-1.64371500	3.90836000	-1.40984400
C	-0.61226500	4.42475900	-0.54300800
F	2.28378100	1.10211200	5.59624800
C	2.08000700	0.74369300	4.27433000
C	2.50094200	-0.51146000	3.79300700
C	1.44207100	1.62238000	3.38607300
C	2.28663000	-0.85365400	2.44513500
F	3.11400900	-1.40161800	4.66110600
C	1.27089200	1.19958500	2.05755800

F	0.99658000	2.86883000	3.81305500
C	1.66336900	-0.01025400	1.48681300
F	2.69357200	-2.13267500	2.07179800
F	0.57015200	2.19717400	1.25082400
B	1.51797200	-0.47320900	-0.12623200
C	3.08985700	-0.91007800	-0.54424900
C	0.39452100	-1.68566600	-0.31976200
C	1.10072600	0.76467800	-1.21565400
C	3.55543000	-2.20475800	-0.87995200
C	4.11883500	0.06308100	-0.56210400
C	-0.51119500	-2.14931100	0.66011400
C	0.20184700	-2.31185400	-1.57716200
H	1.98498700	1.34736900	-1.49547100
H	0.72595100	0.28287100	-2.13683400
C	4.88089600	-2.49820100	-1.26242900
F	2.71035100	-3.31431200	-0.80692500
C	5.45575200	-0.17661300	-0.92766500
F	3.84135700	1.38855200	-0.16001100
C	-1.47643500	-3.15585600	0.45228300
F	-0.53043500	-1.58686800	1.94914300
C	-0.74467100	-3.31689100	-1.84150300
F	1.00443800	-1.94529500	-2.67099100
C	5.84215800	-1.47526500	-1.29720800
F	5.25106500	-3.79731500	-1.58954300
F	6.39263800	0.85360500	-0.92243800
C	-1.59404300	-3.75347800	-0.81084600
F	-2.32907800	-3.54086500	1.48136200
F	-0.85106500	-3.88012400	-3.10956500
F	7.15089200	-1.74341700	-1.67177700
F	-2.54434700	-4.73731900	-1.04587900
C	-3.13320600	4.08012500	-1.22081600
H	-3.43169100	4.06910600	-0.16341100
H	-3.44694800	5.05392600	-1.63547900
H	-3.71526700	3.30602500	-1.73638700
C	-1.67489200	2.69003700	-3.75433400
H	-2.68390900	2.32200300	-3.52783800
H	-1.77846500	3.45838300	-4.54020600
H	-1.10255100	1.85995200	-4.19242300
C	1.47138500	3.18540700	-3.47571200
H	1.26302900	2.24988400	-4.01240000
H	1.47577600	3.99802400	-4.22276300
H	2.48747200	3.11563000	-3.06735100
C	2.01462300	4.63687200	-0.64103200
H	2.83201900	3.95926600	-0.91850100
H	2.25791800	5.63093700	-1.05525600
H	2.01920700	4.73417600	0.45280500
C	-0.83188400	5.18731400	0.74500000
H	-0.05737600	4.97840600	1.49554000
H	-0.80724200	6.27316800	0.54876500
H	-1.80655900	4.96366200	1.19988500
H	-3.13814400	1.04020000	1.95126600
H	-3.30206100	-0.22960100	-2.19622900
Br	-7.47126600	-1.25436200	0.55397200

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Frequencies --	305.6459	313.9037	323.3985
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Frequencies --	1348.5660	1349.0210	1382.7723
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Frequencies --	1451.6457	1461.6937	1466.4550
Frequencies --	1469.7899	1471.7928	1479.8335
Frequencies --	1480.2374	1489.6596	1491.1923
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Frequencies --	1519.2070	1578.8310	1589.9736
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Frequencies --	1616.8114	1621.4729	1630.6087

Frequencies --	3009.8962	3010.9354	3011.6876
Frequencies --	3012.4317	3013.5793	3022.9515
Frequencies --	3098.2731	3100.4865	3102.5336
Frequencies --	3103.6641	3105.7541	3136.3944
Frequencies --	3138.5554	3143.2307	3144.9388
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Frequencies --	3193.2532	3208.8487	3213.2422

Catalyst 8:

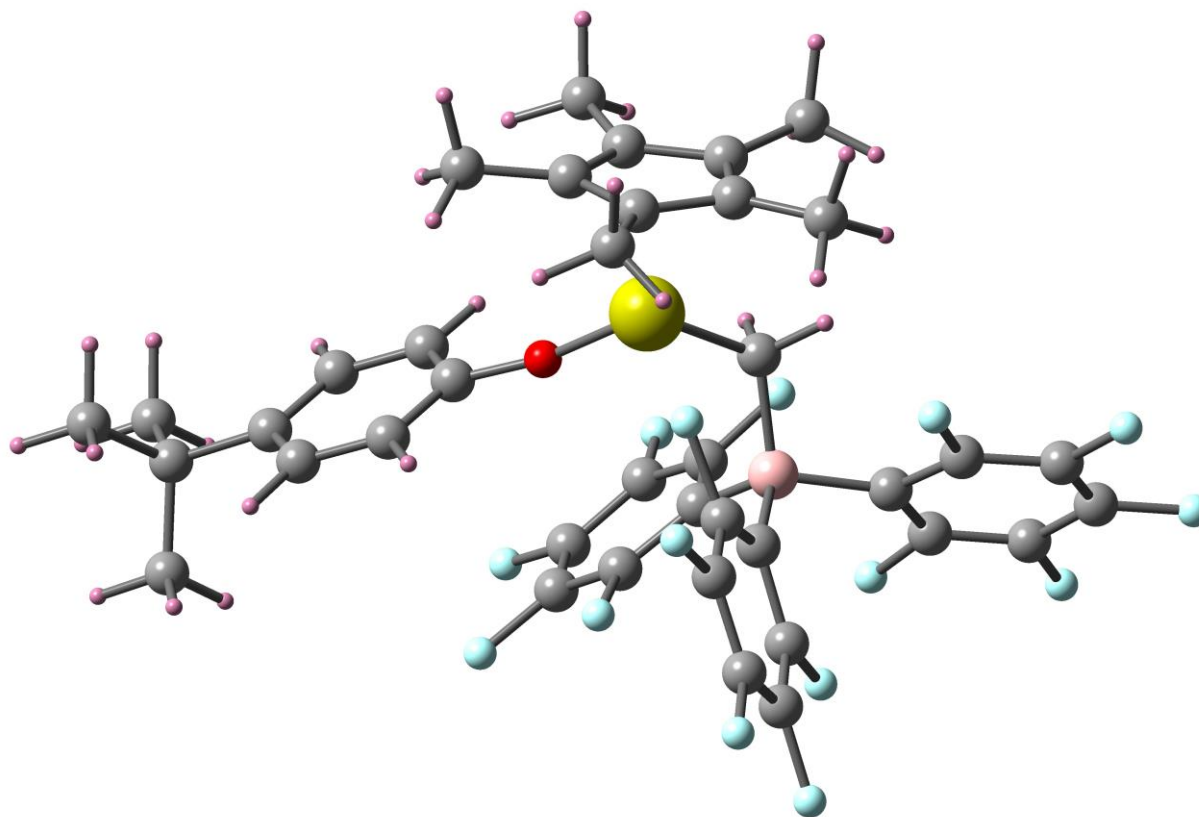
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C	-2.82869400	0.84627400	-0.20841300
C	-3.42091200	0.83919600	1.07654100
C	-3.56744800	0.39756600	-1.32865800
C	-4.74235600	0.38521500	1.23137100
C	-4.89049400	-0.04833100	-1.15856100
C	-5.50985200	-0.06687400	0.12199800
H	-5.18811400	0.40021000	2.22672400
H	-5.43221800	-0.42468300	-2.02726100
C	1.34364500	4.18671900	-1.01217800
C	0.98078200	3.59880400	-2.27299200
C	0.12197000	4.56639100	-0.32093700
C	-0.47356900	3.59462200	-2.35659200
C	-0.99833400	4.23597700	-1.16815700
F	2.39977400	0.62228000	5.67668800
C	2.19869600	0.35993400	4.33166500
C	2.50632900	-0.90256500	3.78806200
C	1.67673300	1.34623500	3.48157900
C	2.29730700	-1.14600200	2.41818200
F	3.00320200	-1.89678900	4.61718200
C	1.50063200	1.01721700	2.12729400
F	1.34687800	2.60600400	3.97049800
C	1.78710300	-0.19280700	1.49669700
F	2.58643400	-2.43681900	1.98015300
F	0.92722800	2.12312900	1.36502900
B	1.64350300	-0.54864000	-0.14374200
C	3.18299600	-1.10315500	-0.54748500

C	0.42275400	-1.64253400	-0.43073300
C	1.37061400	0.77734600	-1.17160500
C	3.54410700	-2.41415200	-0.94290900
C	4.29319500	-0.22562000	-0.48754700
C	-0.54982100	-2.07226100	0.49907800
C	0.21382700	-2.18237700	-1.72492600
H	2.31291400	1.28374300	-1.40801800
H	0.96612600	0.38425900	-2.12164700
C	4.84947000	-2.80258100	-1.31022700
F	2.60472300	-3.44756200	-0.95150400
C	5.61376400	-0.56184200	-0.83600900
F	4.12201800	1.09544200	-0.01790500
C	-1.59534300	-2.97335300	0.21147800
F	-0.55406000	-1.58180300	1.81731200
C	-0.81028500	-3.08218000	-2.06760300
F	1.07936400	-1.83424600	-2.77572200
C	5.89636900	-1.86788600	-1.26761900
F	5.11484500	-4.11046300	-1.69934900
F	6.63560900	0.38088500	-0.75358300
C	-1.72700600	-3.49182500	-1.08473400
F	-2.51072900	-3.33241000	1.19593700
F	-0.92731200	-3.56825900	-3.36643100
F	7.18680200	-2.22987900	-1.62738900
F	-2.75294100	-4.37301000	-1.39712800
C	-1.27146800	3.17825500	-3.57269300
H	-2.30886300	2.92168500	-3.32362400
H	-1.30626500	4.00806400	-4.29995300
H	-0.82513600	2.31748200	-4.09055300
C	1.92012800	3.22135100	-3.39341500
H	1.58947300	2.32642700	-3.93822400
H	1.97750500	4.04721200	-4.12352400
H	2.94001500	3.03457500	-3.03485600
C	2.74683400	4.44554700	-0.51449800
H	3.46817500	3.70839600	-0.88798700
H	3.08740900	5.44023200	-0.85194300
H	2.80711800	4.44083600	0.58226600
C	0.05400200	5.28752200	1.00716400
H	0.81600500	4.93653900	1.71612700
H	0.22512400	6.36752200	0.85689300
H	-0.92602500	5.17987800	1.49160900
C	-2.44796500	4.57166700	-0.90322800
H	-2.68717300	4.58985200	0.16889300
H	-2.67656400	5.57469200	-1.30378200
H	-3.13689100	3.86514000	-1.38304200
H	-2.84624800	1.17381300	1.94083500
H	-3.09786200	0.37266800	-2.31248900
C	-6.91025100	-0.55903000	0.29868800
C	-7.91828400	-0.27112500	-0.66215600
C	-7.27448000	-1.33611000	1.43286500
C	-9.23784000	-0.73892900	-0.49586800
H	-7.67826200	0.34507400	-1.53083300
C	-8.59288700	-1.80642000	1.59953600
H	-6.51621400	-1.60630000	2.16997000
C	-9.58268800	-1.50976000	0.63648000
H	-9.99573700	-0.49662500	-1.24464700
H	-8.84311700	-2.41320400	2.47289400
H	-10.60408400	-1.87513600	0.76474200

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Frequencies --	1295.0788	1301.2339	1314.0504
Frequencies --	1316.5235	1320.6731	1326.1631
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Catalyst 9:

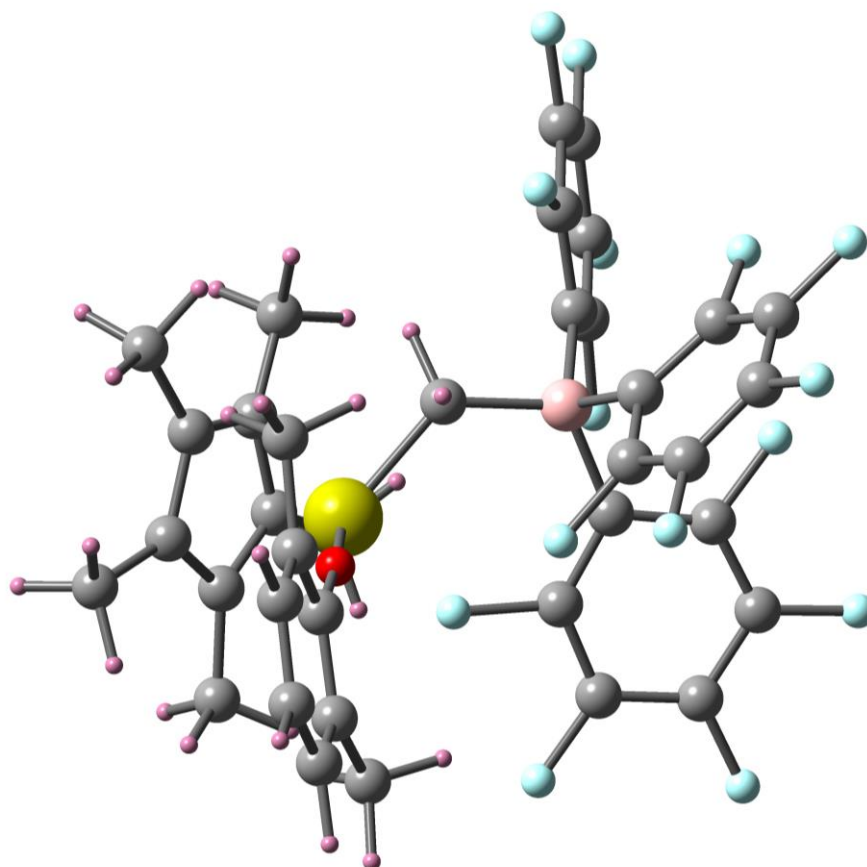
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C	-3.07227300	0.64213600	-0.14869700
C	-3.72081700	0.76085700	1.10266200
C	-3.71104800	-0.03940600	-1.20645600
C	-4.99163700	0.18806000	1.28224600
C	-4.98565900	-0.60732700	-1.00495200
C	-5.65953000	-0.51649000	0.24063400
H	-5.45948400	0.28367900	2.26227400
H	-5.43930200	-1.13880900	-1.83935900
C	0.48569400	3.50939200	-2.43474100
C	-0.97028800	3.44973900	-2.43590700
C	0.89514600	4.17001600	-1.22437700
C	-1.45176200	4.12347700	-1.24836400
C	-0.29975400	4.53374300	-0.48109700
F	2.25469300	0.92254600	5.61781800
C	2.04040600	0.60219900	4.28732100
C	2.38357000	-0.66869000	3.78628400
C	1.46968800	1.53666200	3.41044800
C	2.15919100	-0.97166800	2.43091100
F	2.92984200	-1.61249200	4.64306900
C	1.28186500	1.15029700	2.07288400

F	1.10448800	2.80198500	3.85794700
C	1.59862400	-0.07318400	1.48403100
F	2.48748300	-2.26710500	2.03590600
F	0.66046200	2.20658800	1.27867300
B	1.43713000	-0.49872400	-0.13805500
C	2.99243900	-0.99922500	-0.55242100
C	0.26393100	-1.66085600	-0.35246500
C	1.07320700	0.76797100	-1.20927300
C	3.40620600	-2.30796000	-0.90128200
C	4.06139300	-0.07009100	-0.55198100
C	-0.67230400	-2.09208700	0.61383700
C	0.05533100	-2.26333600	-1.61877200
H	1.98273900	1.30967400	-1.49400300
H	0.66414700	0.31842200	-2.13165800
C	4.72101000	-2.65171100	-1.27893800
F	2.51523800	-3.38237600	-0.84947300
C	5.38958400	-0.36055900	-0.91273500
F	3.83719100	1.26045000	-0.13515900
C	-1.68442000	-3.04583800	0.38271100
F	-0.67530300	-1.54734400	1.91002500
C	-0.93650200	-3.21732700	-1.90481200
F	0.88575200	-1.92305800	-2.69993500
C	5.72427800	-1.66949700	-1.29554500
F	5.03935400	-3.96132000	-1.62014900
F	6.36837200	0.63007000	-0.88964100
C	-1.81847200	-3.62065900	-0.88876100
F	-2.57181000	-3.39850000	1.39537400
F	-1.05828500	-3.75968600	-3.18116500
F	7.02337400	-1.98756700	-1.66588300
F	-2.82051700	-4.54744100	-1.14683200
C	-2.89706000	4.41614300	-0.91774900
H	-3.06785800	4.52300100	0.16213500
H	-3.20135800	5.36675600	-1.38965800
H	-3.57840800	3.63796300	-1.28523800
C	-1.82154700	2.95807300	-3.58595600
H	-1.36305700	2.11053300	-4.11494800
H	-2.82569400	2.65269600	-3.26453200
H	-1.94802600	3.76646800	-4.32717700
C	1.37619100	3.11437200	-3.58867100
H	1.03305700	2.20026300	-4.09213000
H	1.38607100	3.92044700	-4.34277200
H	2.41501800	2.95060000	-3.27561500
C	2.31351000	4.49777600	-0.81865100
H	3.04110700	3.78359200	-1.22339800
H	2.59015700	5.49884100	-1.19348600
H	2.44190400	4.51609200	0.27232100
C	-0.32589000	5.31045600	0.81709600
H	0.52479100	5.06827000	1.46768800
H	-0.27702100	6.39318900	0.60809200
H	-1.24487100	5.13376000	1.39309600
H	-3.22235300	1.27322400	1.92659200
H	-3.20605600	-0.14368500	-2.16760700
C	-7.04816900	-1.16315700	0.50313600
C	-6.91631700	-2.21456200	1.65450300
H	-6.58837000	-1.75471400	2.59796200
H	-7.88808800	-2.69925500	1.83926900
H	-6.18664200	-2.99590400	1.39183700

C	-8.07237700	-0.05626200	0.91874700
H	-8.18927200	0.69207600	0.11903400
H	-9.05939900	-0.50522700	1.11310000
H	-7.76149100	0.47136100	1.83223600
C	-7.61248800	-1.89318400	-0.75075600
H	-7.75409900	-1.20574900	-1.59944200
H	-6.95944800	-2.71765900	-1.07560200
H	-8.59505200	-2.32733800	-0.51163600
Frequencies --	8.4430	16.0799	21.6875
Frequencies --	23.1823	26.6704	29.8270
Frequencies --	31.5192	35.3734	37.8404
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Frequencies --	62.4144	71.0873	73.5779
Frequencies --	78.6673	86.8405	97.4051
Frequencies --	104.6983	110.2262	110.9540
Frequencies --	113.1768	114.4241	119.5899
Frequencies --	123.2027	124.3512	127.5332
Frequencies --	132.2584	134.1559	138.1330
Frequencies --	144.4419	148.6922	157.2087
Frequencies --	159.9348	160.9592	165.4888
Frequencies --	166.3783	169.1282	173.7344
Frequencies --	195.7201	208.2969	213.8642
Frequencies --	219.3043	222.3567	224.8902
Frequencies --	230.7292	244.6744	246.7494
Frequencies --	258.5982	263.9969	264.8312
Frequencies --	265.0386	275.8486	277.5465
Frequencies --	278.9386	287.2687	294.8215
Frequencies --	298.3657	299.4742	303.3759
Frequencies --	305.2024	305.6743	313.8831
Frequencies --	316.6412	324.4634	331.4002
Frequencies --	334.2034	338.6425	356.0087
Frequencies --	363.7785	365.4734	371.8175
Frequencies --	375.4959	377.3322	379.7269
Frequencies --	382.6213	394.0648	396.3017
Frequencies --	411.9011	412.4569	416.3699
Frequencies --	423.2280	431.4353	432.5260
Frequencies --	443.0970	445.2851	454.5874
Frequencies --	459.0030	467.5640	474.9836
Frequencies --	491.8486	534.8223	536.9830
Frequencies --	539.0818	540.9517	546.9773
Frequencies --	553.9786	557.5342	559.7242
Frequencies --	567.8973	580.4359	588.9019
Frequencies --	600.5269	603.7928	610.3222
Frequencies --	624.0269	633.9600	636.0080
Frequencies --	639.5686	640.7453	654.7910
Frequencies --	670.3092	703.9753	714.5387
Frequencies --	717.1030	729.6534	734.6882
Frequencies --	735.2608	745.7877	746.7644
Frequencies --	765.8334	800.7301	804.7765
Frequencies --	821.4591	825.6180	833.7276
Frequencies --	839.5115	843.8988	862.5410
Frequencies --	872.2880	906.3781	910.7933
Frequencies --	925.2005	930.6516	933.1841
Frequencies --	955.6861	964.6175	968.2566
Frequencies --	969.6996	971.2558	978.4563
Frequencies --	1004.7826	1021.6984	1022.2782
Frequencies --	1029.6352	1037.0030	1042.1570
Frequencies --	1042.8593	1043.0114	1044.2611
Frequencies --	1045.8809	1048.0043	1048.3871
Frequencies --	1049.6038	1054.7625	1085.9037
Frequencies --	1087.6345	1091.4755	1121.7205

Frequencies --	1125.9586	1132.0769	1173.4721
Frequencies --	1174.4710	1201.9369	1204.5488
Frequencies --	1208.5748	1211.6855	1216.0683
Frequencies --	1222.9789	1252.3571	1275.5698
Frequencies --	1294.8672	1314.0878	1320.4893
Frequencies --	1326.5668	1338.1819	1344.0622
Frequencies --	1348.8058	1352.0934	1383.2452
Frequencies --	1396.1237	1400.9541	1410.8670
Frequencies --	1412.4660	1413.7111	1416.6423
Frequencies --	1421.1158	1422.5179	1425.1248
Frequencies --	1426.2687	1427.9862	1428.6027
Frequencies --	1429.4558	1435.6755	1449.6746
Frequencies --	1451.4753	1462.4721	1466.3570
Frequencies --	1469.6051	1471.5172	1481.2922
Frequencies --	1482.0114	1487.8273	1490.0851
Frequencies --	1490.6466	1491.2717	1497.2363
Frequencies --	1497.8513	1498.8233	1504.5936
Frequencies --	1505.1406	1509.1146	1509.9491
Frequencies --	1511.5787	1514.3920	1520.7821
Frequencies --	1520.8591	1581.2388	1590.3543
Frequencies --	1593.7320	1598.1659	1616.6866
Frequencies --	1620.0573	1621.5433	1630.2204
Frequencies --	3007.3227	3008.6659	3008.8286
Frequencies --	3009.7352	3010.6655	3011.8667
Frequencies --	3013.2122	3015.5445	3026.3273
Frequencies --	3097.7426	3100.1490	3102.5279
Frequencies --	3103.5853	3104.9516	3108.2992
Frequencies --	3111.1425	3114.6826	3120.7303
Frequencies --	3125.0527	3127.3184	3133.2364
Frequencies --	3136.3790	3139.1224	3143.4868
Frequencies --	3145.4910	3152.6897	3178.1452
Frequencies --	3186.6230	3199.5396	3214.2686

Catalyst 10:

vacuum	toluene-like solvent	D3 dispersion
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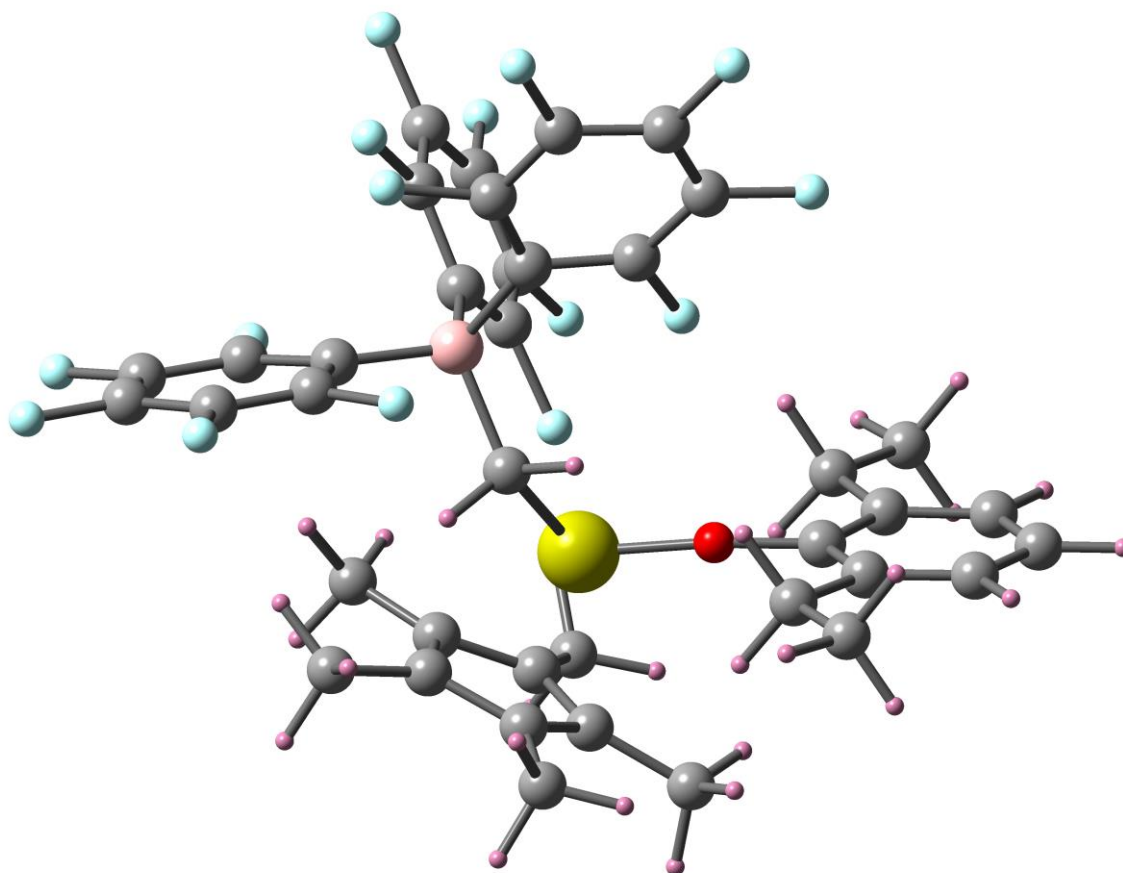
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O	-3.03778900	-0.05086200	-0.55978800
C	-4.12868500	0.79909800	-0.71737300
C	-4.40971200	1.32727900	-2.01170500
C	-4.90497900	1.13960100	0.42977300
C	-5.52597100	2.18563400	-2.14156300
C	-6.00721700	2.00549900	0.24396700
C	-6.32470100	2.52063400	-1.02919500
H	-5.76084600	2.60219700	-3.12299100
H	-6.61300500	2.28374300	1.10859600
H	-7.17960800	3.18838600	-1.15113000
C	-2.11877300	-3.13636000	-1.74071300
C	-0.88968900	-3.46784400	-1.04477000
C	-3.20167100	-3.12725200	-0.77420500
C	-1.19976000	-3.60309300	0.35270000
C	-2.62655200	-3.39009600	0.52281100
F	0.73185000	0.68297200	5.83352000
C	0.83014900	0.55558200	4.45801900
C	1.95509200	1.04331500	3.76498000
C	-0.18911700	-0.06618700	3.72263600
C	2.03035500	0.90481900	2.36712900

F	2.97973300	1.65204600	4.47372900
C	-0.03207600	-0.16174100	2.32920800
F	-1.31898400	-0.57164200	4.35838400
C	1.03670100	0.28991100	1.55696500
F	3.18982100	1.39684900	1.77157200
F	-1.15513600	-0.84370800	1.70455000
B	1.19028000	0.25836700	-0.12330700
C	1.25542300	1.90032300	-0.48537000
C	2.53840700	-0.59953000	-0.59086200
C	-0.07596100	-0.44381500	-1.04488700
C	2.37395600	2.64765300	-0.92846700
C	0.10258500	2.69961000	-0.29886100
C	3.25615100	-1.52537200	0.19732200
C	3.00305500	-0.54397600	-1.92956300
H	-0.57380900	0.36507600	-1.61135300
H	0.39625600	-1.10495600	-1.77894700
C	2.33939900	4.02791900	-1.22019900
F	3.62784800	2.05249000	-1.08117300
C	0.01413600	4.07723400	-0.56808100
F	-1.06664800	2.11395900	0.22426100
C	4.36427900	-2.27433300	-0.25138800
F	2.86654600	-1.79620100	1.52381800
C	4.10274500	-1.26277100	-2.42922900
F	2.33751500	0.26537900	-2.86104300
C	1.14869300	4.75202500	-1.04780700
F	3.48039400	4.68395000	-1.66728500
F	-1.17331900	4.77227600	-0.35740900
C	4.80333100	-2.13420300	-1.57660000
F	5.01327300	-3.16120900	0.60276900
F	4.49913500	-1.12882300	-3.75549600
F	1.09636000	6.10966000	-1.33028300
F	5.89093900	-2.85875300	-2.04378300
C	-3.53687700	1.00959600	-3.21328400
H	-2.51032800	1.38101500	-3.07014900
H	-3.46699400	-0.07223200	-3.39865900
H	-3.93776000	1.47996600	-4.12143000
C	-4.54259800	0.63290700	1.81416300
H	-4.50542800	-0.46580600	1.85920000
H	-3.55405200	1.00552400	2.12527700
H	-5.27589900	0.97190500	2.55841600
C	-0.23927500	-4.02480600	1.44076500
H	-0.59345900	-3.73842200	2.43963200
H	-0.13297100	-5.12377500	1.43941900
H	0.76509700	-3.60371900	1.30693800
C	0.41938400	-3.82322300	-1.70464100
H	0.61155000	-3.23124900	-2.60955000
H	1.27331200	-3.69905500	-1.02919900
H	0.39960900	-4.88311200	-2.01384300
C	-2.25631300	-3.02610500	-3.24293800
H	-1.43858600	-2.44864100	-3.69847600
H	-2.22972100	-4.03233400	-3.69614000
H	-3.20480500	-2.56394500	-3.54344800
C	-4.67394300	-2.99058400	-1.08929600
H	-4.85842400	-2.36772900	-1.97402900
H	-5.10327100	-3.98670500	-1.29445200
H	-5.24464200	-2.55583800	-0.25820200
C	-3.37931700	-3.53343500	1.82756600

H	-4.38487500	-3.09689900	1.77632300
H	-3.50251200	-4.60203400	2.07423300
H	-2.85297400	-3.06884000	2.67410500

Frequencies --	8.2163	17.4658	19.5060
Frequencies --	27.4549	28.8544	33.3747
Frequencies --	33.5569	34.3038	42.1559
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Frequencies --	345.1852	354.7252	360.3748
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Frequencies --	379.3717	391.7774	395.4715
Frequencies --	397.9219	413.4197	430.7541
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Frequencies --	833.8865	860.8580	882.6699
Frequencies --	903.0293	909.9330	915.1928
Frequencies --	921.9707	928.3014	967.9342
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Frequencies --	1000.1013	1002.1619	1023.3292
Frequencies --	1029.8701	1038.5750	1041.3884
Frequencies --	1042.8508	1046.4611	1048.1546
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Frequencies --	1418.8357	1421.5764	1424.6579
Frequencies --	1426.6032	1429.1450	1429.6835
Frequencies --	1431.6162	1435.3688	1451.1673
Frequencies --	1453.6142	1465.7576	1467.0011
Frequencies --	1467.8266	1471.8495	1472.5839
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Frequencies --	1490.6091	1494.7367	1499.2608
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Frequencies --	1505.2503	1508.4840	1510.5580
Frequencies --	1517.8180	1523.2318	1591.2018
Frequencies --	1593.6571	1595.9236	1605.6703
Frequencies --	1608.2134	1616.6472	1618.7387
Frequencies --	1630.2002	3009.7575	3011.2132
Frequencies --	3011.8979	3012.2801	3012.5613
Frequencies --	3013.6125	3020.6256	3023.9561
Frequencies --	3095.4398	3097.3916	3103.2342
Frequencies --	3103.7825	3105.5062	3107.0490
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Frequencies --	3162.6984	3173.5173	3194.5910

Catalyst 11:

vacuum	toluene-like solvent	D3 dispersion
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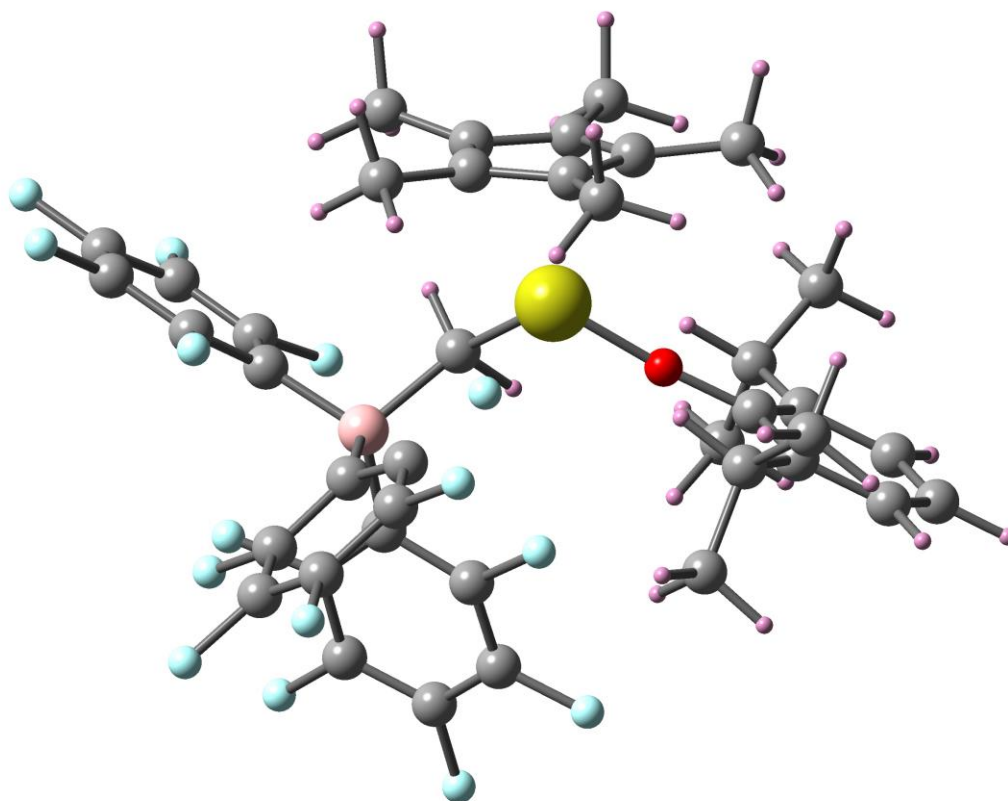
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C	-3.99759900	0.61720900	-0.64746300
C	-4.29987800	1.23382900	-1.89957100
C	-4.79367000	0.80708400	0.52305300
C	-5.47028000	2.02371600	-1.96436100
C	-5.94923600	1.61121900	0.39628800
C	-6.29154600	2.20625900	-0.83397900
H	-5.73953100	2.50996500	-2.90053900
H	-6.58328400	1.78256300	1.26455200
H	-7.18897700	2.82369000	-0.90829100
C	-1.85193200	-3.11938800	-1.93213700
C	-0.58537600	-3.44497400	-1.30199700
C	-2.90051800	-3.23878800	-0.93559300
C	-0.84158700	-3.70342900	0.08855700
C	-2.27018600	-3.57363400	0.31809000
F	1.01292700	0.05352300	5.89917900
C	1.08637400	0.07929900	4.51639300
C	2.18311000	0.67212500	3.86100200
C	0.06851500	-0.48665200	3.73547700

C	2.23388500	0.68694100	2.45525400
F	3.20397300	1.23256800	4.61380900
C	0.19974900	-0.42837300	2.33731700
F	-1.03648100	-1.08700800	4.33186100
C	1.24323800	0.12987300	1.60081600
F	3.36248500	1.28282500	1.89616300
F	-0.92387900	-1.05773700	1.66281800
B	1.36067400	0.28348500	-0.07479900
C	1.31633800	1.95471000	-0.25646300
C	2.74677200	-0.43061200	-0.65730200
C	0.12739000	-0.40856500	-1.04879800
C	2.38067000	2.81382600	-0.62382800
C	0.11971400	2.65533200	0.02533600
C	3.52805500	-1.40308100	0.00377600
C	3.17776600	-0.19300700	-1.98744700
H	-0.39276700	0.41723600	-1.56899200
H	0.62764700	-1.00688800	-1.81762500
C	2.25660000	4.21219600	-0.76639100
F	3.66583800	2.31727100	-0.84959100
C	-0.05807500	4.04525600	-0.09557300
F	-1.00140500	1.94485000	0.49683600
C	4.66281600	-2.03372500	-0.54833100
F	3.18302700	-1.84703400	1.29562800
C	4.30145500	-0.78806000	-2.58635100
F	2.44874000	0.68159700	-2.80564700
C	1.02544300	4.83715900	-0.50986900
F	3.34804500	4.98254500	-1.15019900
F	-1.28293200	4.63795200	0.19815500
C	5.06430700	-1.71541000	-1.85440600
F	5.37558900	-2.97826800	0.18463400
F	4.66077200	-0.47885900	-3.89385800
F	0.88487400	6.21087800	-0.64763800
F	6.17660000	-2.32140200	-2.42189900
C	-3.36225700	1.05074600	-3.09460500
H	-2.36367200	1.42019600	-2.80658900
C	-4.36021300	0.19205300	1.85451000
H	-3.37729600	0.61642000	2.12191600
C	-3.77359200	1.73625800	-4.41577700
H	-3.01927700	1.52533900	-5.19020900
H	-4.74413400	1.37121800	-4.78782100
H	-3.83697900	2.82998200	-4.30829100
C	-5.31583100	0.37973500	3.05303400
H	-6.30989100	-0.05443000	2.86078100
H	-4.89658200	-0.12098200	3.93985900
H	-5.44963900	1.44211100	3.30823200
H	-4.18956300	-0.88759500	1.71243000
H	-3.23334600	-0.02681800	-3.28549700
C	-2.05008700	-2.91115200	-3.41732800
H	-1.27509600	-2.26887300	-3.86051200
H	-2.00012500	-3.88217600	-3.94012400
H	-3.02748600	-2.47076600	-3.65026700
C	0.71722000	-3.68132900	-2.02632800
H	0.75409700	-4.72407300	-2.38768200
H	0.83385600	-3.03485000	-2.90654700
H	1.58825800	-3.53216300	-1.37790300
C	-4.38646900	-3.14280100	-1.19494400
H	-4.62717000	-2.43792000	-2.00114800

H	-4.77658300	-4.13098000	-1.49471800
H	-4.94833300	-2.82647500	-0.30640100
C	0.17372400	-4.16137600	1.11020200
H	0.32179500	-5.25236400	1.02623500
H	1.15550300	-3.69149200	0.97198600
H	-0.15325400	-3.96132700	2.13909700
C	-2.96983000	-3.86444900	1.62796100
H	-4.00528800	-3.50115600	1.63541500
H	-3.00862500	-4.95435600	1.79697600
H	-2.45290400	-3.42534000	2.49362100

Frequencies --	3.6561	15.9062	17.2281
Frequencies --	22.7204	27.2359	28.8663
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Frequencies --	41.0873	43.7744	48.1490
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Frequencies --	113.4648	116.0779	121.1396
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Frequencies --	129.6692	134.1003	137.0181
Frequencies --	141.8596	142.8936	147.3507
Frequencies --	157.6961	158.7723	159.4029
Frequencies --	162.8692	167.1136	173.6210
Frequencies --	177.5428	180.9774	187.3433
Frequencies --	199.8626	214.0665	214.2051
Frequencies --	222.7037	225.5968	246.7395
Frequencies --	259.4387	263.7625	263.9410
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Frequencies --	279.0923	281.0190	286.3920
Frequencies --	289.8900	291.4875	299.1476
Frequencies --	300.4391	301.7352	303.4837
Frequencies --	304.8356	316.9602	323.5662
Frequencies --	326.3910	328.6276	333.2389
Frequencies --	341.8315	344.6809	358.7813
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Frequencies --	431.2135	432.6930	444.2780
Frequencies --	453.4150	459.7343	467.3440
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Frequencies --	532.1279	536.6755	541.8329
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Frequencies --	582.1599	584.2876	598.3773
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Frequencies --	624.7326	633.2603	637.0200
Frequencies --	642.5527	651.6935	679.3751
Frequencies --	698.4619	712.3959	714.3002
Frequencies --	726.3615	729.5953	736.8275
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Frequencies --	772.6313	787.7907	801.5324
Frequencies --	804.1358	819.3526	826.7425
Frequencies --	835.1316	852.6341	861.2123
Frequencies --	882.8112	902.7318	915.2246
Frequencies --	923.4982	930.9991	967.6923
Frequencies --	974.7564	983.2625	992.1609
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Frequencies --	1024.5024	1029.5254	1040.2247
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Frequencies --	1048.4343	1049.4060	1051.5182
Frequencies --	1053.7992	1057.8367	1073.8261

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Frequencies --	1126.3084	1173.0855	1175.9895
Frequencies --	1193.8153	1202.5615	1202.6587
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Frequencies --	1294.9599	1318.9981	1320.0213
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Frequencies --	1345.4030	1350.4868	1380.8952
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Frequencies --	1467.7081	1468.4317	1471.6212
Frequencies --	1480.2891	1481.3453	1490.1554
Frequencies --	1493.1874	1493.8446	1498.6745
Frequencies --	1499.7610	1499.8276	1500.7033
Frequencies --	1504.0872	1505.8314	1506.8955
Frequencies --	1508.0070	1509.3168	1517.4797
Frequencies --	1523.3706	1591.3349	1593.6876
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Frequencies --	1617.0628	1619.0948	1629.7575
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Frequencies --	3012.7522	3013.5141	3019.6093
Frequencies --	3024.9042	3064.8420	3068.4466
Frequencies --	3095.5441	3097.4924	3103.9768
Frequencies --	3105.2453	3107.2509	3113.3852
Frequencies --	3114.3884	3120.2728	3120.3761
Frequencies --	3137.5904	3139.7726	3142.0293
Frequencies --	3147.0208	3151.8718	3158.9840
Frequencies --	3170.2664	3203.6584	3212.9655

Catalyst 12:

vacuum	toluene-like solvent	D3 dispersion
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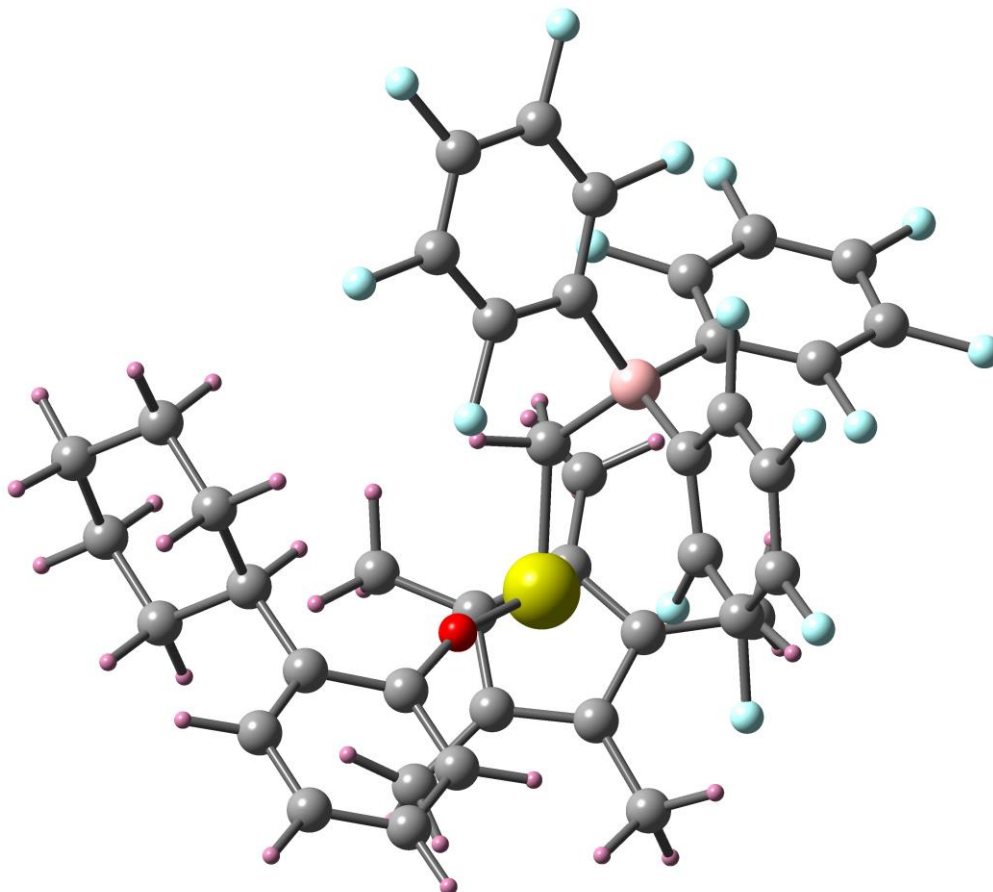
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O	-2.77000400	-0.21900800	-0.50997700
C	-3.92244900	0.56897100	-0.56483600
C	-4.23860300	1.24271400	-1.78680700
C	-4.72622800	0.70272200	0.61181500
C	-5.40586500	2.04179900	-1.80682600
C	-5.87631100	1.52151100	0.52542000
C	-6.22161200	2.18028600	-0.66901000
H	-5.67378200	2.57133500	-2.72161900
H	-6.50517300	1.65245500	1.40634800
H	-7.11449100	2.80729200	-0.70915200
C	-1.64050900	-3.06750400	-2.04865700
C	-0.39334300	-3.40410800	-1.38808300
C	-2.72182900	-3.24142500	-1.09619400
C	-0.69494900	-3.72226100	-0.01834400
C	-2.13190500	-3.61843500	0.16531100
F	1.06778000	-0.05194500	5.91639200
C	1.15580100	-0.00354800	4.53505600
C	2.24929100	0.61720900	3.90083900
C	0.15723000	-0.57587000	3.73434900
C	2.31455000	0.65452400	2.49614000
F	3.25406700	1.18049200	4.67292400
C	0.30058200	-0.49093000	2.33888800

F	-0.94202800	-1.20597300	4.30980400
C	1.34069400	0.09831600	1.62204400
F	3.44503900	1.26743100	1.95967800
F	-0.80041800	-1.13748400	1.64271800
B	1.47962700	0.27074900	-0.05082500
C	1.49480600	1.94554500	-0.21963100
C	2.85249600	-0.47656000	-0.62549600
C	0.22109600	-0.35078600	-1.03437900
C	2.58969200	2.77095100	-0.57484500
C	0.32001700	2.68469100	0.05454600
C	3.62225200	-1.45115200	0.04607500
C	3.29650300	-0.24874200	-1.95301500
H	-0.33944000	0.50564400	-1.45316500
H	0.69881100	-0.86272000	-1.87690600
C	2.51380600	4.17328000	-0.71148600
F	3.85992000	2.23350100	-0.79258400
C	0.18979300	4.08004900	-0.06199500
F	-0.83259800	2.01068000	0.50541900
C	4.75372100	-2.09631200	-0.49602300
F	3.26840500	-1.88387900	1.33916600
C	4.41688800	-0.85911400	-2.54270400
F	2.58960800	0.63859600	-2.77762300
C	1.30210700	4.83794400	-0.46246300
F	3.63391900	4.90834500	-1.08173500
F	-1.02083200	4.70979700	0.21517900
C	5.16569900	-1.79045100	-1.80177100
F	5.45295500	-3.04335500	0.24660700
F	4.78780800	-0.55871700	-3.84901700
F	1.20768300	6.21591600	-0.59643900
F	6.27455600	-2.41141900	-2.35941300
C	-3.34327100	1.16352700	-3.03276500
H	-2.56049000	0.41687900	-2.84412000
C	-4.34513600	0.05421100	1.95129900
H	-3.53058700	-0.65830500	1.76731800
C	-2.62070100	2.52061100	-3.28704700
H	-1.91192200	2.42541000	-4.12555800
H	-3.33788100	3.31673400	-3.53900000
H	-2.06068000	2.84537400	-2.39836300
C	-3.79598900	1.12166400	2.94530800
H	-4.57273100	1.85486000	3.21123600
H	-3.45187100	0.63824700	3.87358100
H	-2.95093200	1.67226200	2.50649200
C	-1.79206500	-2.78880400	-3.52733300
H	-0.94315700	-2.22162600	-3.93436700
H	-1.83917400	-3.74130800	-4.08395300
H	-2.70941800	-2.23397300	-3.75858100
C	0.93414100	-3.60405100	-2.07656700
H	0.96071700	-4.60766800	-2.53635600
H	1.10785800	-2.87982400	-2.88359600
H	1.77672100	-3.54507300	-1.37903900
C	-4.19888600	-3.16417700	-1.40484800
H	-4.41865600	-2.47555500	-2.23031600
H	-4.56749700	-4.16141400	-1.70231700
H	-4.79342300	-2.84094300	-0.54057500
C	0.29084600	-4.20750400	1.01949100
H	0.46406600	-5.29050800	0.89269000
H	1.26690100	-3.71317100	0.93932200

H	-0.07737900	-4.06004200	2.04324800
C	-2.87762700	-3.96515200	1.43520800
H	-3.89451100	-3.55367000	1.44624900
H	-2.97010500	-5.06115400	1.52738100
H	-2.36240900	-3.61065500	2.33944800
C	-5.51252800	-0.75185800	2.58904000
H	-5.91516500	-1.50178800	1.88954000
H	-5.15799600	-1.27667900	3.49064100
H	-6.34551000	-0.10154800	2.89499300
C	-4.11926000	0.70482500	-4.30110000
H	-3.42261400	0.57634900	-5.14522800
H	-4.63771400	-0.25264100	-4.13384900
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Frequencies --	10.1126	17.4913	19.2503
Frequencies --	23.6321	26.3732	31.6207
Frequencies --	33.4545	34.3620	37.2680
Frequencies --	42.9374	48.1845	53.5212
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Frequencies --	73.8212	77.0138	96.2660
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Frequencies --	1116.7707	1120.4103	1126.3402
Frequencies --	1164.0329	1173.1467	1176.2881
Frequencies --	1184.3760	1194.1479	1202.4220
Frequencies --	1205.0902	1210.8270	1213.1117
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Frequencies --	1306.8237	1318.3017	1319.5390
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Frequencies --	1416.0652	1416.6910	1418.0769
Frequencies --	1419.9009	1421.5169	1425.3704
Frequencies --	1426.2098	1428.7887	1431.6419
Frequencies --	1434.9456	1438.6704	1450.6727
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Frequencies --	1468.0153	1472.0082	1474.1864
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Catalyst 13:**distal conformation**

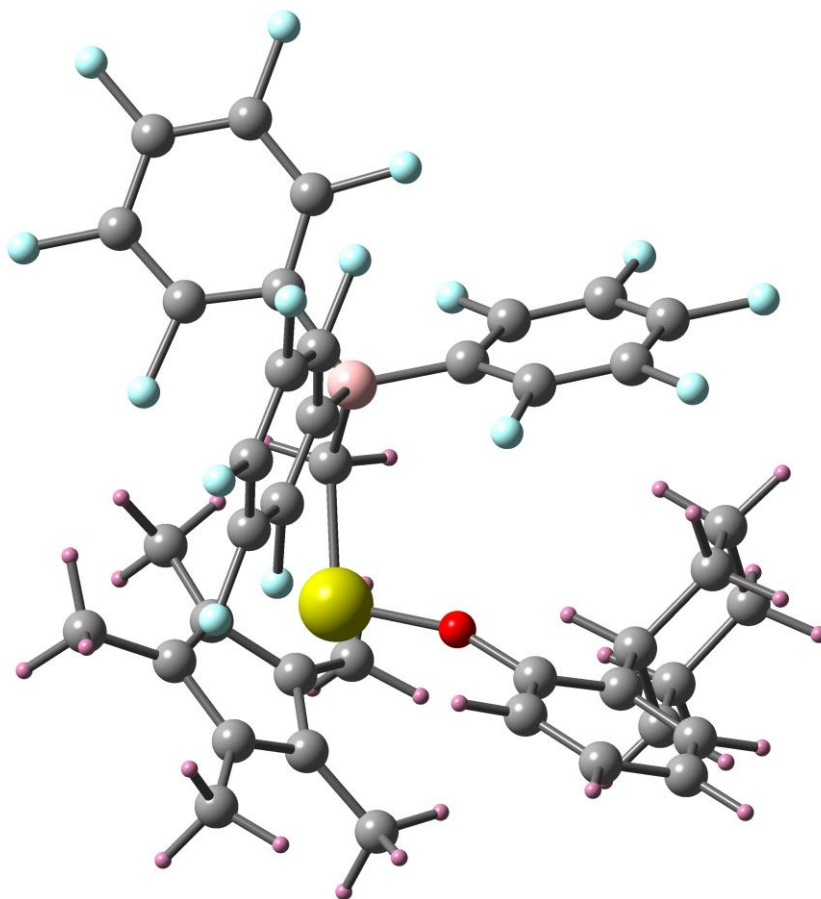
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C	-3.68946800	-0.65050900	0.93478000
C	-4.64147300	0.29587000	0.45109200
C	-3.89328000	-1.35651700	2.14892100
C	-5.80282000	0.48623400	1.24478400
C	-5.05369300	-1.13480700	2.91087500
C	-6.01631800	-0.20829600	2.45171500
H	-6.55490000	1.20267900	0.91187100
H	-5.20027500	-1.67328100	3.84939400
H	-6.92219900	-0.02484300	3.03276900
C	-1.59229400	-2.69330500	-2.54206200
C	-0.17005000	-2.93778400	-2.38493700
C	-2.30045300	-3.43061800	-1.51094500
C	0.00308000	-3.75742500	-1.21456000
C	-1.31307500	-4.06168400	-0.67272800
F	0.65858000	-0.67019200	5.89864800
C	0.85886700	-0.43465500	4.54885200

C	1.62741100	0.65945100	4.11090200
C	0.31113200	-1.29294800	3.58345600
C	1.81009700	0.88803900	2.73218700
F	2.20613800	1.50158400	5.04812900
C	0.53853800	-0.98839500	2.23350500
F	-0.43348000	-2.40667000	3.95938500
C	1.25098300	0.08766900	1.70047500
F	2.64570700	1.95872300	2.41602300
F	0.01055000	-2.01267400	1.33721400
B	1.44852100	0.42378400	0.05995700
C	1.39761800	2.09855500	-0.07127200
C	2.87027600	-0.23570000	-0.52064800
C	0.18812100	-0.14930500	-0.95210800
C	2.45387000	2.95852300	-0.45713100
C	0.20865900	2.80146800	0.23805900
C	3.76677800	-1.06206300	0.19555500
C	3.28336200	-0.02418300	-1.86171300
H	-0.62668900	0.60083900	-0.96061500
H	0.59661900	-0.20440000	-1.96560200
C	2.33063000	4.35526000	-0.60449200
F	3.74436500	2.46290200	-0.66996500
C	0.03422200	4.19194000	0.11948900
F	-0.90572100	2.09902000	0.74071300
C	4.95215000	-1.61480300	-0.33567600
F	3.52184700	-1.41043300	1.53477500
C	4.45170200	-0.54806900	-2.44107800
F	2.51229300	0.78383700	-2.71233800
C	1.10622300	4.98259200	-0.32411500
F	3.41816600	5.12279200	-1.00595000
F	-1.18445100	4.78779400	0.43801900
C	5.30419900	-1.35474000	-1.66817700
F	5.76950700	-2.42154500	0.44942600
F	4.77172900	-0.27834200	-3.76764200
F	0.96248400	6.35567000	-0.46511600
F	6.46141100	-1.89035100	-2.21497800
C	1.30946600	-4.31340400	-0.69714800
H	1.30189200	-4.45752500	0.39171900
H	1.50615600	-5.29937100	-1.15318500
H	2.16155400	-3.66774400	-0.94084700
C	0.89132400	-2.57161700	-3.39330100
H	1.89830900	-2.58419000	-2.96245800
H	0.88090000	-3.30404200	-4.21940000
H	0.73033600	-1.58146100	-3.84018800
C	-2.22797900	-1.95446900	-3.69856400
H	-1.62355500	-1.09772000	-4.02830800
H	-2.32984600	-2.63021300	-4.56579900
H	-3.23333600	-1.58599900	-3.45735900
C	-3.80136100	-3.57461200	-1.40883800
H	-4.32539700	-2.63157900	-1.61143800
H	-4.15538200	-4.31476100	-2.14705600
H	-4.12070300	-3.92131900	-0.41809000
C	-1.58535800	-4.96634700	0.50908800
H	-2.55906100	-4.76436000	0.97532000
H	-1.59571500	-6.02027500	0.18121200
H	-0.81690000	-4.88095400	1.28988400
H	-3.13470000	-2.06119300	2.49121100
C	-4.43977200	1.08453000	-0.84586300

C	-5.55168500	0.79503700	-1.90387100
C	-4.33832700	2.62215400	-0.59111900
H	-3.48089500	0.77208500	-1.28568900
C	-5.30245900	1.57220200	-3.22224700
H	-6.53498400	1.08565600	-1.49643300
H	-5.60741600	-0.28830000	-2.10819400
C	-4.08165400	3.39753700	-1.90753700
H	-5.27597700	2.98467700	-0.13611100
H	-3.53339400	2.82687100	0.12939300
C	-5.16204600	3.09506900	-2.97486500
H	-6.12797600	1.37663600	-3.92837900
H	-4.38015800	1.19596300	-3.70256900
H	-4.04809900	4.47929300	-1.69559100
H	-3.08656600	3.12610200	-2.30510700
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H	-6.13328500	3.50100300	-2.63763400

proximal conformation



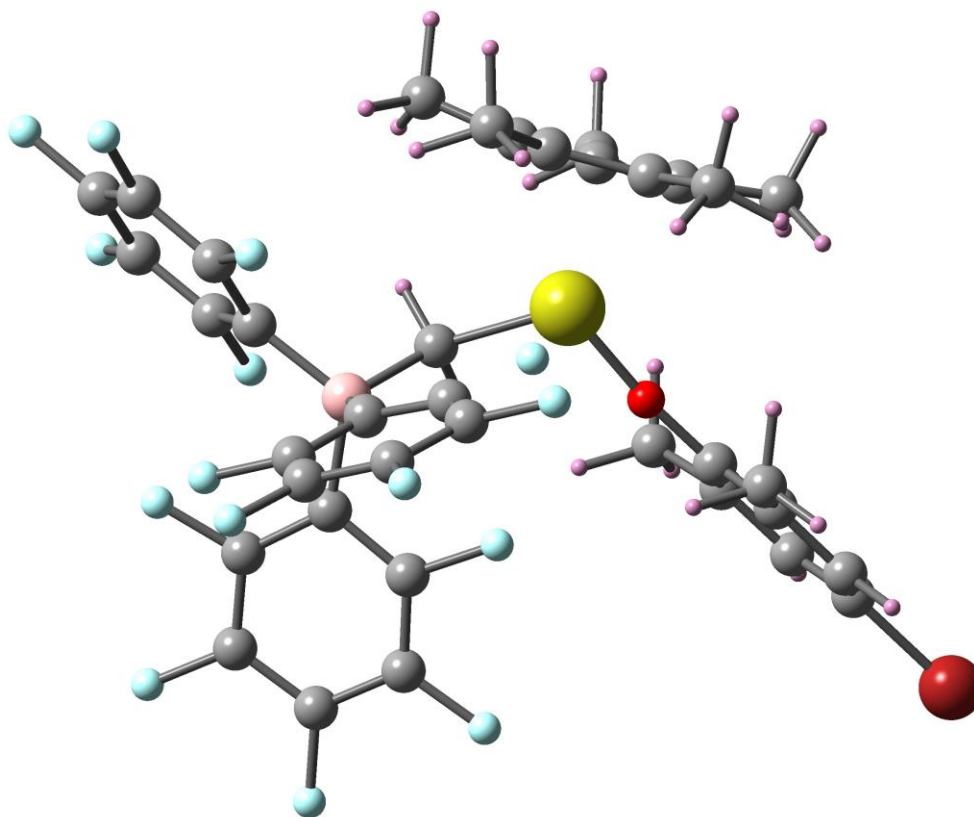
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C	3.15216900	-0.76155400	1.23774500

C	3.00574500	-1.42698700	2.48288800
C	4.28367300	0.06164400	0.96098700
C	3.98576600	-1.29331900	3.48084800
C	5.25329300	0.16887200	1.99348900
C	5.12066800	-0.49068000	3.23050900
H	3.85962500	-1.79929400	4.43998800
H	6.13247800	0.79233000	1.82583800
H	5.88973800	-0.37199100	3.99609100
C	0.40583500	-2.88185900	-2.80943700
C	1.81887500	-2.56943000	-2.67533800
C	0.06972300	-3.83052700	-1.78375800
C	2.36704600	-3.38646200	-1.60732600
C	1.27841000	-4.13412400	-1.03221700
F	-3.42294800	-2.61627000	4.63348600
C	-2.92624600	-1.90855800	3.55162800
C	-3.37044200	-0.60036900	3.27744400
C	-1.96376500	-2.47816100	2.70559800
C	-2.85425100	0.09739900	2.17020200
F	-4.30770200	-0.01132400	4.11252500
C	-1.50205400	-1.70936300	1.62407100
F	-1.48428300	-3.76414100	2.93547900
C	-1.88762700	-0.41921300	1.26519000
F	-3.32310000	1.39884500	2.00325300
F	-0.49325000	-2.41745900	0.84566800
B	-1.38762400	0.47004600	-0.07899100
C	-2.85004700	0.82362400	-0.84053800
C	-0.51895800	1.81132300	0.37616300
C	-0.43772900	-0.34581900	-1.24049600
C	-3.48014400	2.08717300	-0.95563400
C	-3.60924500	-0.21754000	-1.42578200
C	0.01170300	2.07065200	1.65938800
C	-0.17909400	2.80984300	-0.57107800
H	-1.07324300	-0.68470800	-2.06233300
H	0.28097200	0.38724900	-1.65940300
C	-4.69664900	2.31014100	-1.63448800
F	-2.93610000	3.22187600	-0.35069700
C	-4.82770400	-0.05325100	-2.10873500
F	-3.16331000	-1.55281700	-1.31898500
C	0.74145500	3.22691600	2.00557200
F	-0.14373100	1.14390300	2.70478800
C	0.54342200	3.97940300	-0.28111100
F	-0.58654100	2.66739900	-1.90741500
C	-5.37665400	1.23367700	-2.22660400
F	-5.23957700	3.58742300	-1.71061900
F	-5.49046500	-1.14786100	-2.65920800
C	1.00148600	4.19938100	1.02886900
F	1.22315600	3.40112200	3.29876600
F	0.82295100	4.91195300	-1.27548900
F	-6.57319100	1.43306200	-2.90031600
F	1.73228000	5.33871900	1.33919600
C	3.82670200	-3.52201100	-1.24241200
H	3.97992100	-3.72068600	-0.17318000
H	4.26775100	-4.36785300	-1.79813700
H	4.40673000	-2.62791900	-1.49723500
C	2.59932400	-1.68615400	-3.62381700
H	2.05335700	-0.76451500	-3.87190300
H	3.57948300	-1.40308000	-3.22338400

H	2.77269100	-2.22211100	-4.57307100
C	-0.48799600	-2.42618600	-3.93748600
H	-0.25465400	-1.40613700	-4.27206800
H	-0.35594400	-3.09226200	-4.80803600
H	-1.55014300	-2.45531800	-3.66440800
C	-1.27246800	-4.49583200	-1.58748600
H	-2.10639600	-3.84980500	-1.88517500
H	-1.32718200	-5.41021300	-2.20424700
H	-1.43829000	-4.80146000	-0.54583300
C	1.38566000	-5.14371400	0.08962900
H	0.49547700	-5.15380600	0.73374900
H	1.49278500	-6.16027300	-0.32700700
H	2.26046400	-4.96271200	0.72887300
H	2.11343300	-2.02748100	2.66414000
C	4.46612300	0.82435700	-0.35594700
C	4.42769200	2.37103300	-0.13980500
C	5.78029600	0.43171300	-1.10329300
H	3.62260000	0.57251900	-1.01682500
C	4.57858100	3.14385700	-1.47394300
H	5.24043500	2.66833700	0.54448700
H	3.48659100	2.64893000	0.35561000
C	5.93917500	1.20515500	-2.43745100
H	6.65037300	0.64925500	-0.46137900
H	5.79851300	-0.65468600	-1.29132900
C	5.86905200	2.73773400	-2.22592300
H	4.58119800	4.22797900	-1.27188200
H	3.70158700	2.94792800	-2.11716700
H	6.89806800	0.93063100	-2.91004500
H	5.14219300	0.90017800	-3.14047300
H	5.91879200	3.25507800	-3.19895400
H	6.75034600	3.06790200	-1.64634400
Frequencies --	7.4162	18.6146	23.0598
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Frequencies --	163.0995	163.8163	170.5843
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Frequencies --	454.2987	459.0252	467.3942
Frequencies --	489.3538	495.8746	512.2296
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Frequencies --	821.8178	839.5082	862.3936
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Frequencies --	1327.9670	1338.7393	1345.2921
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Frequencies --	1361.6845	1362.2625	1370.4044
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Frequencies --	1421.5420	1421.7469	1425.9628
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Catalyst 14:

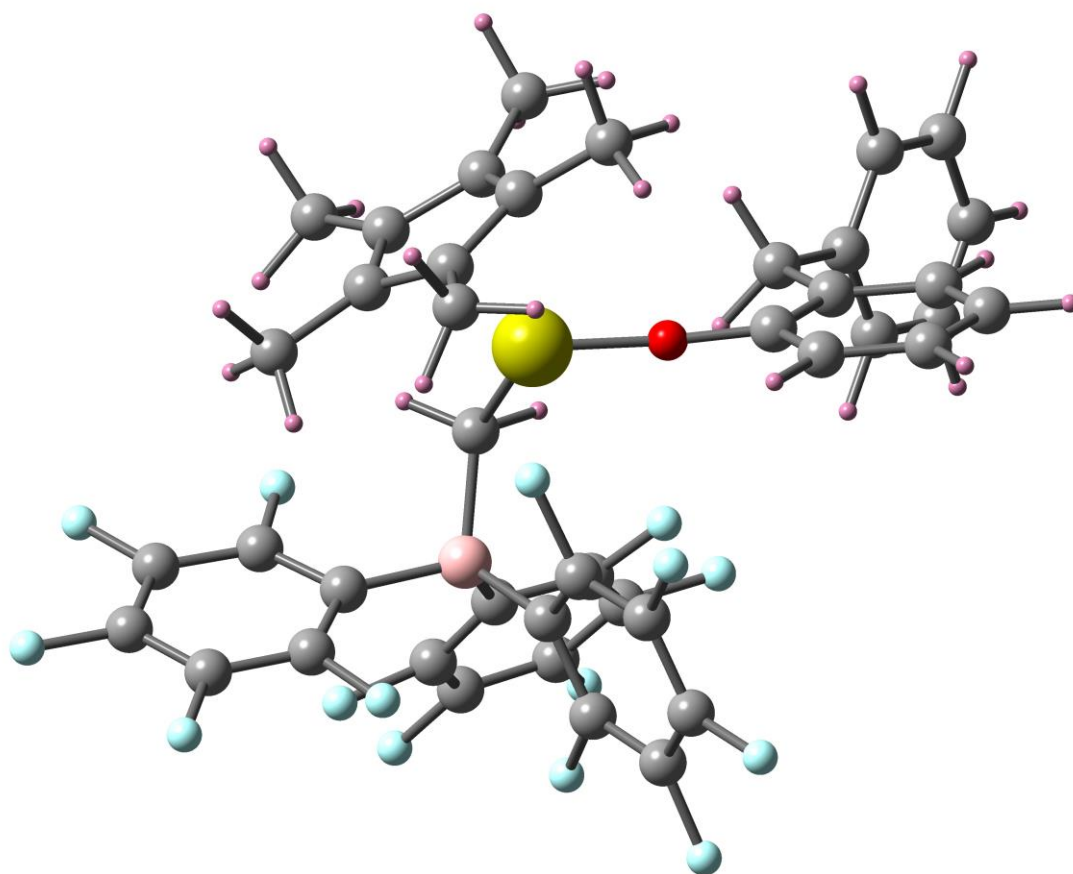
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C	-3.58062300	-0.48582400	-0.36583000
C	-4.08911100	0.02356700	-1.59638900
C	-4.34454700	-0.45130600	0.83798700
C	-5.40627500	0.53727700	-1.61161700
C	-5.65549600	0.07464100	0.78334000
C	-6.17564700	0.55277500	-0.43345700
H	-5.81472600	0.93052700	-2.54194000
H	-6.25381400	0.11420400	1.69281100
C	-0.62216200	-3.60553200	-1.80892900
C	0.69952600	-3.60528500	-1.21119500
C	-1.58582500	-3.96494500	-0.78461100
C	0.54870400	-3.90306100	0.18779500
C	-0.86216100	-4.12309100	0.45415400
F	1.85020400	0.22713000	5.84333900
C	1.81460900	0.26180400	4.45952100
C	2.69117800	1.09217500	3.73401800
C	0.90396200	-0.53185800	3.74711300
C	2.63571500	1.11046100	2.32860100
F	3.60382600	1.88070200	4.41764500
C	0.91773100	-0.45255700	2.34392200
F	0.01643400	-1.37131300	4.41314300

C	1.74580900	0.32973800	1.54096500
F	3.54888500	1.95098900	1.69596800
F	-0.07404700	-1.33050400	1.74214700
B	1.70664600	0.49520700	-0.13690600
C	1.24006800	2.10297400	-0.29655900
C	3.18118500	0.13883500	-0.82016600
C	0.61616500	-0.48838200	-1.03160600
C	2.03474600	3.19610300	-0.72120500
C	-0.06977100	2.49037000	0.07253300
C	4.21598200	-0.61373500	-0.22389300
C	3.45295900	0.47039400	-2.17164400
H	-0.13142000	0.18023200	-1.49837600
H	1.19432900	-0.94045400	-1.84425700
C	1.56341600	4.52151200	-0.83348600
F	3.38365300	3.02930800	-1.03916800
C	-0.58992600	3.79410300	-0.01571000
F	-0.95002300	1.52802500	0.60613900
C	5.43148300	-0.95072000	-0.85529500
F	4.07033100	-1.12799300	1.07987600
C	4.64590400	0.16446100	-2.84921700
F	2.48180100	1.13987200	-2.92899800
C	0.23704700	4.82683700	-0.48742000
F	2.40543600	5.53477600	-1.27565200
F	-1.90025100	4.06786100	0.36512100
C	5.65743600	-0.54725000	-2.17998700
F	6.39756800	-1.69355800	-0.18310600
F	4.83286600	0.54832700	-4.17258900
F	-0.24329900	6.12391100	-0.59384900
F	6.84362300	-0.86626600	-2.82563200
C	-3.25002900	0.04957400	-2.86165500
H	-2.36904500	0.69807900	-2.73855100
H	-2.88177400	-0.95089300	-3.13044300
H	-3.83141100	0.43360500	-3.71052600
C	-3.76705000	-0.92376100	2.15992200
H	-3.44782500	-1.97591100	2.11722000
H	-2.88684000	-0.32521300	2.44137800
H	-4.50622900	-0.83230000	2.96689400
Br	-8.00533700	1.27147500	-0.48418700
C	1.67232000	-4.08926800	1.18147800
H	1.32351800	-4.01604300	2.21966600
H	2.11418100	-5.09372500	1.06049800
H	2.48362900	-3.36281100	1.04511400
C	2.00097900	-3.53229300	-1.97106400
H	2.83618600	-3.21272600	-1.33786500
H	2.25324200	-4.53343500	-2.36277300
H	1.94908900	-2.85628500	-2.83499600
C	-0.89914200	-3.45761600	-3.28844900
H	-0.32008600	-2.64216800	-3.74579800
H	-0.61686300	-4.38584900	-3.81476100
H	-1.96062600	-3.27854100	-3.49940400
C	-3.05565400	-4.24341300	-1.00190600
H	-3.47121800	-3.67732700	-1.84538600
H	-3.20085100	-5.31483000	-1.22440500
H	-3.66488700	-4.01003000	-0.11880400
C	-1.44186400	-4.55400300	1.78390700
H	-2.53353600	-4.44581100	1.81465700
H	-1.21779900	-5.61966800	1.96246100

H	-1.02350300	-3.99329000	2.63251100
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Frequencies --	376.2357	379.8683	386.1299
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Frequencies --	1417.3758	1420.5600	1422.4285
Frequencies --	1424.3116	1425.3689	1425.5233
Frequencies --	1429.0125	1432.1326	1433.1957

Frequencies --	1435.1601	1450.4060	1453.1712
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Frequencies --	1503.4210	1504.8263	1508.6782
Frequencies --	1510.5623	1516.3141	1522.7374
Frequencies --	1588.9697	1591.4324	1592.2278
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Frequencies --	3137.1218	3137.4905	3142.1544
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Catalyst 15:**distal conformation**

vacuum	toluene-like solvent	D3 dispersion
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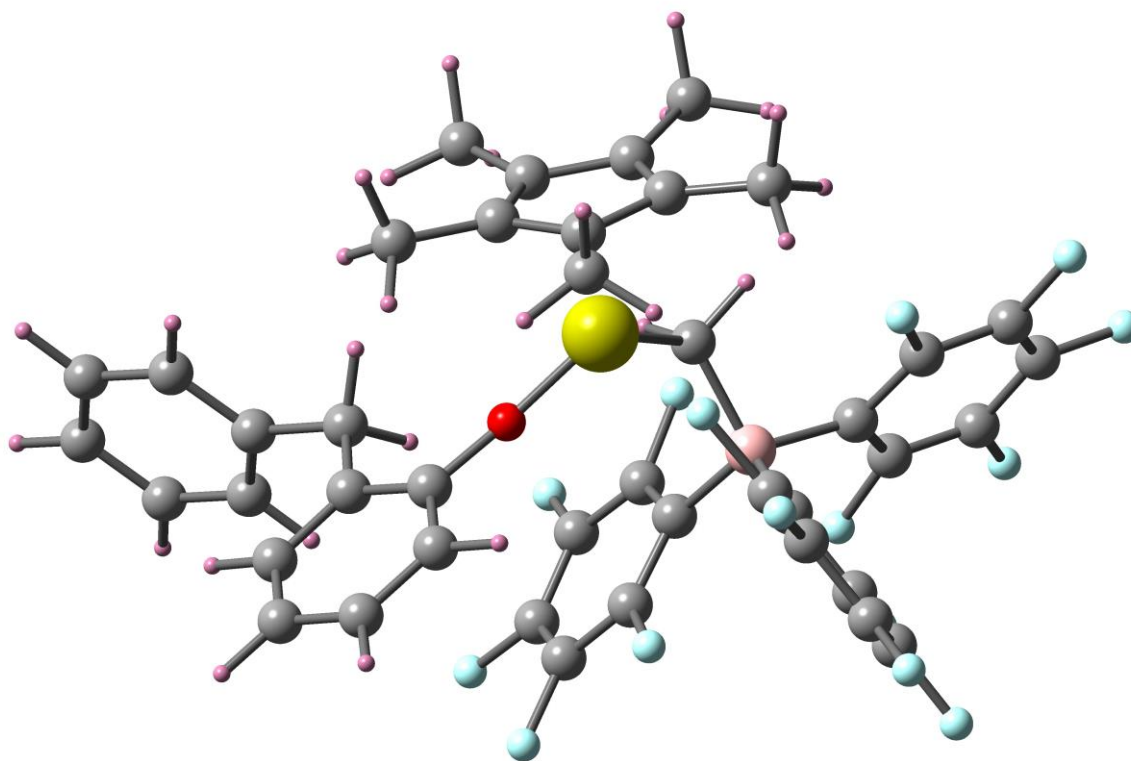
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C	-4.30731400	-0.85085400	0.32429000
C	-3.28782000	-2.42196900	1.95377900
C	-5.49773700	-0.91670100	1.08669900
C	-4.48564800	-2.46034100	2.69160600
C	-5.59485600	-1.70568300	2.25317100
H	-6.35878300	-0.33087600	0.76699300
H	-4.54639800	-3.06633000	3.59788300
H	-6.52895500	-1.72421400	2.81794000
C	-0.99788800	-3.20006400	-2.57172700
C	0.37490300	-2.78015500	-2.83414300
C	-0.98067300	-4.14316600	-1.47387200
C	1.21835600	-3.41479400	-1.86173500
C	0.38036100	-4.23707000	-1.00303200
F	0.29848900	-0.79934400	5.75742900
C	0.57183000	-0.45635400	4.44401700

C	0.94556400	0.85545900	4.10079400
C	0.49165300	-1.41538800	3.42242200
C	1.21179200	1.18798700	2.75638700
F	1.05668900	1.81243200	5.09797900
C	0.76240300	-0.99733400	2.11266400
F	0.14600100	-2.73307800	3.70632900
C	1.11189700	0.28090800	1.66922000
F	1.64257500	2.49831300	2.54960500
F	0.73400000	-2.09861100	1.15227700
B	1.41437500	0.67772100	0.06053300
C	1.01236900	2.29482600	-0.13902700
C	3.00873200	0.35603100	-0.33832700
C	0.42732400	-0.17247400	-1.05599800
C	1.89119500	3.35784900	-0.45739000
C	-0.32593200	2.72752100	0.02206300
C	4.00500200	-0.15733000	0.52491900
C	3.49890500	0.57931400	-1.65134300
H	-0.54393500	0.35232700	-1.14227700
H	0.92049300	-0.11582400	-2.02926000
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F	3.27359100	3.15393200	-0.53217700
C	-0.78236500	4.04392800	-0.16416400
F	-1.31060500	1.80923000	0.44446700
C	5.33795700	-0.42911400	0.14759800
F	3.72660300	-0.43833400	1.87292700
C	4.81366300	0.32819100	-2.08049300
F	2.65788400	1.13170700	-2.63205300
C	0.13355800	5.04267800	-0.53135200
F	2.41770500	5.66994000	-0.99700800
F	-2.12596700	4.36581300	0.02003700
C	5.75202400	-0.18484400	-1.16960000
F	6.24311100	-0.94007600	1.07176400
F	5.19520200	0.58675300	-3.39333200
F	-0.28651900	6.34925000	-0.73469600
F	7.05525900	-0.44721800	-1.56600000
C	2.72490200	-3.34778100	-1.78568700
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H	3.16137800	-4.26820500	-2.21081100
H	3.12984200	-2.50318900	-2.35309000
C	0.81570500	-1.97271000	-4.03220800
H	1.79756800	-1.50632700	-3.89070500
H	0.89090900	-2.63260200	-4.91413700
H	0.10390700	-1.17476800	-4.28569800
C	-2.18964800	-2.86825000	-3.44292000
H	-2.17090600	-1.82965000	-3.80299400
H	-2.19469200	-3.51768500	-4.33553800
H	-3.14178900	-3.02682200	-2.92021500
C	-2.15841800	-4.94464800	-0.96923700
H	-3.10720300	-4.39885500	-1.05148200
H	-2.25897700	-5.86808900	-1.56590200
H	-2.04091500	-5.24905000	0.07909600
C	0.88373200	-5.14420200	0.09782800
H	0.12108700	-5.34160600	0.86371900
H	1.17967500	-6.11986000	-0.32515100
H	1.76511700	-4.73166500	0.60662800
H	-2.41793300	-2.99174400	2.28088000
C	-4.18338000	-0.01106100	-0.95536900

H	-3.22165100	0.51809300	-0.91890100
H	-4.12018100	-0.70374900	-1.81170200
C	-5.29862000	0.99884100	-1.21779700
C	-6.40583500	0.67086000	-2.04024500
C	-5.23780100	2.30163100	-0.66023300
C	-7.42794000	1.61174200	-2.29534100
H	-6.46980500	-0.32493400	-2.48801800
C	-6.25670200	3.24541600	-0.91164000
H	-4.38904500	2.58305200	-0.03375800
C	-7.35709200	2.90382400	-1.72951400
H	-8.27071900	1.33908900	-2.93528900
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Frequencies --	6.3394	9.7501	18.1046
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proximal conformation

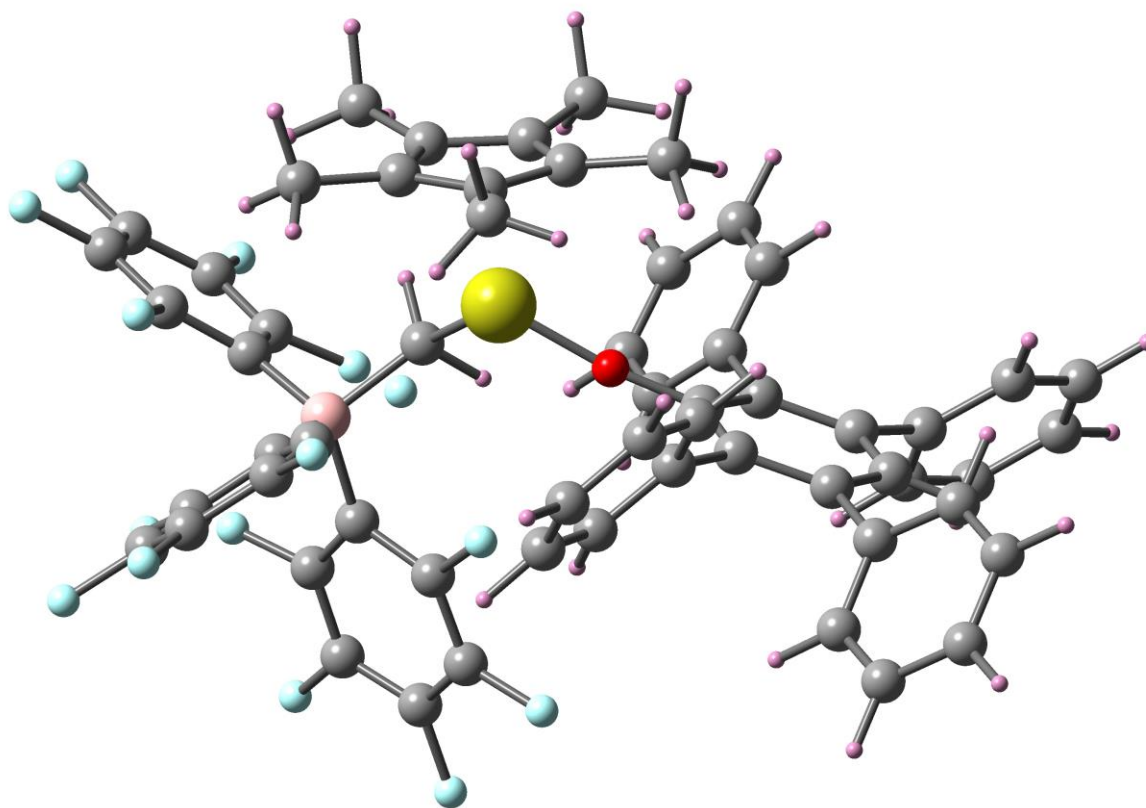
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C	-3.94942600	0.46001600	0.86539300
C	-3.64398400	1.80862900	3.37803100
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H	-3.51794200	2.31221500	4.33845900
H	-5.86879000	-0.14633800	1.65601700
H	-5.61751800	1.01617500	3.83598700
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C	-1.33734900	2.84635900	-2.70158100
C	0.65878000	3.80846200	-1.96705700
C	-1.66500100	3.77007400	-1.63197300
C	-0.42763500	4.33384200	-1.15291300
F	3.93514900	2.20106400	4.59068600
C	3.34212300	1.56586100	3.51239000
C	3.55447600	0.19371500	3.27582600
C	2.51012700	2.27550100	2.63403900
C	2.94444600	-0.42987000	2.17195700
F	4.35768800	-0.52953600	4.14435400
C	1.94141100	1.57365300	1.55817800
F	2.25984800	3.63037300	2.82838900

C	2.10202700	0.22724400	1.23543200
F	3.17808800	-1.79739400	2.04306700
F	1.08212200	2.42531800	0.74286700
B	1.47660000	-0.58511400	-0.10178100
C	2.85576900	-1.23943900	-0.81675700
C	0.33963800	-1.71284300	0.34649100
C	0.75153200	0.37999100	-1.30256600
C	3.20798800	-2.60830400	-0.90658400
C	3.83023700	-0.38721200	-1.39049000
C	-0.26368000	-1.83180600	1.61833400
C	-0.19063100	-2.62608400	-0.59947700
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C	5.00096900	-0.81399300	-2.04283300
F	3.67725900	1.01398700	-1.30188700
C	-1.25160400	-2.78169100	1.95198500
F	0.07620300	-0.95555900	2.66280300
C	-1.17198500	-3.59307400	-0.32216500
F	0.27728100	-2.60831900	-1.92323500
C	5.26704900	-2.18934400	-2.14023100
F	4.62453200	-4.45537100	-1.61214000
F	5.89245800	0.10854000	-2.58489900
C	-1.70773100	-3.67748600	0.97412300
F	-1.79406300	-2.82178200	3.23182800
F	-1.62700000	-4.45568700	-1.31440200
F	6.40780900	-2.64469500	-2.78572000
F	-2.69844000	-4.60668900	1.26924200
C	-3.05231800	4.15287900	-1.17073100
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H	-3.39918300	5.03597000	-1.73505500
H	-3.78630900	3.35390800	-1.33466600
C	-2.31809300	2.10630500	-3.58428500
H	-1.98282800	1.08760700	-3.82865900
H	-3.31533100	2.03288100	-3.13355400
H	-2.43370600	2.64219700	-4.54244800
C	0.81863500	2.27059600	-4.09788200
H	0.44343700	1.26402900	-4.32872600
H	0.67686100	2.88762400	-5.00223300
H	1.89945000	2.19336700	-3.92538700
C	2.10870200	4.22283200	-1.86841600
H	2.79412700	3.42241500	-2.17257800
H	2.29664100	5.08674000	-2.52985100
H	2.38570700	4.53049900	-0.85131500
C	-0.28608600	5.37619700	-0.06540400
H	0.63704100	5.25381800	0.51721500
H	-0.25427100	6.38483400	-0.51284900
H	-1.13003800	5.36218800	0.63785800
H	-1.69770000	2.41507600	2.62079300
C	-4.07317400	-0.27209600	-0.47924800
H	-3.88386700	0.45343600	-1.28489100
H	-3.25284800	-1.00352800	-0.54467500
C	-5.39904000	-0.97984100	-0.75334000
C	-6.48464000	-0.28482900	-1.34476300
C	-5.57273200	-2.35200800	-0.44231300
C	-7.70663700	-0.93683900	-1.61730300

H	-6.37602800	0.77429400	-1.59475500
C	-6.79256900	-3.00992700	-0.71267500
H	-4.75515800	-2.91470000	0.01219900
C	-7.86490100	-2.30477800	-1.30182600
H	-8.52808200	-0.38217000	-2.07729100
H	-6.90041800	-4.06919000	-0.46833600
H	-8.80744000	-2.81394500	-1.51588700
Frequencies --	7.3524	16.1502	18.8992
Frequencies --	21.3904	24.8681	27.5335
Frequencies --	30.2301	32.4191	35.0965
Frequencies --	38.2851	39.9751	42.0113
Frequencies --	47.0189	55.0010	61.3214
Frequencies --	79.0111	80.5043	92.6994
Frequencies --	93.2040	97.3219	108.5743
Frequencies --	109.8427	111.1820	113.9712
Frequencies --	119.4068	122.3838	124.5747
Frequencies --	130.1022	134.0534	137.6745
Frequencies --	140.5141	143.6600	148.4670
Frequencies --	158.1282	159.1095	160.9272
Frequencies --	162.5733	164.3779	169.2087
Frequencies --	169.9373	183.6595	200.7842
Frequencies --	209.7109	214.3562	220.9814
Frequencies --	224.2645	226.6717	242.8182
Frequencies --	247.0763	263.6775	264.7828
Frequencies --	265.1652	275.0201	277.1343
Frequencies --	278.9487	284.3330	290.2968
Frequencies --	300.0961	301.9023	305.5598
Frequencies --	306.3514	310.7089	314.3651
Frequencies --	317.6835	322.4650	330.8636
Frequencies --	333.8949	340.5131	354.0689
Frequencies --	363.1647	370.4844	375.5340
Frequencies --	377.0651	379.6134	389.5086
Frequencies --	395.5025	404.7633	406.1818
Frequencies --	413.2591	430.8818	432.2602
Frequencies --	441.0955	443.6990	452.2494
Frequencies --	458.6100	462.4268	467.0925
Frequencies --	478.1046	500.5923	534.0648
Frequencies --	536.2119	537.3995	541.1295
Frequencies --	543.6756	547.6063	556.1320
Frequencies --	563.1750	572.1916	580.3765
Frequencies --	588.0391	599.4982	603.2968
Frequencies --	610.3805	619.7181	623.8776
Frequencies --	624.1497	633.8593	635.5624
Frequencies --	640.8022	653.3780	663.0794
Frequencies --	672.8392	703.7181	704.9563
Frequencies --	710.6361	717.0159	729.3391
Frequencies --	734.8701	744.1636	745.7448
Frequencies --	747.2545	764.5592	765.7852
Frequencies --	800.8335	804.2860	806.3881
Frequencies --	821.5562	831.1985	840.1618
Frequencies --	860.3024	861.6769	863.5100
Frequencies --	873.6571	905.9196	911.5160
Frequencies --	926.7452	929.8059	935.8485
Frequencies --	962.9401	967.9001	969.9529
Frequencies --	972.4735	986.9596	997.1657
Frequencies --	1004.1187	1006.5852	1021.8782
Frequencies --	1022.3474	1028.2302	1039.5144
Frequencies --	1043.1699	1044.7211	1045.5351
Frequencies --	1048.2114	1049.3685	1050.8507
Frequencies --	1052.4807	1053.4182	1055.9564
Frequencies --	1082.4012	1086.6670	1090.1174

Frequencies --	1093.7372	1105.6181	1125.4791
Frequencies --	1173.0843	1174.7711	1179.8629
Frequencies --	1182.6203	1191.2586	1199.1886
Frequencies --	1202.4935	1203.8963	1209.3608
Frequencies --	1213.0877	1219.1520	1239.5158
Frequencies --	1286.4066	1295.6182	1314.4449
Frequencies --	1316.8765	1320.6587	1338.3842
Frequencies --	1344.8625	1349.7031	1349.8246
Frequencies --	1374.6413	1379.5450	1383.7603
Frequencies --	1409.3869	1412.1840	1414.9290
Frequencies --	1416.3948	1421.2612	1424.3728
Frequencies --	1426.3382	1428.9304	1430.8142
Frequencies --	1435.4622	1444.9797	1447.6744
Frequencies --	1453.0480	1454.7535	1464.1965
Frequencies --	1466.4729	1467.6263	1471.4527
Frequencies --	1478.6158	1481.3309	1490.0257
Frequencies --	1491.8393	1495.2429	1497.4464
Frequencies --	1500.0263	1501.6723	1504.1357
Frequencies --	1505.5330	1510.0981	1517.2623
Frequencies --	1523.0202	1588.7633	1591.0002
Frequencies --	1593.6337	1597.3216	1604.6501
Frequencies --	1614.9680	1616.8821	1619.8632
Frequencies --	1627.2543	1630.4816	3005.1164
Frequencies --	3009.8767	3010.3131	3011.8960
Frequencies --	3012.1877	3013.4042	3041.9940
Frequencies --	3090.8619	3095.0228	3100.4224
Frequencies --	3101.3836	3105.0565	3107.5367
Frequencies --	3137.2595	3142.2229	3144.3321
Frequencies --	3144.9830	3149.5082	3152.4711
Frequencies --	3154.1263	3158.3706	3167.4943
Frequencies --	3170.2169	3181.7160	3182.4396
Frequencies --	3195.3763	3196.5885	3208.4580

Catalyst 16:

vacuum	toluene-like solvent	D3 dispersion
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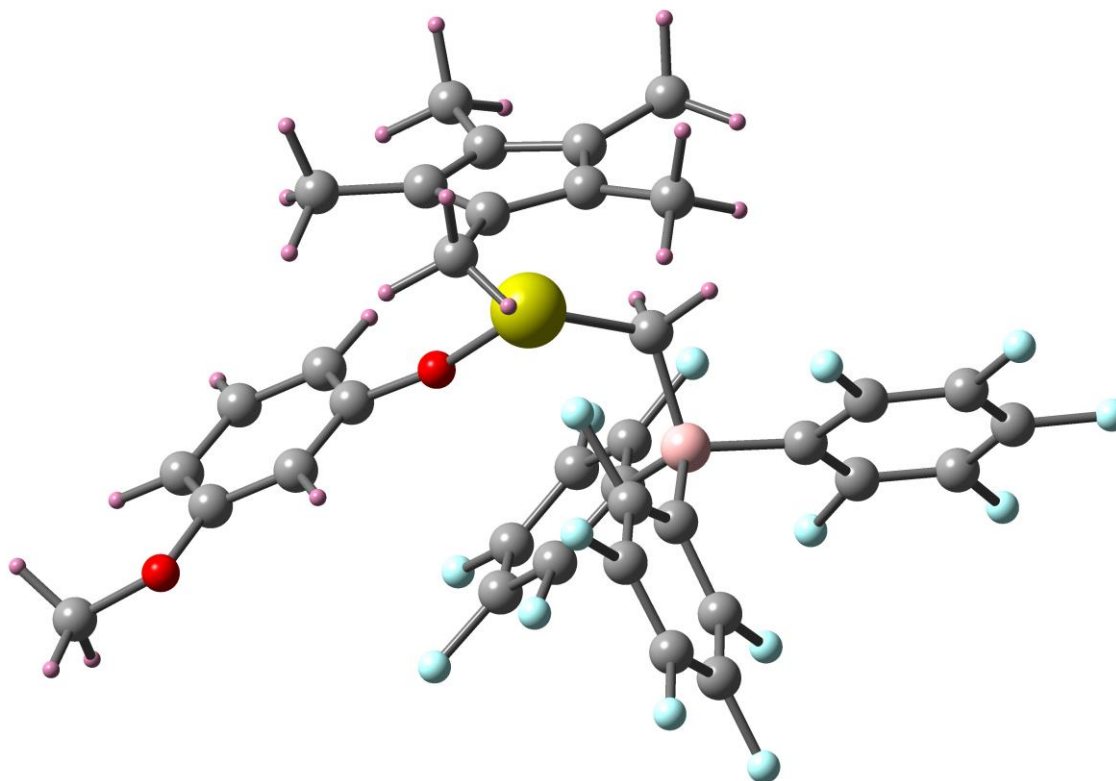
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C	-3.26958200	1.54166900	-0.35186000
C	-3.68446200	-0.91851400	-0.05113100
C	-4.62562900	1.79717700	0.01832100
C	-5.03278900	-0.63068600	0.31933800
C	-5.47494000	0.71044000	0.31988400
H	-6.49498400	0.92099600	0.63792900
C	-0.00469000	0.32475400	-3.84589400
C	1.35758400	-0.15748700	-3.70224800
C	-0.89776400	-0.81694800	-3.79890100
C	1.30242500	-1.57912000	-3.51703200
C	-0.08984500	-1.98926400	-3.56470700
F	0.95059900	1.88886200	5.90355500
C	1.36690500	1.49859800	4.63861500
C	2.64474800	1.83814100	4.16498600
C	0.52321200	0.74370600	3.80818200
C	3.05057000	1.43342600	2.87507200
F	3.50427300	2.56572800	4.97962700
C	0.97870400	0.37031000	2.53100800
F	-0.74223400	0.36655300	4.25300300
C	2.23444500	0.70392200	1.97487200

F	4.35650400	1.79434700	2.53950400
F	0.08369400	-0.42596500	1.78852800
B	2.63666200	0.15900600	0.43236000
C	4.01595700	0.86445300	-0.17941000
C	2.83778600	-1.48743100	0.70755700
C	1.43929400	0.62293900	-0.68965200
C	5.08123300	0.20110900	-0.82457200
C	4.14339500	2.27571400	-0.22175600
C	2.02575700	-2.52050800	0.23791000
C	3.87125700	-1.97646900	1.55085000
H	0.70769500	1.25973800	-0.16282400
H	1.92579900	1.25689700	-1.43947700
C	6.19917400	0.84270300	-1.39757900
F	5.06908200	-1.19971500	-0.97339800
C	5.23464500	2.96787500	-0.77419900
F	3.12229000	3.07993600	0.30669700
C	2.18667900	-3.89817100	0.47205000
F	0.87139600	-2.23372200	-0.59067100
C	4.08917700	-3.33303300	1.84989500
F	4.76750400	-1.07705700	2.12552300
C	6.28567300	2.24267500	-1.36336900
F	7.20547700	0.10107200	-2.01007600
F	5.28366500	4.35804900	-0.75096200
C	3.24177100	-4.31242900	1.29804900
F	1.33701000	-4.83705800	-0.10402200
F	5.13633400	-3.72114800	2.67260700
F	7.37441800	2.90029500	-1.91967900
F	3.44237600	-5.65795800	1.56319200
C	2.48626300	-2.51371400	-3.43544700
H	2.23751700	-3.45730800	-2.93323200
H	2.82207300	-2.77332800	-4.45504400
H	3.34449600	-2.06767600	-2.91837100
C	2.59865300	0.66449200	-3.94585100
H	3.48427800	0.23498500	-3.46505200
H	2.80334500	0.70725300	-5.03022400
H	2.49155200	1.70206100	-3.60181900
C	-0.37429000	1.73932200	-4.22659400
H	0.14085600	2.49232100	-3.61519500
H	-0.08876900	1.92201100	-5.27750900
H	-1.44952800	1.92627300	-4.14042000
C	-2.38352400	-0.79767700	-4.07259600
H	-2.84337700	0.16189500	-3.80436100
H	-2.56433000	-0.96037600	-5.14962300
H	-2.91689500	-1.58554900	-3.52728500
C	-0.57359500	-3.42020500	-3.51459700
H	-1.64920600	-3.48885100	-3.32072900
H	-0.37985100	-3.91150800	-4.48433600
H	-0.06125200	-4.01371800	-2.74505600
C	-5.20847800	3.17957400	0.16049100
C	-6.33767100	3.55796800	-0.61173700
C	-4.71263800	4.10106500	1.11881400
C	-6.94253900	4.82218000	-0.44622900
H	-6.73967300	2.86254300	-1.35220400
C	-5.31965800	5.36213700	1.29225000
H	-3.85920900	3.82774600	1.74027400
C	-6.43507500	5.73099700	0.50798700
H	-7.80609100	5.09423600	-1.05804300

H	-4.92403900	6.05233900	2.04110100
H	-6.90351100	6.70885200	0.64167400
C	-6.02098700	-1.67756600	0.76463700
C	-7.24136800	-1.85156300	0.06116900
C	-5.80598600	-2.44957500	1.93560300
C	-8.20956000	-2.77922900	0.50153800
H	-7.43014100	-1.26431400	-0.84047900
C	-6.77473300	-3.37175200	2.38263300
H	-4.88665000	-2.31918500	2.50736300
C	-7.97952400	-3.54452200	1.66581600
H	-9.13833900	-2.90157300	-0.06099000
H	-6.58996000	-3.95009900	3.29096200
H	-8.72881300	-4.26034800	2.01177300
C	-2.36592800	2.69571000	-0.69529000
C	-2.64989700	3.51995500	-1.81504400
C	-1.27663200	3.05404100	0.13859900
C	-1.87201200	4.66225000	-2.09437900
H	-3.49691700	3.27771200	-2.45942100
C	-0.49306800	4.19497700	-0.13776700
H	-1.06165800	2.45515800	1.02413200
C	-0.78815600	5.00485400	-1.25620700
H	-2.11721900	5.28705700	-2.95665200
H	0.34160900	4.45040700	0.51806700
H	-0.18652800	5.89232100	-1.46485300
C	-3.20899100	-2.34656200	-0.06656200
C	-3.77866900	-3.28505800	-0.96579500
C	-2.27243300	-2.81588800	0.88967600
C	-3.43189900	-4.65076900	-0.90856500
H	-4.51935600	-2.94934300	-1.69400500
C	-1.92992800	-4.18288000	0.95375100
H	-1.83591800	-2.11721800	1.60293100
C	-2.50714800	-5.10682000	0.05598800
H	-3.89349900	-5.35654700	-1.60340800
H	-1.22112400	-4.52695000	1.70989800
H	-2.24383800	-6.16530200	0.11149100
Frequencies --	9.1397	10.8600	12.4526
Frequencies --	14.5052	22.5803	24.3599
Frequencies --	27.7256	30.9721	33.1073
Frequencies --	35.0528	35.1253	40.8610
Frequencies --	41.6378	45.5779	46.4881
Frequencies --	49.2014	52.1502	55.1263
Frequencies --	60.2748	62.5339	67.4179
Frequencies --	74.2099	78.5076	82.0508
Frequencies --	88.7880	100.5651	103.7096
Frequencies --	105.9757	108.4950	116.9690
Frequencies --	117.2164	118.5292	123.1808
Frequencies --	126.3468	130.2433	135.6318
Frequencies --	139.2122	141.2510	142.9805
Frequencies --	144.9576	147.5208	148.1891
Frequencies --	157.8745	159.7905	162.9378
Frequencies --	165.8802	166.2015	175.1166
Frequencies --	178.0280	192.6878	197.3681
Frequencies --	205.6711	211.0019	213.2066
Frequencies --	214.0123	217.4704	224.2932
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Frequencies --	257.1336	261.7482	263.7460
Frequencies --	264.1076	265.0147	273.5221
Frequencies --	274.4272	279.0425	280.8496

Frequencies --	290.5035	292.2766	299.5684
Frequencies --	300.4950	302.1368	303.1501
Frequencies --	304.3896	321.7096	324.6507
Frequencies --	325.9310	329.3108	333.6399
Frequencies --	344.7526	354.7026	360.4205
Frequencies --	374.9921	376.8848	379.4022
Frequencies --	381.3726	388.8007	394.3280
Frequencies --	397.5068	403.7166	405.1433
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Frequencies --	516.6368	518.0190	529.2300
Frequencies --	531.2095	536.2813	541.1232
Frequencies --	542.9440	544.7496	546.2184
Frequencies --	551.3854	555.8085	557.7839
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Frequencies --	615.8989	617.8055	620.2346
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Frequencies --	725.0253	734.0863	735.8888
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Frequencies --	783.4415	796.3764	803.3270
Frequencies --	804.0573	806.2309	826.7992
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Frequencies --	861.4685	861.9985	866.5286
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Frequencies --	912.6003	914.6477	933.9923
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Frequencies --	959.2118	968.2924	973.9139
Frequencies --	984.8138	985.5240	988.1831
Frequencies --	991.9083	995.2004	995.5837
Frequencies --	1001.5527	1005.1647	1006.4903
Frequencies --	1007.7547	1011.2988	1014.8074
Frequencies --	1019.9848	1020.4585	1024.2855
Frequencies --	1027.7874	1038.6450	1041.0034
Frequencies --	1041.9049	1043.8693	1047.0385
Frequencies --	1047.7853	1049.1669	1050.8123
Frequencies --	1051.1446	1051.4826	1051.9963
Frequencies --	1053.2854	1053.9096	1070.6059
Frequencies --	1089.2534	1089.3408	1090.6678
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Frequencies --	1126.8164	1128.5507	1128.7976
Frequencies --	1175.0422	1177.3694	1182.7443
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Frequencies --	1202.3703	1204.0375	1205.4649
Frequencies --	1207.2474	1208.4261	1210.4906
Frequencies --	1212.7478	1228.9789	1261.7021
Frequencies --	1281.2176	1296.6324	1303.4772
Frequencies --	1318.8850	1320.1119	1321.1775
Frequencies --	1327.9705	1332.1263	1332.2272
Frequencies --	1334.9368	1338.9956	1346.2615
Frequencies --	1350.7999	1366.8777	1368.5489
Frequencies --	1369.9901	1370.7427	1378.7098
Frequencies --	1394.3697	1409.2065	1411.5487
Frequencies --	1416.4487	1416.7217	1420.6492
Frequencies --	1425.8507	1427.0755	1429.5807

Frequencies --	1433.1501	1436.0640	1440.5065
Frequencies --	1443.2173	1446.0102	1447.5447
Frequencies --	1451.1339	1455.3319	1455.7192
Frequencies --	1466.6106	1466.9292	1467.4602
Frequencies --	1470.5226	1480.9261	1492.4177
Frequencies --	1494.4555	1496.8699	1497.2939
Frequencies --	1498.7240	1501.4545	1502.3198
Frequencies --	1503.7052	1507.7112	1508.4956
Frequencies --	1512.1832	1519.7105	1525.1678
Frequencies --	1526.7906	1588.6229	1591.8281
Frequencies --	1593.8436	1594.7240	1595.7218
Frequencies --	1596.0113	1597.2037	1599.2497
Frequencies --	1617.0273	1619.2601	1623.0038
Frequencies --	1623.6505	1623.9954	1624.3775
Frequencies --	1626.8356	3010.9479	3011.3391
Frequencies --	3011.8050	3012.1613	3013.2756
Frequencies --	3029.4715	3102.8353	3105.8061
Frequencies --	3107.0687	3108.9194	3110.1437
Frequencies --	3135.1206	3151.2357	3151.7884
Frequencies --	3151.8702	3154.5964	3154.8572
Frequencies --	3156.3306	3159.4782	3159.9304
Frequencies --	3161.9159	3165.4338	3166.2528
Frequencies --	3166.5963	3168.3219	3171.9151
Frequencies --	3172.2732	3178.1223	3179.3610
Frequencies --	3185.3240	3185.3953	3186.8110
Frequencies --	3190.4507	3194.2843	3197.4554
Frequencies --	3197.8623	3201.3233	3208.8431

Catalyst 17:**distal conformation**

vacuum	toluene-like solvent	D3 dispersion
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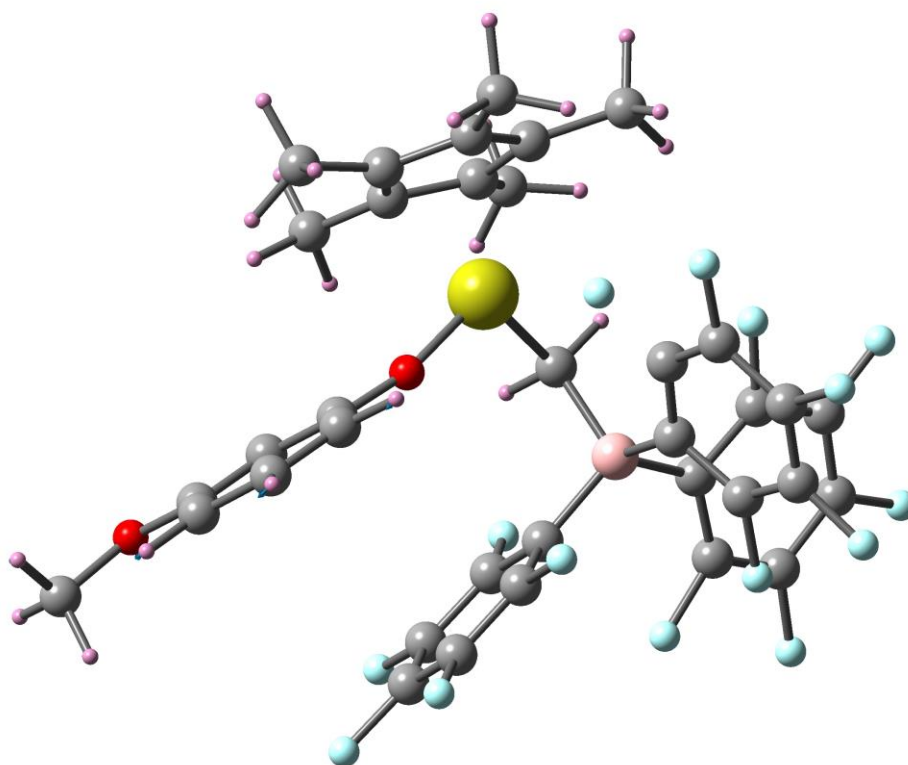
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C	-4.14823900	-0.27873600	0.77165700
C	-3.87967300	-1.00566600	-1.56593600
C	-5.30765800	-1.08317400	0.88551600
C	-5.03404300	-1.79857300	-1.43362100
C	-5.75718200	-1.84743200	-0.22125900
H	-5.37314500	-2.39729300	-2.28156100
H	-6.64058000	-2.47871900	-0.15144200
C	-0.42587000	3.39415600	-2.44435400
C	-1.80581900	2.96413000	-2.62426400
C	-0.34781900	4.09814200	-1.19235200
C	-2.58428600	3.45888500	-1.50678800
C	-1.67735500	4.12594800	-0.60428400
F	1.33572900	1.18232400	5.66132800
C	1.28312100	0.82894200	4.32322700
C	1.94619200	-0.32163600	3.85372600
C	0.56203100	1.60789100	3.40604200
C	1.88329000	-0.65951900	2.48950900

F	2.64663600	-1.11564000	4.74932900
C	0.55207400	1.19651900	2.06289400
F	-0.11763400	2.74843600	3.82018600
C	1.18570600	0.08770500	1.50329100
F	2.53168700	-1.83801500	2.12550300
F	-0.25421700	2.07986100	1.22500700
B	1.23180300	-0.34857800	-0.12351900
C	2.88409300	-0.46419200	-0.43458600
C	0.37744900	-1.74724900	-0.41033100
C	0.64989200	0.81203100	-1.22044900
C	3.61707900	-1.63672300	-0.74058300
C	3.70193600	0.69068200	-0.37508200
C	-0.49840200	-2.38970100	0.49292600
C	0.40064500	-2.37027200	-1.68365100
H	1.42857400	1.54656600	-1.45318600
H	0.40688100	0.28966200	-2.16369100
C	4.99814300	-1.65897300	-1.02704800
F	3.00362900	-2.89123200	-0.73421900
C	5.08223900	0.72332000	-0.64405200
F	3.14425000	1.92932800	0.01181100
C	-1.24490800	-3.54942100	0.20079500
F	-0.71437500	-1.87078200	1.78141500
C	-0.32274200	-3.52487300	-2.02939600
F	1.20091300	-1.83702100	-2.70806300
C	5.74074500	-0.46800000	-0.98906100
F	5.63800500	-2.85512700	-1.33130800
F	5.79607600	1.91677100	-0.56702500
C	-1.15459000	-4.12965700	-1.07228000
F	-2.09121400	-4.10600600	1.15477400
F	-0.22879400	-4.07097600	-3.30642300
F	7.09999800	-0.46914100	-1.26903400
F	-1.89102900	-5.26355300	-1.38976800
C	-4.08474500	3.36479700	-1.35542100
H	-4.40008900	3.30957600	-0.30446600
H	-4.55880900	4.26183800	-1.79069200
H	-4.50379100	2.49203300	-1.87171000
C	-2.35349100	2.29410800	-3.86525500
H	-3.26109900	1.70889900	-3.66635800
H	-2.61889400	3.05823800	-4.61681500
H	-1.61625500	1.62729500	-4.33408500
C	0.66973400	3.27925200	-3.47671200
H	0.64717800	2.32082200	-4.01314200
H	0.55687900	4.07907900	-4.22910100
H	1.66821100	3.38855600	-3.03492100
C	0.88044000	4.76560300	-0.61801600
H	1.80571000	4.23398900	-0.87318400
H	0.97041200	5.79174600	-1.01557000
H	0.83614100	4.84697300	0.47618600
C	-2.05666100	4.82597700	0.68200100
H	-1.27346000	4.75088100	1.44841400
H	-2.22103900	5.90062100	0.49102300
H	-2.98510200	4.42897100	1.11490000
H	-3.80186600	0.28347200	1.63699100
H	-3.31035600	-0.98579400	-2.49429500
O	-5.92446900	-1.03828800	2.13941100
C	-7.08284800	-1.90201100	2.39325500
H	-6.82304600	-2.96614700	2.26776200

H	-7.35244500	-1.70851200	3.43839300
H	-7.93078700	-1.64140800	1.73744500
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Frequencies --	22.0786	25.5672	27.1981
Frequencies --	33.1216	33.6404	38.4951
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Frequencies --	69.5707	77.2198	79.6292
Frequencies --	81.9662	95.0135	101.5583
Frequencies --	105.6778	108.8369	110.8936
Frequencies --	112.9294	116.9480	120.3988
Frequencies --	123.0570	126.8115	133.6748
Frequencies --	138.3348	143.7660	145.8084
Frequencies --	148.9505	157.8099	159.2279
Frequencies --	161.0387	162.6665	165.8279
Frequencies --	169.1143	170.7709	194.5256
Frequencies --	199.6767	214.5158	219.0774
Frequencies --	220.8943	224.1336	234.3853
Frequencies --	246.3630	255.9129	263.6918
Frequencies --	264.4184	264.5632	274.9026
Frequencies --	277.5100	278.1691	285.0632
Frequencies --	291.9876	297.8578	302.1157
Frequencies --	305.5225	305.8685	308.6042
Frequencies --	313.0723	321.8644	326.5957
Frequencies --	331.9201	339.2720	357.8785
Frequencies --	363.6350	371.8991	376.1594
Frequencies --	377.4445	380.0396	384.5628
Frequencies --	391.5540	398.9197	404.9901
Frequencies --	417.0429	431.3155	432.4105
Frequencies --	443.5177	449.3200	454.0714
Frequencies --	458.8330	467.2698	474.1130
Frequencies --	492.6880	534.1370	537.1223
Frequencies --	539.4440	541.3820	547.2683
Frequencies --	556.3619	559.2343	565.9929
Frequencies --	580.3519	588.2335	600.6585
Frequencies --	603.1896	606.2257	610.6986
Frequencies --	624.2735	634.3152	636.0871
Frequencies --	641.2845	652.2364	658.8767
Frequencies --	672.0066	677.0636	704.4524
Frequencies --	716.8389	729.7027	735.6978
Frequencies --	746.0130	747.3550	761.1266
Frequencies --	765.9888	782.2631	800.4661
Frequencies --	804.3285	823.4737	829.8306
Frequencies --	843.4807	865.2554	867.2158
Frequencies --	873.3760	906.6253	911.4931
Frequencies --	949.4367	962.9119	969.0020
Frequencies --	970.8704	973.1765	987.4613
Frequencies --	1005.2827	1021.9207	1024.3672
Frequencies --	1030.4193	1041.8046	1043.0944
Frequencies --	1044.0011	1045.8441	1047.4334
Frequencies --	1048.3598	1049.7815	1055.3310
Frequencies --	1086.7263	1087.4343	1092.7626
Frequencies --	1097.5579	1125.1964	1126.2829
Frequencies --	1163.4539	1173.1107	1173.8257
Frequencies --	1174.1039	1200.0675	1202.7615
Frequencies --	1208.7571	1212.7777	1273.6541
Frequencies --	1295.3948	1300.1855	1313.6512
Frequencies --	1321.6029	1338.0572	1344.5193
Frequencies --	1349.1723	1385.4465	1386.2446
Frequencies --	1409.9929	1412.3899	1414.0257
Frequencies --	1416.9555	1421.4426	1424.6861
Frequencies --	1426.9664	1427.3266	1429.5609

Frequencies --	1435.0203	1445.9766	1448.3367
Frequencies --	1451.4324	1455.5615	1462.4415
Frequencies --	1466.1873	1469.6515	1471.5551
Frequencies --	1480.1730	1483.4486	1485.0900
Frequencies --	1488.1619	1489.8052	1491.7691
Frequencies --	1496.3313	1498.2899	1504.9031
Frequencies --	1505.1820	1509.4928	1514.4820
Frequencies --	1520.1422	1590.4696	1590.7055
Frequencies --	1593.4021	1598.0067	1616.3168
Frequencies --	1619.1800	1621.7487	1630.5262
Frequencies --	2997.1284	3008.7847	3009.9846
Frequencies --	3010.8062	3011.6798	3012.9362
Frequencies --	3022.9305	3097.5540	3098.2973
Frequencies --	3100.6175	3102.4523	3103.0080
Frequencies --	3105.6609	3136.4101	3138.5271
Frequencies --	3142.3366	3144.3701	3146.3657
Frequencies --	3149.2592	3160.9564	3174.6660
Frequencies --	3209.8814	3216.4430	3220.9922

proximal conformation



vacuum	toluene-like solvent	D3 dispersion
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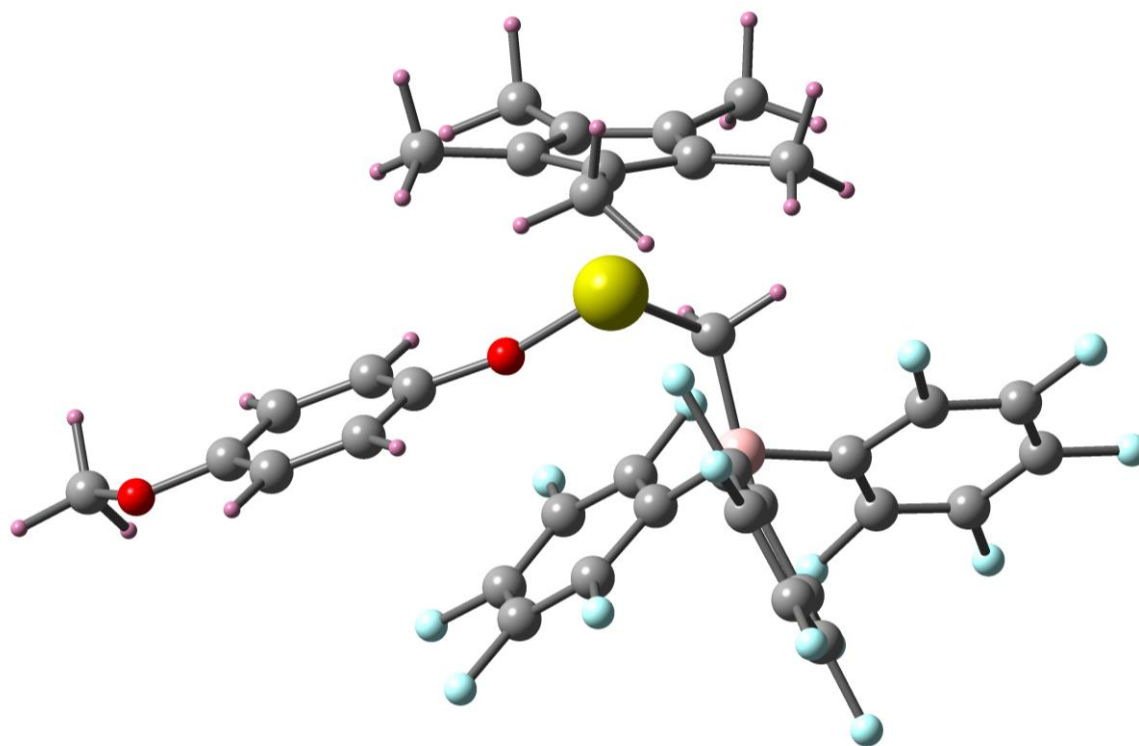
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C	-3.42798600	0.27808900	0.46191400
C	-3.83020100	0.45538800	1.80978300
C	-4.18388000	-0.50794800	-0.42876900

C	-5.00577900	-0.18008500	2.24898600
C	-5.36445100	-1.13904200	0.03195200
C	-5.78201700	-0.97559500	1.37711200
H	-5.32056900	-0.06462400	3.28813400
H	-6.68117200	-1.45944200	1.75295800
C	-0.47954600	3.16908100	-2.62603200
C	-1.90588800	2.90524300	-2.49948300
C	-0.09249800	4.01408900	-1.52821000
C	-2.40412100	3.64247700	-1.35584300
C	-1.27760200	4.29558000	-0.73372400
F	2.78296100	1.87529400	5.16053100
C	2.38138100	1.34305500	3.94645300
C	2.79496300	0.05651600	3.54939500
C	1.54671300	2.07339400	3.08754200
C	2.37730700	-0.46311500	2.31048400
F	3.60332400	-0.68865500	4.39464900
C	1.17854000	1.47842300	1.86933500
F	1.10250300	3.34436100	3.43719800
C	1.54601800	0.22317700	1.38541200
F	2.79892700	-1.76005000	2.02464100
F	0.29096100	2.33651200	1.08829300
B	1.15620300	-0.44290800	-0.11150200
C	2.65325800	-0.88561300	-0.74564100
C	0.07874600	-1.70430100	0.03156900
C	0.50720600	0.64601700	-1.24082700
C	3.11085600	-2.19873000	-1.01408200
C	3.61907800	0.10311400	-1.05585900
C	-0.60860000	-2.08958400	1.20399000
C	-0.30672500	-2.46753200	-1.09956900
H	1.30605300	1.23732900	-1.70133100
H	0.03805100	0.05219800	-2.04548900
C	4.36048900	-2.50280900	-1.59309700
F	2.34216600	-3.31328500	-0.66984200
C	4.88045500	-0.14527200	-1.62679700
F	3.35919600	1.46005700	-0.76112900
C	-1.54938200	-3.13728300	1.27672700
F	-0.41384700	-1.40218700	2.41522100
C	-1.23891600	-3.51939000	-1.08522600
F	0.27225100	-2.20198900	-2.35264000
C	5.25398400	-1.46824000	-1.91356900
F	4.72532500	-3.82230400	-1.83531400
F	5.75642600	0.90127800	-1.90468700
C	-1.86933600	-3.86454700	0.12167400
F	-2.18418300	-3.43702300	2.47843500
F	-1.54693800	-4.21570100	-2.24994200
F	6.48727100	-1.74684500	-2.48583200
F	-2.80818900	-4.88707400	0.16407600
C	-3.85204000	3.77192300	-0.94351100
H	-3.96893900	3.95776100	0.13290200
H	-4.31336700	4.62412700	-1.47240200
H	-4.44021400	2.87875900	-1.18942100
C	-2.74061900	2.14903600	-3.50960100
H	-2.22442800	1.25844700	-3.89613800
H	-3.70510300	1.82634500	-3.09762800
H	-2.95693900	2.79653400	-4.37708800
C	0.38043300	2.77444900	-3.80220500
H	0.12722200	1.77987200	-4.19371900

H	0.23806500	3.49677000	-4.62479200
H	1.44950700	2.77221700	-3.55458300
C	1.28705300	4.57922900	-1.28059500
H	2.08265100	3.91029900	-1.63255800
H	1.40244100	5.53756000	-1.81663500
H	1.46952100	4.78177000	-0.21663400
C	-1.33251800	5.20033300	0.47779900
H	-0.42254400	5.14008600	1.08994800
H	-1.43876300	6.25155600	0.15849500
H	-2.18753800	4.97210300	1.12901300
H	-3.22062500	1.04937000	2.48979900
H	-3.86025800	-0.66543100	-1.45588300
O	-6.03046700	-1.89858800	-0.93469900
C	-7.18964300	-2.70342800	-0.53275200
H	-7.48982700	-3.23588600	-1.44308900
H	-6.91745400	-3.43051700	0.24997800
H	-8.02070800	-2.06701000	-0.18450200

Frequencies --	8.1723	14.7664	18.1089
Frequencies --	24.0198	27.2928	30.9379
Frequencies --	33.9997	34.7291	38.5840
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Frequencies --	106.1843	110.4078	114.5650
Frequencies --	117.2703	119.3055	124.4521
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Frequencies --	265.0155	265.3687	275.9616
Frequencies --	278.2910	279.1494	283.1268
Frequencies --	289.4655	299.0075	301.9583
Frequencies --	303.7316	304.7175	306.8571
Frequencies --	315.2645	320.8945	325.1028
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Frequencies --	365.2963	374.9632	377.2584
Frequencies --	380.0670	381.2256	387.8708
Frequencies --	393.2726	399.1147	409.3034
Frequencies --	420.1207	431.4328	432.3304
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Frequencies --	458.8828	467.6277	473.7136
Frequencies --	498.6306	535.0001	536.6062
Frequencies --	539.3538	542.3009	547.4569
Frequencies --	555.8550	557.5333	568.3449
Frequencies --	580.0116	588.8056	601.3271
Frequencies --	602.9349	606.5150	612.9963
Frequencies --	624.3371	635.0881	636.7377
Frequencies --	641.5141	652.9208	660.1558
Frequencies --	673.6364	677.3644	705.4357
Frequencies --	717.1224	729.9084	736.1409
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Frequencies --	970.5400	982.5925	987.5165
Frequencies --	1008.2864	1022.1796	1024.2070
Frequencies --	1032.4390	1040.8387	1043.3493
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Frequencies --	1505.0133	1509.5163	1514.5050
Frequencies --	1521.1511	1590.2870	1590.5429
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Frequencies --	1619.7040	1621.6168	1629.8796
Frequencies --	2998.1033	3009.8548	3010.3357
Frequencies --	3011.1902	3011.6607	3012.9689
Frequencies --	3026.9189	3098.2647	3099.0199
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Frequencies --	3206.2710	3217.8304	3221.2674

Catalyst 18:

vacuum	toluene-like solvent	D3 dispersion
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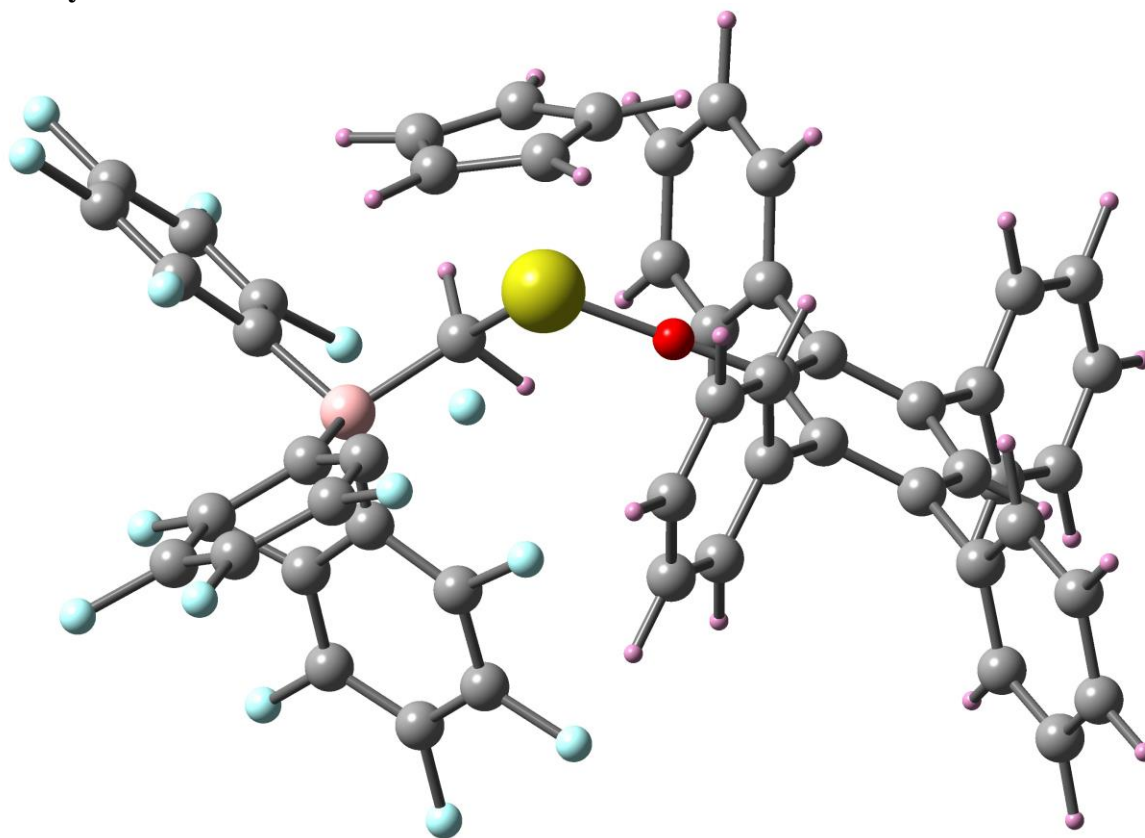
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C	-4.08319700	0.44614800	1.30458400
C	-4.04267700	-0.61598300	-0.90492200
C	-5.30548700	-0.18205600	1.58128500
C	-5.27169800	-1.24785600	-0.62934900
C	-5.91028600	-1.03293800	0.61836600
H	-5.80394400	-0.03989200	2.53981500
H	-5.70441000	-1.90487000	-1.38177700
C	0.04724900	4.08486400	-1.33513100
C	-0.24749200	3.31451600	-2.51377300
C	-1.19932500	4.32065100	-0.62497400
C	-1.67878800	3.04974300	-2.52256800
C	-2.27002300	3.71385200	-1.37883600
F	2.43836800	1.58985100	5.38953700
C	2.12927200	1.12200600	4.12307800
C	2.60497000	-0.12660000	3.67802800
C	1.32749200	1.88041800	3.25720700
C	2.28153500	-0.58059300	2.38606900
F	3.38060400	-0.90077600	4.52784700
C	1.05493200	1.35186800	1.98459000
F	0.82229500	3.11468300	3.65252700
C	1.49126600	0.13937400	1.45070600
F	2.75568100	-1.84851200	2.05474800

F	0.18609000	2.22860100	1.20463400
B	1.21129300	-0.44331600	-0.10469400
C	2.74761100	-0.85466400	-0.66153300
C	0.12978600	-1.70967200	-0.10439100
C	0.63900200	0.70880900	-1.21281000
C	3.22255100	-2.15284100	-0.96947300
C	3.73140200	0.14595500	-0.85450500
C	-0.63384700	-2.15765700	0.99652500
C	-0.17690900	-2.40909600	-1.29893600
H	1.46612600	1.32926400	-1.57381500
H	0.24017200	0.16086300	-2.08532500
C	4.50688800	-2.42976500	-1.48203000
F	2.43398200	-3.28218300	-0.73413500
C	5.02742600	-0.07573500	-1.35461800
F	3.45335300	1.48601400	-0.50488600
C	-1.57569900	-3.20609800	0.94889100
F	-0.52107300	-1.53908700	2.25394400
C	-1.10802300	-3.45655100	-1.40471000
F	0.48441700	-2.07794200	-2.49416500
C	5.41920600	-1.38249100	-1.68746300
F	4.88681700	-3.73574600	-1.77050300
F	5.91943600	0.98139300	-1.51769700
C	-1.81647400	-3.86708200	-0.26359700
F	-2.28906000	-3.57000100	2.08639100
F	-1.34265100	-4.08321900	-2.62613000
F	6.68718800	-1.63398500	-2.19250200
F	-2.75869100	-4.88507900	-0.34303300
C	-2.43166100	2.36356900	-3.64133700
H	-3.38822900	1.94403800	-3.30364800
H	-2.65784100	3.08814400	-4.44295100
H	-1.84949500	1.55096700	-4.09854600
C	0.70986600	2.99556000	-3.63659000
H	0.50755400	2.02016800	-4.09968400
H	0.62146000	3.75984000	-4.42823900
H	1.75521700	2.99451900	-3.30274200
C	1.40228100	4.62736600	-0.94196500
H	2.21960800	3.93913000	-1.19361700
H	1.59734000	5.57461000	-1.47468900
H	1.46741700	4.84373200	0.13248800
C	-1.35212600	5.14793000	0.63259700
H	-0.51683800	5.00931500	1.33251300
H	-1.38456500	6.22096600	0.37624600
H	-2.27998800	4.91690400	1.17371000
C	-3.74800300	3.83000600	-1.08547500
H	-3.95684700	3.95740800	-0.01474000
H	-4.15959800	4.71392900	-1.60336900
H	-4.31610500	2.95710900	-1.43151800
H	-3.61020900	1.08291600	2.05306100
H	-3.54011500	-0.79037700	-1.85671300
O	-7.12491200	-1.60030000	1.01179800
C	-7.78836400	-2.55269600	0.11428400
H	-7.14697900	-3.42681500	-0.08660500
H	-8.68636200	-2.87081700	0.65712400
H	-8.08016300	-2.07339400	-0.83561600

Frequencies -- 7.5647 12.7391 15.2558
Frequencies -- 19.8669 25.0064 27.1103

Frequencies --	31.2519	32.1054	35.6522
Frequencies --	40.6437	48.4536	56.3366
Frequencies --	73.5716	76.1605	83.1641
Frequencies --	86.4432	95.0224	100.2605
Frequencies --	104.6187	107.4687	111.3391
Frequencies --	111.5086	116.9911	120.2884
Frequencies --	123.1302	126.5800	129.7674
Frequencies --	130.0174	136.9543	137.6414
Frequencies --	145.0189	149.0128	156.6973
Frequencies --	158.4963	161.2974	164.1070
Frequencies --	168.6305	172.7447	193.2254
Frequencies --	209.5854	215.7981	220.6307
Frequencies --	222.8953	228.2324	231.2048
Frequencies --	255.3099	264.1380	264.8702
Frequencies --	265.0971	268.9195	275.8341
Frequencies --	278.6083	279.7267	285.5858
Frequencies --	290.2914	294.4481	300.7279
Frequencies --	303.0237	304.7184	306.6469
Frequencies --	315.6267	325.2129	332.1564
Frequencies --	339.2847	354.6142	365.2000
Frequencies --	374.3988	377.0359	379.0673
Frequencies --	379.9801	384.5483	396.8160
Frequencies --	398.2983	405.9234	415.9195
Frequencies --	417.5906	424.7006	431.4109
Frequencies --	432.2203	443.4779	451.4194
Frequencies --	458.8293	467.7702	474.0789
Frequencies --	504.8203	519.6024	534.5153
Frequencies --	537.0852	539.4267	542.4210
Frequencies --	547.4220	555.2808	566.1587
Frequencies --	579.7776	582.6162	593.9831
Frequencies --	604.1461	606.1281	614.4366
Frequencies --	624.6335	634.4691	636.5153
Frequencies --	637.0322	641.4871	656.1767
Frequencies --	673.0962	705.4153	713.3269
Frequencies --	717.3965	730.0023	736.1006
Frequencies --	746.3448	747.9194	765.5560
Frequencies --	768.2223	800.6902	803.0658
Frequencies --	804.4378	823.6683	828.0896
Frequencies --	840.3844	868.7560	873.9193
Frequencies --	906.3113	911.1672	922.3615
Frequencies --	947.1629	966.2672	966.4714
Frequencies --	971.0611	981.7480	990.3888
Frequencies --	1008.0763	1010.5719	1022.2394
Frequencies --	1032.4533	1040.7467	1043.3805
Frequencies --	1044.4946	1045.2741	1047.9769
Frequencies --	1048.9892	1050.1900	1055.9210
Frequencies --	1086.5138	1088.8137	1116.7370
Frequencies --	1120.8233	1124.8992	1125.9873
Frequencies --	1172.2647	1173.6401	1174.6931
Frequencies --	1187.1938	1202.2068	1208.6043
Frequencies --	1211.7938	1228.5753	1261.1170
Frequencies --	1295.3498	1313.2947	1314.3526
Frequencies --	1320.0236	1337.5374	1344.0184
Frequencies --	1348.0887	1361.4953	1388.9718
Frequencies --	1409.8783	1412.6300	1415.3040
Frequencies --	1416.1110	1420.5923	1424.0580
Frequencies --	1424.8794	1427.9812	1430.8378
Frequencies --	1433.8069	1437.2031	1449.8653
Frequencies --	1451.2727	1454.9739	1463.1087
Frequencies --	1466.3301	1469.4925	1471.7696
Frequencies --	1480.6384	1484.9734	1487.3702
Frequencies --	1488.5232	1492.3904	1496.2166
Frequencies --	1497.7065	1502.6402	1505.1885

Frequencies --	1506.2590	1508.0887	1513.6738
Frequencies --	1519.0574	1583.1983	1590.4064
Frequencies --	1593.5630	1598.1476	1616.6710
Frequencies --	1621.0827	1626.6671	1630.2048
Frequencies --	2996.4934	3009.2345	3009.9799
Frequencies --	3010.9759	3012.0220	3013.2258
Frequencies --	3026.0117	3096.9002	3098.2571
Frequencies --	3099.9199	3102.2356	3103.2808
Frequencies --	3105.3201	3134.1025	3137.7997
Frequencies --	3143.2291	3145.1033	3147.1871
Frequencies --	3151.2882	3161.6619	3187.8266
Frequencies --	3191.8894	3211.6239	3216.1068

Catalyst 19:

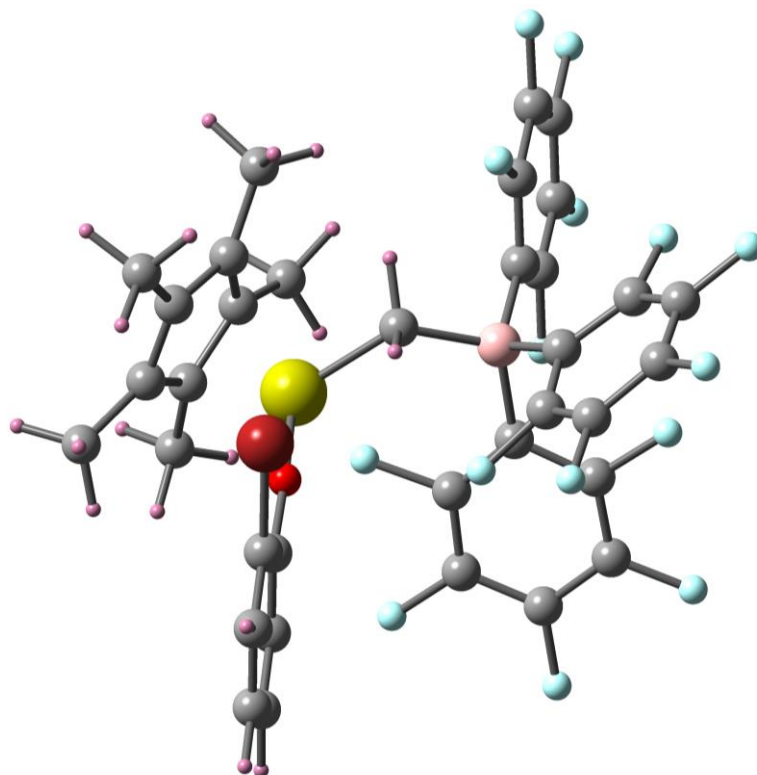
vacuum	toluene-like solvent	D3 dispersion
-3729.222843	-3729.2393371	-0.75515753

Ti	0.09081100	-0.38725900	-1.89443500
O	-1.56120000	-0.05913500	-1.33376900
C	-2.85376000	0.19696900	-0.89544200
C	-3.24946600	1.55434600	-0.69296500
C	-3.68196400	-0.92142900	-0.57582000
C	-4.51569300	1.78950200	-0.08139100
C	-4.94084600	-0.65999000	0.03910900
C	-5.31500100	0.68162100	0.28726700
H	-6.28806700	0.87261400	0.73802300
C	0.73856800	0.89213400	-3.82337500
C	1.87482200	0.05211400	-3.57074800
C	-0.37578800	0.04686300	-4.16935800
C	1.46272700	-1.30838300	-3.73791400
C	0.07220200	-1.31470600	-4.10640100
F	1.01401200	0.90499300	6.01401600
C	1.38837200	0.72042700	4.69062200
C	2.64904900	1.13959900	4.23534100
C	0.51800700	0.09700900	3.78167500
C	3.01198300	0.94473100	2.88537000
F	3.53317200	1.73811100	5.12488900
C	0.92793500	-0.07084800	2.44684500
F	-0.72936400	-0.35326200	4.20718900
C	2.16748400	0.35675100	1.91143200

F	4.30353900	1.36404300	2.56298200
F	0.00704800	-0.74964100	1.62152800
B	2.51759600	0.07307000	0.29078500
C	3.84942500	0.87839400	-0.29227500
C	2.74669900	-1.59610800	0.30177000
C	1.23582800	0.71639600	-0.63760300
C	4.85002900	0.33202500	-1.12545000
C	3.99652900	2.27549500	-0.09983700
C	3.84019400	-2.17951300	0.99700500
C	1.91182300	-2.57197100	-0.24357500
H	0.41933100	1.03355500	0.03153700
H	1.60844200	1.62088400	-1.13422600
C	5.93675800	1.05752700	-1.65699900
F	4.79452600	-1.01901500	-1.51911800
C	5.06026000	3.04631600	-0.60061100
F	3.02567500	2.98186600	0.62384400
C	4.07916000	-3.56191800	1.09880400
F	4.77399900	-1.35398200	1.61877900
C	2.07914400	-3.96709500	-0.19740300
F	0.70376900	-2.17841200	-0.95202300
C	6.05323800	2.42871100	-1.38153800
F	6.88145600	0.43054900	-2.46331200
F	5.13601800	4.41012300	-0.34046500
C	3.19228000	-4.47165100	0.49201500
F	5.18486600	-4.04193300	1.78394200
F	1.18180500	-4.82897600	-0.81303900
F	7.11276000	3.16609600	-1.89053500
F	3.41028400	-5.83717900	0.57303000
C	-5.05321600	3.16729300	0.20144900
C	-5.34255000	4.08735100	-0.83895000
C	-5.34702600	3.54944500	1.53673200
C	-5.90070100	5.35097400	-0.55356500
H	-5.14530500	3.81154400	-1.87543100
C	-5.89759300	4.81597500	1.82597700
H	-5.13020000	2.85828700	2.35413900
C	-6.17750400	5.72303300	0.78052000
H	-6.12077400	6.04114400	-1.37148000
H	-6.10507400	5.09228100	2.86243800
H	-6.60625800	6.70318900	1.00155000
C	-5.90333300	-1.74437700	0.44441400
C	-6.48878400	-2.62005800	-0.50587400
C	-6.29394100	-1.86906700	1.80346500
C	-7.43086000	-3.59221200	-0.10952500
H	-6.21835800	-2.53444100	-1.55900600
C	-7.22981400	-2.84604100	2.20398600
H	-5.85239600	-1.20843500	2.55276400
C	-7.80323300	-3.71243400	1.24761800
H	-7.87400900	-4.25190100	-0.85933300
H	-7.50736300	-2.93031000	3.25731900
H	-8.52996700	-4.46814400	1.55452100
C	-2.33103400	2.68924000	-1.06564900
C	-2.19910900	3.10872200	-2.41381900
C	-1.60279700	3.38774900	-0.06973600
C	-1.37116600	4.19903200	-2.75768500
H	-2.76838800	2.59780000	-3.19424600
C	-0.76449600	4.47007400	-0.40980300
H	-1.69382300	3.08453700	0.97501700

C	-0.64749400	4.88246600	-1.75549400
H	-1.30165500	4.52045900	-3.80006600
H	-0.20638300	4.98891000	0.37235200
H	-0.00579300	5.72673000	-2.01714800
C	-3.19834100	-2.32361400	-0.82990500
C	-3.18098300	-2.86141300	-2.14245700
C	-2.77776600	-3.14889600	0.24361900
C	-2.77166400	-4.19223100	-2.37478000
H	-3.51549000	-2.24562000	-2.98101000
C	-2.36367200	-4.47719400	0.01362400
H	-2.77708800	-2.75081700	1.25970600
C	-2.36206500	-5.00556500	-1.29570500
H	-2.78283600	-4.59475000	-3.39087100
H	-2.04282800	-5.09673300	0.85396500
H	-2.04319500	-6.03488700	-1.47244500
H	2.09069700	-2.18500200	-3.60689600
H	2.86568900	0.38785700	-3.29240900
H	0.71941000	1.97581100	-3.76197700
H	-1.37754800	0.38041500	-4.42080800
H	-0.53420800	-2.19742000	-4.28960800
Frequencies --	-3.7725	6.8849	11.5397
Frequencies --	15.4379	21.5998	25.3561
Frequencies --	29.1955	30.9721	33.0668
Frequencies --	37.1086	37.4379	39.3815
Frequencies --	41.6101	44.8511	45.5476
Frequencies --	49.9215	54.0205	56.0034
Frequencies --	57.7435	62.2279	66.5287
Frequencies --	69.0287	74.6168	86.4932
Frequencies --	105.2658	109.3858	114.4322
Frequencies --	116.2059	120.0732	126.4832
Frequencies --	130.9312	133.4476	136.2012
Frequencies --	140.8117	146.8744	148.4328
Frequencies --	155.4420	158.1867	168.2468
Frequencies --	168.8070	183.3003	194.1114
Frequencies --	198.2848	208.3913	211.1780
Frequencies --	214.3010	218.1316	223.1429
Frequencies --	228.6135	236.0893	246.3144
Frequencies --	249.2034	251.5656	264.2836
Frequencies --	264.5438	264.5884	270.5078
Frequencies --	273.3757	277.8096	281.5671
Frequencies --	290.0978	300.3287	304.8577
Frequencies --	306.5795	319.1360	324.3028
Frequencies --	328.0797	330.5834	332.4714
Frequencies --	347.0556	354.8580	362.9538
Frequencies --	375.4394	377.4674	379.5037
Frequencies --	394.4943	402.6587	403.9332
Frequencies --	404.3730	406.6142	407.0033
Frequencies --	409.1043	420.3667	430.4239
Frequencies --	430.9481	431.8849	444.9716
Frequencies --	454.1850	459.4457	468.9109
Frequencies --	488.8782	517.2924	526.1710
Frequencies --	526.2012	541.3262	542.9123
Frequencies --	544.9522	548.4494	552.8000
Frequencies --	560.9766	569.3715	577.7995
Frequencies --	588.5151	610.4916	612.0321
Frequencies --	616.1687	617.4046	619.4168
Frequencies --	624.2333	625.6520	632.2511
Frequencies --	633.3926	636.9340	643.1265
Frequencies --	644.5737	652.7606	654.8627
Frequencies --	679.0694	690.1824	698.0213

Frequencies --	702.0193	709.4052	709.8069
Frequencies --	713.5135	714.5876	715.7006
Frequencies --	726.9750	738.1885	741.8176
Frequencies --	742.3429	744.6824	746.9440
Frequencies --	764.3541	765.8496	772.2188
Frequencies --	776.8008	783.3383	793.8426
Frequencies --	797.3069	808.2124	808.3897
Frequencies --	828.4490	837.3015	840.7713
Frequencies --	841.9773	857.9964	859.0655
Frequencies --	859.6255	860.6293	864.8393
Frequencies --	867.0026	868.6742	880.3557
Frequencies --	901.0515	904.9338	911.8112
Frequencies --	914.5236	934.1124	935.1844
Frequencies --	941.3059	943.2760	971.6695
Frequencies --	984.7199	985.3623	992.3246
Frequencies --	993.8487	994.9594	995.9814
Frequencies --	1000.7998	1004.2537	1004.5751
Frequencies --	1010.2303	1012.3238	1014.2457
Frequencies --	1020.0063	1022.7720	1028.4108
Frequencies --	1029.0172	1033.0881	1038.6453
Frequencies --	1039.3537	1045.8291	1046.8378
Frequencies --	1049.1296	1049.8107	1053.2996
Frequencies --	1053.9109	1059.5251	1068.0819
Frequencies --	1087.5790	1088.7834	1089.7256
Frequencies --	1091.0219	1091.5168	1092.4384
Frequencies --	1127.8373	1128.9830	1142.5209
Frequencies --	1183.2883	1183.4214	1184.0618
Frequencies --	1184.6582	1203.5346	1203.7848
Frequencies --	1204.6434	1205.6761	1206.4770
Frequencies --	1210.9863	1215.1222	1236.0662
Frequencies --	1268.8866	1281.8763	1284.9214
Frequencies --	1296.8925	1309.0374	1316.1030
Frequencies --	1321.4397	1323.9401	1327.0153
Frequencies --	1329.1179	1332.4434	1334.6125
Frequencies --	1338.1758	1344.7391	1349.5031
Frequencies --	1366.8097	1367.7458	1369.2715
Frequencies --	1371.0697	1379.5873	1390.5056
Frequencies --	1396.1457	1403.2680	1411.1706
Frequencies --	1418.0203	1421.8400	1442.4402
Frequencies --	1442.6987	1443.8217	1444.9332
Frequencies --	1446.1365	1450.1562	1459.9958
Frequencies --	1466.4151	1467.7672	1471.6461
Frequencies --	1496.3203	1496.5774	1501.8545
Frequencies --	1510.7439	1533.1521	1589.0341
Frequencies --	1590.0989	1592.8394	1594.1873
Frequencies --	1595.2258	1595.6352	1597.2149
Frequencies --	1598.9313	1616.1936	1619.3010
Frequencies --	1623.3321	1624.2413	1624.4956
Frequencies --	1624.8572	1628.9991	3040.7931
Frequencies --	3131.8837	3148.0259	3148.5889
Frequencies --	3153.7632	3154.0164	3160.6970
Frequencies --	3160.8041	3161.8114	3161.9362
Frequencies --	3170.0407	3170.4716	3173.8139
Frequencies --	3173.9116	3179.2147	3181.5218
Frequencies --	3185.4827	3185.9887	3193.6371
Frequencies --	3195.7958	3196.0195	3196.5162
Frequencies --	3196.8959	3240.1914	3250.2489
Frequencies --	3259.0848	3271.2403	3299.6922

Catalyst 20:**distal conformation**

vacuum	toluene-like solvent	D3 dispersion
-3014.4739881	-3014.484886	-0.53393418

Ti	-1.35198000	-1.59496000	-0.30151000
O	-2.75438600	-0.50764300	-0.00915700
C	-3.87245600	0.19280400	0.37183200
C	-4.58066700	1.02760500	-0.53402300
C	-4.32144900	0.10645800	1.71657700
C	-5.70614000	1.75882100	-0.10425400
C	-5.44299800	0.83859400	2.14646900
C	-6.13824000	1.66510900	1.23623100
H	-6.23524100	2.40098000	-0.80846000
H	-5.76730600	0.76751500	3.18634700
H	-7.00659200	2.24007100	1.56159800
C	-1.94582000	-3.13505200	-1.97709600
C	-0.52031700	-3.36527700	-1.78065900
C	-2.64168100	-3.53722600	-0.77049100
C	-0.33697900	-3.83981800	-0.43710100
C	-1.64523000	-3.93367800	0.19372300
F	-0.04884000	0.88738400	5.80016500
C	0.28428800	0.73901300	4.46413400
C	1.23732200	1.57909100	3.85807500
C	-0.31234000	-0.26352700	3.68499600

C	1.55111500	1.41987400	2.49405400
F	1.86270700	2.55582100	4.61772400
C	0.06006600	-0.35213700	2.33512700
F	-1.24707100	-1.13535200	4.23656800
C	0.95839600	0.45455800	1.63685700
F	2.55291300	2.25968500	2.01027200
F	-0.54923700	-1.49856100	1.66706600
B	1.31838100	0.36128100	-0.00664300
C	1.36459400	1.95653000	-0.53099000
C	2.74002600	-0.47652500	-0.26040800
C	0.13216400	-0.40160500	-0.98262400
C	2.48304900	2.66660400	-1.02845100
C	0.19116300	2.74750000	-0.48200800
C	3.49431500	-1.16152600	0.71975700
C	3.29225800	-0.60879900	-1.56096300
H	-0.58582600	0.36481800	-1.34022900
H	0.65343600	-0.79778000	-1.85806200
C	2.43331700	3.99229200	-1.50649800
F	3.75861400	2.09381500	-1.02800300
C	0.08819000	4.07508600	-0.93455600
F	-0.98148400	2.21272100	0.08560300
C	4.68345600	-1.87793600	0.46511100
F	3.08110700	-1.19169100	2.06289900
C	4.47080300	-1.30936700	-1.87065800
F	2.65822500	0.00143400	-2.65400800
C	1.22382200	4.70439900	-1.47004400
F	3.57841400	4.61107900	-1.99549000
F	-1.11619200	4.76721100	-0.85073100
C	5.18400200	-1.95054500	-0.84311800
F	5.35527300	-2.52244900	1.49879500
F	4.93717600	-1.37497200	-3.17937500
F	1.15513200	6.00966700	-1.93628700
F	6.34842600	-2.65210900	-1.12003200
C	0.96233800	-4.27396300	0.19915500
H	1.03910200	-3.96876300	1.25242900
H	1.04007300	-5.37486900	0.17751100
H	1.83614000	-3.87587400	-0.32897200
C	0.52435500	-3.30130300	-2.86850000
H	1.53537700	-3.14860500	-2.47471700
H	0.53183500	-4.25244500	-3.42884600
H	0.32728400	-2.50122400	-3.59465400
C	-2.59124600	-2.73789200	-3.28609600
H	-1.97179300	-2.03587400	-3.86115800
H	-2.73718500	-3.63240300	-3.91628700
H	-3.57385100	-2.27163400	-3.14418500
C	-4.13955400	-3.59879900	-0.58155300
H	-4.67100400	-2.88133100	-1.21996600
H	-4.50568000	-4.60623700	-0.84566900
H	-4.44036800	-3.40713300	0.45751900
C	-1.91475200	-4.48020500	1.57782900
H	-2.85315900	-4.09952400	2.00423800
H	-2.00196400	-5.57980900	1.53503600
H	-1.10789800	-4.24778300	2.28542700
H	-3.76976400	-0.52589700	2.41317100
Br	-4.00429500	1.18998700	-2.39965300

Frequencies --

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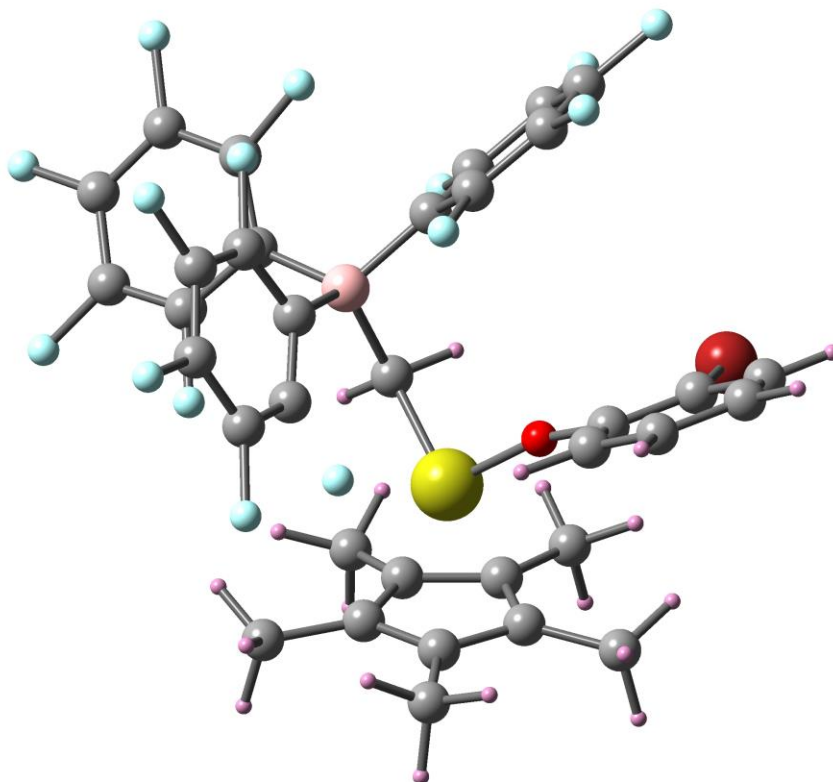
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18.2285

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proximal conformation



vacuum	toluene-like solvent	D3 dispersion
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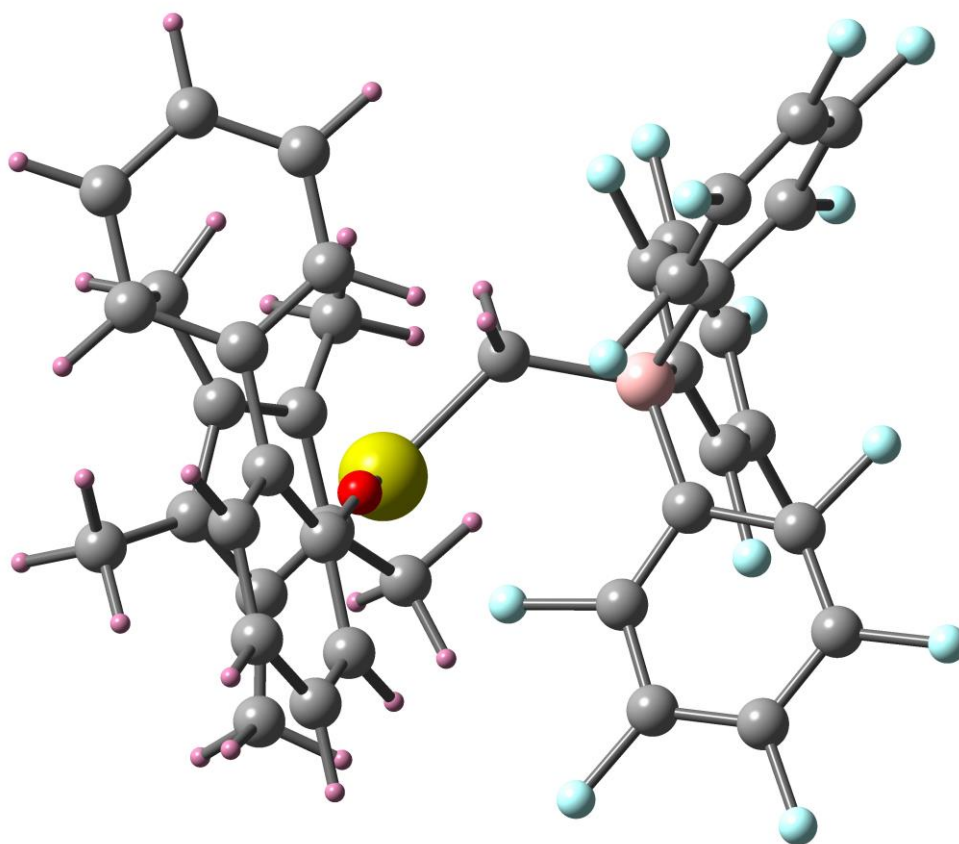
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C	3.55157700	-0.35934000	2.25212800
C	4.26086700	1.00038600	0.35012200
C	4.56993800	0.20660000	3.03934000
C	5.28277500	1.56831800	1.13766700
C	5.43853500	1.17147100	2.48286100
H	4.67732800	-0.09638400	4.08235800
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H	6.22668700	1.62252600	3.08756500
C	0.71544800	-3.15039800	-2.49790500
C	2.03923900	-2.57194800	-2.63101900

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C	2.04072000	-3.90933500	-0.71654100
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C	-1.96633900	-1.46370300	4.05831600
C	-2.58288600	-0.26225300	3.65712000
C	-1.09064000	-2.09687900	3.16428800
C	-2.31710000	0.27107900	2.38255500
F	-3.44108100	0.38616800	4.53198000
C	-0.88254800	-1.49392300	1.91257000
F	-0.45126500	-3.28299300	3.51185500
C	-1.44646400	-0.31640300	1.42507400
F	-2.94697700	1.47740600	2.08616600
F	0.05496700	-2.25308400	1.09073200
B	-1.25391800	0.35994100	-0.10900300
C	-2.83729000	0.38045800	-0.68060200
C	-0.52429000	1.84963600	-0.03232200
C	-0.35152600	-0.53527200	-1.24887200
C	-3.65720300	1.51385800	-0.90264200
C	-3.50025200	-0.83809400	-0.96232200
C	0.16208200	2.38983100	1.07725900
C	-0.45534700	2.68154900	-1.17820300
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C	-4.80849400	-0.95538200	-1.46468400
F	-2.84630900	-2.06450100	-0.71019400
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C	0.16455100	3.94182700	-1.22131600
F	-1.04275700	2.25606400	-2.38028400
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F	0.16666000	4.69621700	-2.38977600
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H	4.90133000	-3.65796600	-1.93621000
H	4.68765600	-1.90257000	-1.82275400
C	2.51640700	-1.73899600	-3.79936100
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H	2.88489100	-2.40106800	-4.60251000
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H	-0.42093800	-2.09809600	-4.03298000
H	-0.22856600	-3.83895300	-4.29982900
H	-1.37751900	-3.25288600	-3.08472200
C	-0.44094200	-4.80031100	-0.80809200
H	-1.41516200	-4.34657300	-1.02790700
H	-0.41853500	-5.78781400	-1.30148700
H	-0.39143200	-4.97901300	0.27401300
C	2.48999600	-4.67794900	0.50666600

H	1.70389200	-4.75097300	1.27117200
H	2.76024300	-5.71029600	0.22430400
H	3.37621200	-4.23042600	0.97719800
H	2.86286800	-1.09117500	2.67599500
Br	4.07257800	1.58793600	-1.51177200

Frequencies --	8.6014	19.0755	24.8614
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Catalyst 21:**distal conformation**

vacuum	toluene-like solvent	D3 dispersion
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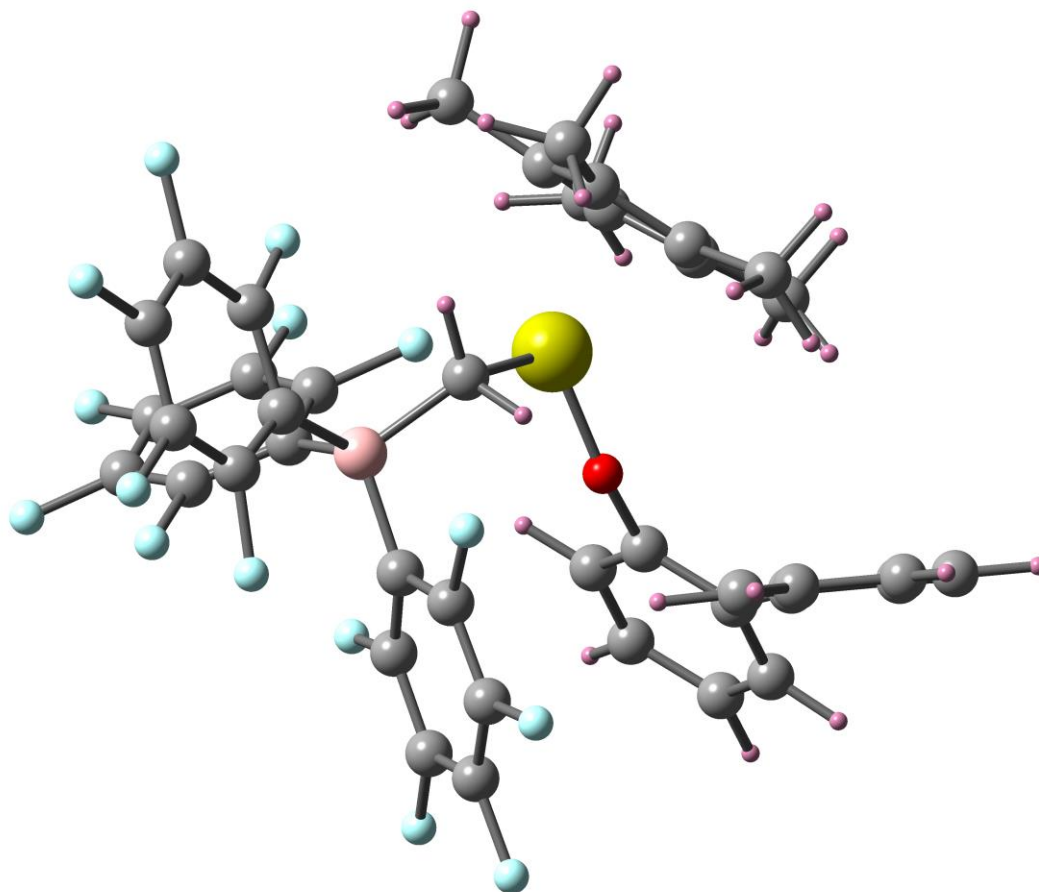
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C	-5.14882800	-0.03872000	3.03045900
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H	-7.03219200	1.05379300	2.97366500
C	-2.07739800	-2.52553700	-2.29739900
C	-0.69123000	-2.93351800	-2.14014300
C	-2.84178700	-3.06917300	-1.18929000
C	-0.58956300	-3.65782500	-0.90091800
C	-1.91736000	-3.73775200	-0.30966600
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C	0.81610000	-0.07476100	4.57055600

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C	1.23548100	0.15811300	1.68895400
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C	0.57421300	2.86715200	0.03554300
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C	1.74871900	4.84849000	-0.71838200
F	4.03829200	4.60748600	-1.44523600
F	-0.52729500	5.03635000	0.09078700
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H	0.26422600	-3.60218600	-3.94134400
H	0.32842000	-1.84517700	-3.73466700
C	-2.65051900	-1.81522900	-3.50357300
H	-1.91533900	-1.15602300	-3.98446100
H	-2.96586000	-2.55615000	-4.25914600
H	-3.52944500	-1.20640800	-3.25684400
C	-4.34529100	-3.03284400	-1.04650800
H	-4.79086400	-2.16558600	-1.54892800
H	-4.77850900	-3.93720700	-1.50871300
H	-4.67139300	-3.01617300	0.00189400
C	-2.27366000	-4.48504900	0.95642300
H	-3.19614800	-4.10681600	1.41747900
H	-2.43880700	-5.55266000	0.72951900
H	-1.47720100	-4.43652300	1.71150000
H	-3.23267800	-1.02232200	2.75950000
C	-4.67532600	1.39656800	-1.06547000

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C	-3.55023900	2.16325300	-1.46860000
C	-5.64679600	1.73486600	-3.30625000
H	-6.59914300	0.61036000	-1.71571000
C	-3.47563200	2.70864600	-2.76750700
H	-2.75413200	2.36287600	-0.75407800
C	-4.52075000	2.49464200	-3.69363000
H	-6.46419100	1.56609800	-4.01145500
H	-2.60953700	3.31227500	-3.04898200
H	-4.46293500	2.92137400	-4.69748800

Frequencies --	7.8014	15.8826	22.6321
Frequencies --	23.7060	28.6256	31.0137
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Frequencies --	43.2242	47.6186	51.1945
Frequencies --	54.7726	60.4875	81.4860
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Frequencies --	124.0895	124.9300	125.9970
Frequencies --	128.4675	132.4846	136.7026
Frequencies --	137.9870	142.7281	146.8937
Frequencies --	150.2347	157.4484	159.6979
Frequencies --	161.1114	167.2459	170.2120
Frequencies --	181.0900	200.2068	213.6681
Frequencies --	219.5257	223.2519	231.0817
Frequencies --	252.8937	263.9607	264.3161
Frequencies --	265.0279	269.9165	276.3109
Frequencies --	278.0726	281.4647	285.0254
Frequencies --	291.0322	292.0652	298.0065
Frequencies --	298.8830	299.3356	303.8456
Frequencies --	304.8884	312.0017	321.4279
Frequencies --	330.4348	333.3984	334.9228
Frequencies --	345.1934	359.3575	372.9180
Frequencies --	375.9257	380.4470	380.8338
Frequencies --	385.3308	390.3284	396.0474
Frequencies --	398.6402	408.9841	418.3996
Frequencies --	431.4470	432.6684	442.4488
Frequencies --	453.4911	457.6888	465.2751
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Frequencies --	541.5956	545.8089	549.3652
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Frequencies --	581.0368	587.6085	597.8320
Frequencies --	605.2414	609.8252	614.3593
Frequencies --	621.6870	625.7894	635.9555
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Frequencies --	713.3661	719.0939	729.0841
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Frequencies --	743.9694	748.1289	764.5999
Frequencies --	767.0253	780.3134	801.0396
Frequencies --	804.2699	819.2699	839.8966
Frequencies --	857.2855	866.8344	875.6127
Frequencies --	876.5375	905.3594	912.8470
Frequencies --	916.6609	939.4957	959.4326
Frequencies --	966.6131	973.9382	989.2966
Frequencies --	991.9793	992.7067	998.6124
Frequencies --	1005.7651	1009.8139	1020.0251
Frequencies --	1026.8285	1036.9187	1040.0205
Frequencies --	1043.6909	1044.1741	1044.5180
Frequencies --	1046.0059	1047.9838	1048.6679

Frequencies --	1050.2920	1055.3528	1061.8439
Frequencies --	1065.5834	1088.2003	1090.0431
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Frequencies --	1172.3928	1175.5114	1183.9820
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Frequencies --	1210.6716	1213.1379	1226.4502
Frequencies --	1265.4857	1297.7757	1300.0072
Frequencies --	1315.8827	1318.3775	1337.5001
Frequencies --	1337.8085	1342.2265	1344.8853
Frequencies --	1357.4906	1371.4855	1396.0823
Frequencies --	1410.8316	1412.0544	1412.5158
Frequencies --	1415.0191	1419.2747	1424.3699
Frequencies --	1428.2641	1428.5928	1430.3536
Frequencies --	1433.8578	1435.9158	1447.6002
Frequencies --	1452.5542	1453.4406	1462.7096
Frequencies --	1467.2941	1469.1103	1473.4798
Frequencies --	1480.5721	1480.7771	1490.8783
Frequencies --	1492.2489	1497.5975	1500.1906
Frequencies --	1503.4796	1506.6341	1508.6724
Frequencies --	1509.6797	1516.2646	1522.1922
Frequencies --	1579.5151	1589.9514	1593.8837
Frequencies --	1595.6105	1595.8709	1611.9603
Frequencies --	1617.2757	1618.8251	1623.7348
Frequencies --	1631.6134	2998.5363	3010.0735
Frequencies --	3010.8362	3011.6466	3013.2744
Frequencies --	3015.5894	3099.8685	3104.8050
Frequencies --	3105.4640	3107.0136	3108.8243
Frequencies --	3137.2306	3146.9407	3152.1315
Frequencies --	3154.0272	3154.3631	3159.7615
Frequencies --	3163.5792	3164.9055	3167.1551
Frequencies --	3175.5027	3178.9792	3190.6517
Frequencies --	3195.4133	3208.1836	3227.2347

proximal conformation

vacuum	toluene-like solvent	D3 dispersion
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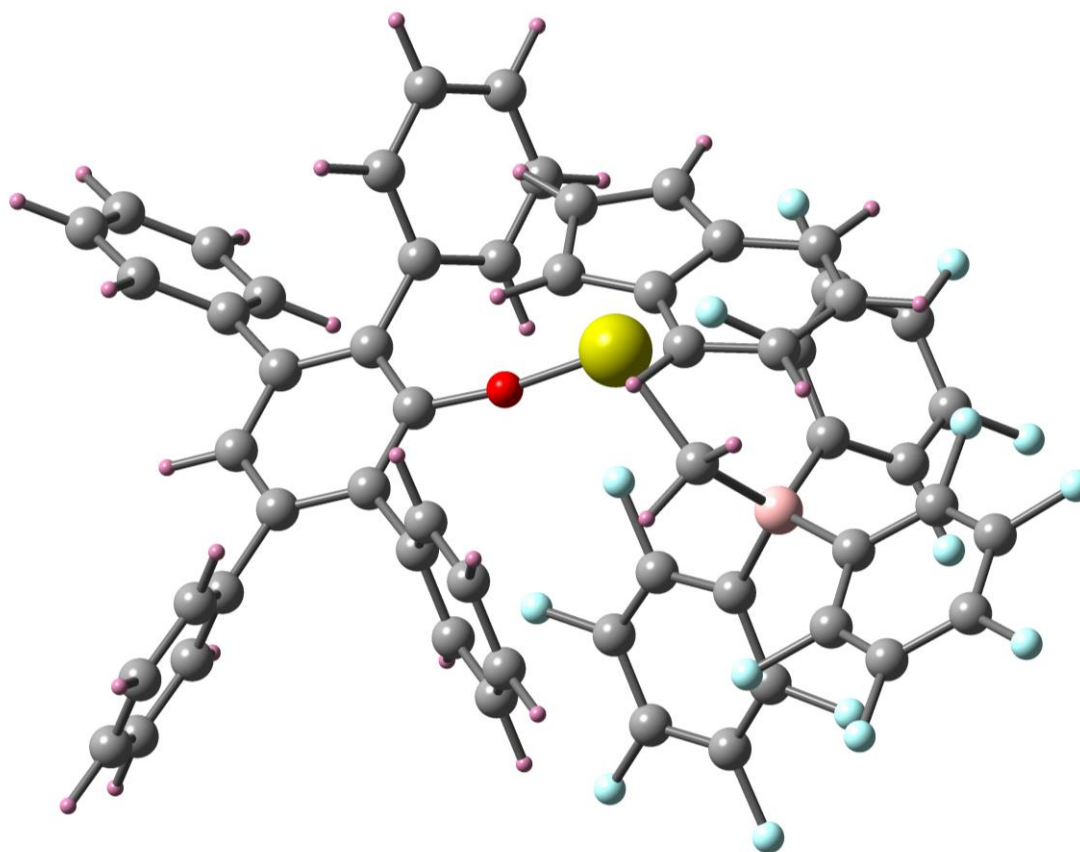
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C	3.08828500	-0.83883000	2.57687600
C	4.38684400	0.51156300	0.95347000
C	4.04947300	-0.60799800	3.57638400
C	5.34253900	0.71562900	1.98701000
C	5.18893000	0.17016900	3.27591600
H	3.90437200	-1.02200700	4.57603200
H	6.20620900	1.34739600	1.77529800
H	5.93985800	0.36797000	4.04273900
C	0.58487800	-3.69329300	-1.79093000
C	0.85281200	-2.71232200	-2.80649200
C	1.79678600	-3.87740600	-1.00503500
C	2.22465700	-2.26078700	-2.63182600
C	2.82005600	-3.02142800	-1.54809600
F	-3.19701900	-3.02892100	4.49607500
C	-2.74882000	-2.23791000	3.45132600
C	-3.33841700	-0.98637500	3.18775700

C	-1.69072400	-2.66363100	2.63520700
C	-2.86999200	-0.20219100	2.11751500
F	-4.37105800	-0.53758200	3.99703900
C	-1.28613100	-1.81751400	1.58928800
F	-1.06584700	-3.88668000	2.85935300
C	-1.81632800	-0.57626900	1.24059000
F	-3.48297300	1.03995300	1.96432300
F	-0.15990900	-2.37083700	0.84789800
B	-1.37149800	0.39131300	-0.06482600
C	-2.83955700	0.66296900	-0.84934500
C	-0.60879500	1.77986600	0.44372400
C	-0.35985200	-0.33822700	-1.22480800
C	-3.54000400	1.88834100	-0.96617200
C	-3.52362700	-0.41512500	-1.46109800
C	-0.14496100	2.05174400	1.75035100
C	-0.29626700	2.81554100	-0.47231900
H	-0.96909400	-0.80102500	-2.00557000
H	0.23898300	0.46022800	-1.70812800
C	-4.75125700	2.04835800	-1.67130600
F	-3.07890700	3.04453000	-0.33242400
C	-4.73446700	-0.31388800	-2.16938200
F	-3.00452000	-1.72436900	-1.35627200
C	0.50671800	3.24071200	2.14058000
F	-0.29040700	1.10496500	2.77954300
C	0.34941300	4.01830000	-0.13917400
F	-0.64733900	2.67808200	-1.82562000
C	-5.35395900	0.94058700	-2.28869400
F	-5.36589700	3.29281000	-1.74737600
F	-5.32102200	-1.43856600	-2.74464600
C	0.74992900	4.24249100	1.18903900
F	0.92257200	3.42133800	3.45512900
F	0.61029900	4.97917600	-1.11184000
F	-6.54465200	1.07747500	-2.98790100
F	1.39434300	5.41845900	1.54496700
C	2.95602100	-1.31984400	-3.56280100
H	3.77717700	-0.78683700	-3.06936500
H	3.39230200	-1.89297800	-4.39991800
H	2.28784600	-0.56657300	-4.00182800
C	-0.05260500	-2.34251500	-3.95658500
H	0.03467000	-1.28446300	-4.23951100
H	0.21360000	-2.94020800	-4.84567700
H	-1.10807200	-2.54358200	-3.73428000
C	-0.69437700	-4.48109200	-1.62807600
H	-1.58296800	-3.89737100	-1.89745200
H	-0.67199900	-5.36798000	-2.28556200
H	-0.83067900	-4.84638500	-0.60178800
C	1.97701000	-4.87480400	0.11834300
H	1.07315000	-4.98725300	0.73235800
H	2.21104200	-5.87057800	-0.29685000
H	2.80514300	-4.60160800	0.78674700
C	4.27368000	-2.99931200	-1.13738300
H	4.76568200	-2.05621800	-1.40197500
H	4.41154200	-3.15749800	-0.05888800
H	4.81520900	-3.80922300	-1.65682500
H	2.19863400	-1.43060800	2.79355100
C	4.61644400	1.15264900	-0.38121400
C	5.89016100	1.06685200	-1.00748700

C	3.61214700	1.92727800	-1.01918400
C	6.14924200	1.73117200	-2.22487000
H	6.67991800	0.47168800	-0.54431800
C	3.87043300	2.60146500	-2.23053500
H	2.63772900	2.02703800	-0.54825100
C	5.14068100	2.50506900	-2.84084200
H	7.13603600	1.64906300	-2.68660500
H	3.08715600	3.21155500	-2.68599300
H	5.34360400	3.03123500	-3.77622200

Frequencies --	8.2249	18.0542	24.5933
Frequencies --	25.5349	27.3079	28.1580
Frequencies --	32.5557	34.3201	39.5124
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Frequencies --	56.8972	60.7206	80.8441
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Frequencies --	123.7462	125.2311	131.1472
Frequencies --	133.4714	135.4433	139.5939
Frequencies --	142.4862	144.5729	148.3808
Frequencies --	156.6721	158.3198	160.2032
Frequencies --	163.8172	165.2551	169.4724
Frequencies --	169.9210	197.3869	213.0803
Frequencies --	217.3222	217.9446	224.4571
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Frequencies --	264.5383	265.1956	275.2400
Frequencies --	277.3049	278.8071	281.3837
Frequencies --	290.1349	293.6505	297.6055
Frequencies --	300.5366	302.4219	305.4908
Frequencies --	307.1372	310.3748	321.4823
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Frequencies --	351.0731	361.1529	363.8949
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Frequencies --	1086.8904	1088.4654	1091.6126
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Frequencies --	1173.1157	1175.2979	1185.7761
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Frequencies --	1511.3451	1517.8666	1522.6804
Frequencies --	1579.9254	1591.6289	1593.5036
Frequencies --	1596.0463	1596.9678	1612.8688
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Frequencies --	3195.1570	3206.3334	3238.1189

Catalyst 22:

vacuum	toluene-like solvent	D3 dispersion
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C	-3.14938700	1.48438100	-0.66801800
C	-3.80754500	-0.92887400	-0.40030300
C	-4.46878600	1.87223100	-0.29016700
C	-5.11689800	-0.51459800	-0.01385900
C	-5.40915500	0.86796300	0.03589000
H	-6.40927200	1.17436900	0.33929000
C	-0.41953400	-0.82447900	-3.78414400
C	1.01969000	-0.68429100	-3.99453900
C	-0.66510700	-2.19264700	-3.38992500
C	1.64573800	-1.92186700	-3.55959400
C	0.58569700	-2.82681100	-3.14882500
F	3.27954200	-5.45791000	2.63623500
C	3.08772700	-4.18140800	2.13234400
C	3.88449000	-3.10567200	2.56887000
C	2.08848800	-3.93362400	1.17928600
C	3.67019400	-1.82036200	2.03990400
F	4.87240900	-3.32894100	3.51641200
C	1.93709900	-2.61957200	0.70065400
F	1.27382500	-4.96813700	0.72874300

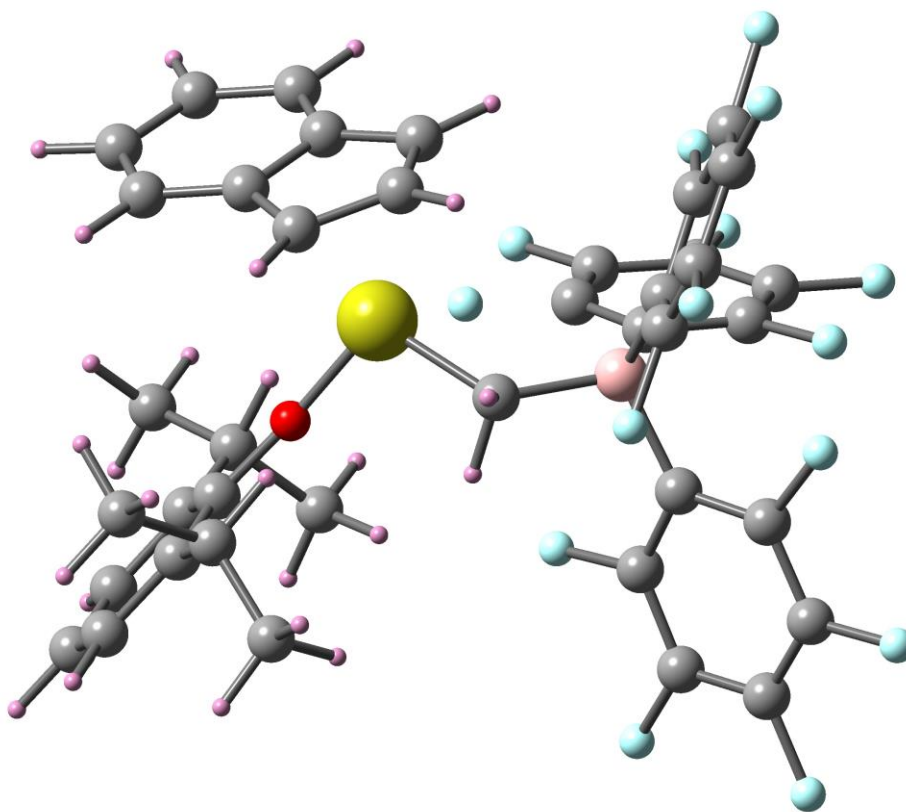
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B	2.45518500	0.07108200	0.53412800
C	1.80052500	0.78630700	1.89861800
C	3.85347200	0.79227800	-0.01061800
C	1.48308700	0.27841000	-0.85125700
C	2.45034300	1.66873000	2.79694100
C	0.49038200	0.45954100	2.31052500
C	4.98484600	0.10399400	-0.50173000
C	3.92690700	2.19227700	-0.21788300
H	0.97379300	1.25494200	-0.75666900
H	2.16149200	0.33937900	-1.71571600
C	1.83989700	2.22445000	3.94166200
F	3.78135400	2.04178300	2.60824700
C	-0.16930000	0.98453800	3.43544300
F	-0.24382700	-0.49493800	1.57866700
C	6.10995800	0.72441600	-1.08071300
F	5.03454900	-1.30134600	-0.47690400
C	5.02516700	2.86220900	-0.78384300
F	2.83601700	3.00413300	0.12353100
C	0.51353400	1.89100800	4.26220900
F	2.54238200	3.09838400	4.76285800
F	-1.47723700	0.61057900	3.73692100
C	6.13899800	2.12091000	-1.21546900
F	7.18039700	-0.03777300	-1.54252000
F	5.01441400	4.24527200	-0.93840900
F	-0.10541000	2.43309800	5.37991900
F	7.23379900	2.75581200	-1.78788600
C	-4.92062800	3.30580900	-0.20329700
C	-4.93879900	4.15842900	-1.33711200
C	-5.40688000	3.81639500	1.02910400
C	-5.42298100	5.47968100	-1.24117500
H	-4.58561000	3.78738000	-2.29961900
C	-5.88395600	5.14034000	1.12965000
H	-5.39699000	3.17962400	1.91631600
C	-5.89457400	5.97840200	-0.00677000
H	-5.43239600	6.11695100	-2.12864500
H	-6.24258400	5.51465900	2.09135100
H	-6.26467800	7.00350700	0.06798800
C	-6.21413000	-1.47357900	0.36200000
C	-7.46004700	-1.42743400	-0.31774700
C	-6.06865100	-2.39275600	1.43341000
C	-8.52160300	-2.28114300	0.04936700
H	-7.59520000	-0.72870500	-1.14631000
C	-7.13075500	-3.24179200	1.80758700
H	-5.13015800	-2.43440200	1.98708000
C	-8.36108900	-3.19352400	1.11522100
H	-9.46808900	-2.23334100	-0.49442600
H	-6.99800100	-3.93551800	2.64110100
H	-9.18215500	-3.85357600	1.40430900
C	-2.09688900	2.50833900	-1.00070800
C	-1.71772800	2.75689100	-2.34407400
C	-1.48943000	3.27704300	0.02364500
C	-0.76234800	3.74735400	-2.65689000
H	-2.19268100	2.19291300	-3.15032500
C	-0.52880300	4.26265500	-0.28449300

H	-1.77475200	3.10746900	1.06334600
C	-0.16115600	4.50233200	-1.62636200
H	-0.49433900	3.93388100	-3.69999400
H	-0.06575300	4.83870600	0.51931300
H	0.58430100	5.26433300	-1.86264100
C	-3.46349600	-2.38610800	-0.55304300
C	-4.07048200	-3.14975100	-1.58470700
C	-2.56614900	-3.04022000	0.32948500
C	-3.79281500	-4.52527300	-1.72936500
H	-4.77352400	-2.66783200	-2.26650700
C	-2.28972300	-4.41797500	0.18998400
H	-2.10688400	-2.47800000	1.14351000
C	-2.90099400	-5.16551200	-0.84021200
H	-4.27844100	-5.09503300	-2.52510900
H	-1.60243000	-4.90419400	0.88455200
H	-2.69051800	-6.23223300	-0.94402400
H	-1.17500500	-0.11878200	-4.11560700
H	-1.64084100	-2.64013100	-3.23037700
H	0.72240100	-3.84192400	-2.78567900
C	1.81599300	0.37622000	-4.50686000
H	1.35627500	1.30599700	-4.84614300
C	3.20411500	0.19621800	-4.57971700
H	3.83296100	0.99055500	-4.98762900
C	3.82370500	-1.01408800	-4.12964200
H	4.90881400	-1.11220100	-4.19731300
C	3.06062700	-2.06938900	-3.61404300
H	3.54063800	-2.99049600	-3.27916200

Frequencies --	8.0991	11.8464	14.9317
Frequencies --	16.7111	22.9713	23.3801
Frequencies --	28.0066	31.4905	32.8850
Frequencies --	35.4565	39.6285	40.2160
Frequencies --	44.5915	46.8692	47.9384
Frequencies --	51.1782	53.6222	55.4107
Frequencies --	61.3444	62.8343	64.4137
Frequencies --	68.5093	71.2203	73.7895
Frequencies --	79.1921	103.4554	105.6995
Frequencies --	113.4453	118.3292	120.8991
Frequencies --	126.2256	126.8624	131.1973
Frequencies --	133.4971	138.0373	143.7890
Frequencies --	146.7896	149.8650	158.7025
Frequencies --	158.7959	165.2806	174.0674
Frequencies --	190.1961	192.8468	195.5633
Frequencies --	206.9515	212.4672	213.2535
Frequencies --	223.0155	224.7451	230.9336
Frequencies --	233.9288	245.2573	255.0405
Frequencies --	261.0693	263.7145	263.9913
Frequencies --	264.2908	272.6562	273.8881
Frequencies --	276.2090	279.4978	281.5214
Frequencies --	300.7482	303.2459	307.7259
Frequencies --	313.2182	324.4026	326.6187
Frequencies --	330.0453	333.7212	346.9258
Frequencies --	357.8228	363.1201	374.6593
Frequencies --	375.8270	379.7070	386.8496
Frequencies --	390.3529	402.6926	403.7521
Frequencies --	406.0001	407.2916	409.4676
Frequencies --	412.1576	414.1736	431.1434
Frequencies --	433.3804	435.1219	437.9087
Frequencies --	441.4695	452.6341	458.1130
Frequencies --	467.3909	490.4604	507.6517

Frequencies --	519.5664	529.6534	539.4583
Frequencies --	541.3136	542.6550	545.8154
Frequencies --	547.6087	549.5999	552.7470
Frequencies --	559.6755	572.1753	593.0671
Frequencies --	599.7295	606.9000	612.6301
Frequencies --	616.3812	616.9955	619.3738
Frequencies --	624.2486	624.9620	631.4996
Frequencies --	632.7035	636.8891	642.4856
Frequencies --	643.0039	653.8174	658.8015
Frequencies --	674.8659	689.0662	695.4485
Frequencies --	707.5950	709.5166	710.9284
Frequencies --	713.1406	714.2200	716.7180
Frequencies --	726.1484	735.0907	735.9649
Frequencies --	738.0805	744.3092	744.7086
Frequencies --	747.5976	750.8110	765.8201
Frequencies --	770.0789	774.2742	775.4409
Frequencies --	778.9061	792.6284	795.6438
Frequencies --	806.6652	821.8509	832.3562
Frequencies --	839.7574	858.7607	859.9989
Frequencies --	860.5028	864.8538	867.3291
Frequencies --	869.4459	873.8696	880.6469
Frequencies --	881.0683	889.7471	894.1121
Frequencies --	906.7121	914.5344	916.3079
Frequencies --	932.5609	939.5598	942.1915
Frequencies --	945.2728	970.0420	972.3598
Frequencies --	983.8843	985.3758	987.1060
Frequencies --	991.0726	994.9394	995.7371
Frequencies --	1005.2238	1005.7621	1008.3999
Frequencies --	1009.0209	1009.8310	1012.5523
Frequencies --	1014.0873	1016.1246	1020.1558
Frequencies --	1025.8999	1030.5588	1030.9642
Frequencies --	1037.3218	1044.4230	1045.3377
Frequencies --	1050.6389	1052.2446	1052.7773
Frequencies --	1053.7341	1054.9002	1055.9216
Frequencies --	1075.8124	1089.1530	1089.7103
Frequencies --	1091.7624	1092.6917	1092.9477
Frequencies --	1129.3486	1137.2411	1138.1144
Frequencies --	1183.1764	1183.3224	1183.6141
Frequencies --	1185.2400	1185.8865	1201.8079
Frequencies --	1203.7630	1204.1448	1206.1744
Frequencies --	1206.8279	1209.6662	1211.2838
Frequencies --	1214.0160	1235.0757	1240.8162
Frequencies --	1263.2120	1266.0388	1282.8128
Frequencies --	1300.5027	1308.1228	1321.9908
Frequencies --	1322.7549	1325.0250	1327.3203
Frequencies --	1331.7725	1332.7576	1336.1418
Frequencies --	1339.0984	1346.0129	1352.1181
Frequencies --	1355.1358	1367.5136	1368.4602
Frequencies --	1369.6340	1369.8481	1371.2326
Frequencies --	1380.4684	1382.0111	1410.1018
Frequencies --	1416.1754	1418.8869	1422.9087
Frequencies --	1425.1535	1442.5177	1443.7107
Frequencies --	1445.5151	1447.3015	1460.2865
Frequencies --	1465.6229	1466.5589	1467.7870
Frequencies --	1470.6465	1496.6910	1497.0265
Frequencies --	1497.8981	1502.4941	1510.8804
Frequencies --	1532.0057	1568.3846	1589.6014
Frequencies --	1591.8777	1594.0398	1594.2929
Frequencies --	1595.3885	1596.2422	1597.4877
Frequencies --	1599.8744	1618.5586	1619.8333
Frequencies --	1622.1413	1624.1640	1624.5066
Frequencies --	1624.8006	1626.6579	1627.5018
Frequencies --	3013.4970	3103.8311	3149.3906

Frequencies --	3153.1630	3154.4585	3158.0532
Frequencies --	3160.7813	3161.6946	3163.8665
Frequencies --	3166.7075	3170.6026	3171.7307
Frequencies --	3173.5280	3174.7089	3175.3759
Frequencies --	3181.7061	3181.9634	3186.3105
Frequencies --	3186.8781	3187.3142	3188.3963
Frequencies --	3194.5790	3197.3815	3197.9488
Frequencies --	3198.3651	3200.2899	3203.3426
Frequencies --	3237.8185	3244.4625	3269.9128

Catalyst 23:

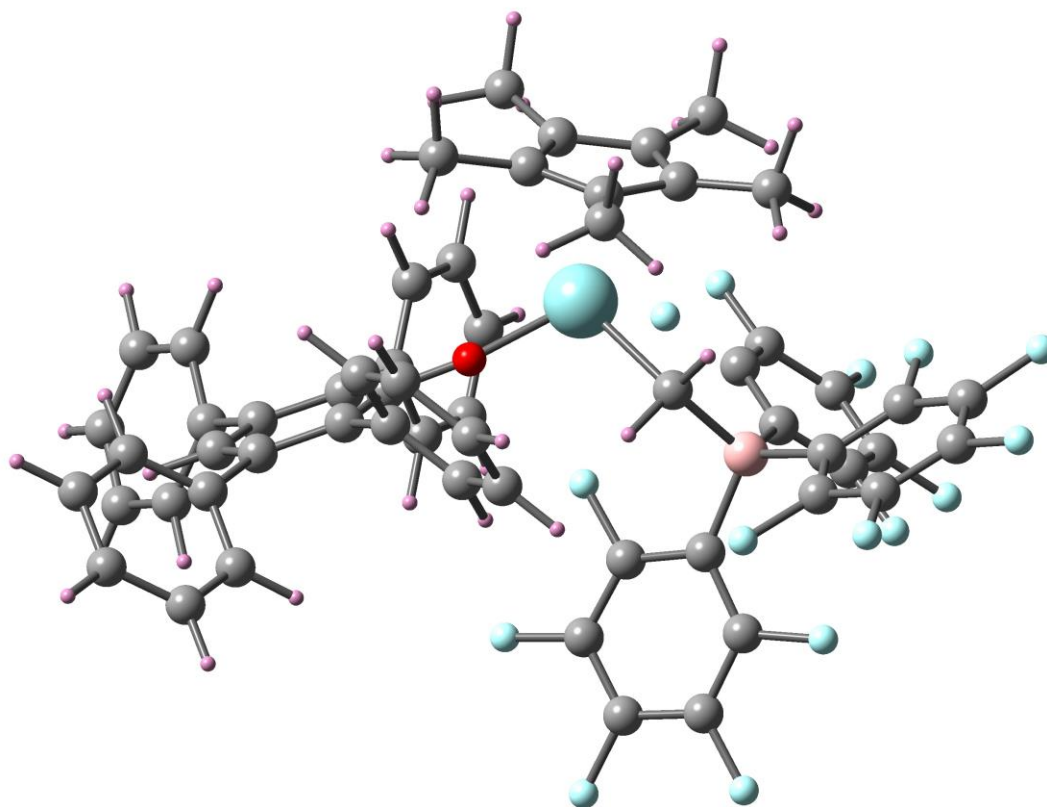
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Ti	-1.53136300	-0.96954400	-0.43639800
O	-2.86425600	0.19287800	-0.58778300
C	-3.95956900	1.04196100	-0.75654600
C	-4.20162000	1.60207200	-2.04878300
C	-4.76936800	1.33959000	0.38448500
C	-5.30371300	2.48067300	-2.17372500
C	-5.85035200	2.23000300	0.19110500
C	-6.12076900	2.79302700	-1.07126500
H	-5.51968900	2.93128000	-3.14306900
H	-6.48739500	2.48907900	1.03673600
H	-6.96254800	3.47758500	-1.19307300
H	0.34677100	-2.63635600	-2.23435800
C	-0.55815500	-2.79963600	-1.66236100
C	-0.62361600	-3.26622700	-0.31922700
C	-1.89684300	-2.50929600	-2.12047600
H	0.22273900	-3.52739400	0.30788200
C	-2.02456200	-3.41554600	0.03918400
H	-2.16983000	-2.18861200	-3.12186100
C	-2.82325200	-2.97430000	-1.09808100
F	3.18669500	5.88733900	-0.03013600
C	2.83189900	4.54636900	-0.03876700
C	3.72814500	3.56956400	-0.50169600
C	1.57371100	4.13654700	0.43210600

C	3.34799000	2.21125200	-0.50437800
F	4.99011900	3.95084700	-0.94116500
C	1.24275700	2.76967200	0.40262800
F	0.67516900	5.07747900	0.92576200
C	2.08017400	1.73720500	-0.08753800
F	4.34454600	1.32723900	-0.92423800
F	-0.02135100	2.45149800	0.94364100
B	1.54138100	0.14114500	-0.08184600
C	2.54119100	-0.92566100	-0.87917800
C	1.43940800	-0.19679900	1.56448000
C	0.08078400	0.13496000	-0.94085600
C	3.03183600	-2.15078000	-0.37564000
C	2.91423600	-0.70320900	-2.22940900
C	0.30486500	-0.55994400	2.28984300
C	2.56923300	-0.04915600	2.41340500
H	-0.42034900	1.11529600	-0.86062900
H	0.31776400	-0.01531700	-2.00577000
C	3.85191300	-3.04634000	-1.09384500
F	2.68484200	-2.58940300	0.91676600
C	3.72915600	-1.55846900	-2.99199600
F	2.46394600	0.44731200	-2.89500200
C	0.19952900	-0.76763500	3.67556700
F	-0.96168100	-0.77993200	1.60419100
C	2.55390400	-0.23728100	3.80750900
F	3.80397100	0.27606700	1.85605000
C	4.21531900	-2.74483600	-2.41522800
F	4.28758800	-4.23074900	-0.50932400
F	4.05641800	-1.24546200	-4.30609000
C	1.35496300	-0.59803300	4.45306000
F	-1.00690100	-1.12984700	4.26331900
F	3.70946700	-0.07950200	4.55683600
F	5.01974500	-3.60807200	-3.14403400
F	1.31598300	-0.78663300	5.82424900
C	-3.30923400	1.30174500	-3.26325200
H	-2.53993200	0.58244800	-2.95227300
C	-4.44926500	0.77482700	1.77715900
H	-3.77581700	-0.08413100	1.64946600
C	-2.55844000	2.57645600	-3.74912900
H	-1.87465300	2.32446200	-4.57562600
H	-3.25586200	3.34676900	-4.11176100
H	-1.96222300	3.01893300	-2.93643500
C	-4.10384900	0.63880900	-4.42584800
H	-4.60991000	-0.28085800	-4.09081300
H	-4.87279400	1.31172900	-4.83412800
H	-3.42179800	0.37611200	-5.25073000
C	-3.68814100	1.82851400	2.63833900
H	-2.77539000	2.17710700	2.13246800
H	-4.31882500	2.70869300	2.83790000
H	-3.39765600	1.39039900	3.60685900
C	-5.70139300	0.24033000	2.52643500
H	-6.40505000	1.04315900	2.79407200
H	-6.24446300	-0.50009900	1.91854700
H	-5.39091500	-0.24795600	3.46387200
C	-2.66723800	-3.87936800	1.22727600
H	-2.07849100	-4.20425900	2.08664500
C	-4.06396500	-3.94306100	1.25160300
H	-4.57226200	-4.32038900	2.14125500

C	-4.84927800	-3.52893400	0.12366600
H	-5.93694900	-3.60660800	0.17960200
C	-4.24848400	-3.03263700	-1.03631800
H	-4.85378100	-2.71204800	-1.88579100
Frequencies --	9.4477	12.7093	16.2548
Frequencies --	22.2633	24.9089	28.0500
Frequencies --	31.5749	33.6423	36.5467
Frequencies --	41.3024	43.1431	43.9791
Frequencies --	46.7330	53.3563	59.7681
Frequencies --	65.0398	76.3927	79.6717
Frequencies --	105.4149	108.8378	114.6885
Frequencies --	115.8654	121.6450	124.3726
Frequencies --	127.8120	134.0434	136.3648
Frequencies --	142.0400	148.1575	154.1419
Frequencies --	158.3313	159.9044	163.4619
Frequencies --	169.6396	177.2133	184.6397
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Frequencies --	223.5023	225.9180	232.4676
Frequencies --	244.8605	252.1705	261.0757
Frequencies --	262.5888	263.8622	264.3357
Frequencies --	265.2408	271.1624	273.4553
Frequencies --	275.2972	278.1491	279.6828
Frequencies --	291.5095	299.5640	302.5911
Frequencies --	306.1026	313.1659	314.3185
Frequencies --	322.1514	328.1293	331.7634
Frequencies --	338.7372	347.2155	361.6889
Frequencies --	369.7337	375.0984	377.3827
Frequencies --	380.3100	392.4166	392.6610
Frequencies --	408.6119	424.7461	427.4130
Frequencies --	431.0012	431.9855	434.8248
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Frequencies --	458.7194	468.2871	500.9051
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Frequencies --	548.3855	561.9273	572.7414
Frequencies --	587.5923	596.2195	598.4851
Frequencies --	603.0580	613.8305	626.0603
Frequencies --	627.7410	634.6863	636.8452
Frequencies --	642.3250	652.6373	672.8304
Frequencies --	707.3144	717.0602	721.4930
Frequencies --	723.7461	729.7116	736.2234
Frequencies --	738.4906	744.7177	748.9354
Frequencies --	762.2513	766.1199	768.5230
Frequencies --	794.8115	797.4392	816.2715
Frequencies --	821.5208	828.6522	843.6515
Frequencies --	866.4584	866.8836	874.3533
Frequencies --	876.0781	879.6402	881.7954
Frequencies --	901.2073	907.2897	912.4558
Frequencies --	924.3877	928.5743	929.5856
Frequencies --	938.8162	939.7199	960.5331
Frequencies --	967.0567	973.9635	977.1246
Frequencies --	993.2359	1005.6625	1006.8415
Frequencies --	1012.8519	1023.0144	1032.8754
Frequencies --	1045.1793	1049.5399	1054.6801
Frequencies --	1056.1226	1058.6535	1073.6722
Frequencies --	1078.2612	1084.5186	1113.7450
Frequencies --	1118.1989	1121.9138	1138.0821
Frequencies --	1162.7050	1182.0499	1184.5677
Frequencies --	1197.5715	1203.8380	1204.9648
Frequencies --	1210.4555	1210.7148	1215.3932
Frequencies --	1237.8570	1257.0445	1268.1603
Frequencies --	1276.2590	1297.0269	1308.2577

Frequencies --	1314.9018	1317.7901	1319.8101
Frequencies --	1324.5190	1337.0505	1337.7110
Frequencies --	1343.6258	1349.1823	1358.4933
Frequencies --	1371.5430	1382.9273	1390.2461
Frequencies --	1399.2862	1399.6472	1411.6330
Frequencies --	1415.7666	1416.6284	1417.7663
Frequencies --	1419.0229	1420.9643	1428.2489
Frequencies --	1437.4717	1466.6052	1466.6617
Frequencies --	1468.6279	1471.5230	1474.5738
Frequencies --	1485.5583	1487.2254	1488.3820
Frequencies --	1490.3672	1495.3096	1498.4951
Frequencies --	1504.4249	1505.8630	1509.1472
Frequencies --	1559.8547	1590.2072	1592.9384
Frequencies --	1595.2424	1596.6280	1603.8043
Frequencies --	1616.6594	1619.4955	1626.9893
Frequencies --	1630.0916	3005.4377	3008.3937
Frequencies --	3011.6654	3012.2047	3020.6779
Frequencies --	3070.9015	3072.8778	3100.4010
Frequencies --	3103.7677	3108.1350	3112.8699
Frequencies --	3115.0888	3116.9185	3119.5084
Frequencies --	3127.6761	3128.0885	3165.7898
Frequencies --	3167.8948	3176.0414	3186.8112
Frequencies --	3188.9381	3200.2723	3200.8465
Frequencies --	3240.8489	3257.0223	3290.7551

Catalyst 24:

vacuum	toluene-like solvent	D3 dispersion
-3914.1756929	-3914.1899681	-0.85037141

O	-1.62064500	0.04193200	-0.90655800
C	-2.92091500	0.17872600	-0.43195900
C	-3.48301900	1.48764800	-0.29773300
C	-3.63623300	-1.00727100	-0.07050900
C	-4.82894000	1.59378100	0.17018300
C	-4.98491800	-0.87576800	0.37324100
C	-5.54989900	0.41602800	0.46915500
H	-6.57841600	0.50914400	0.81501700
C	0.55923600	0.92340900	-3.82076300
C	1.67341900	-0.00102600	-3.78011300
C	-0.65465200	0.15667300	-4.05653600
C	1.15059100	-1.33452200	-3.93777800
C	-0.28505500	-1.23763700	-4.12739000
F	0.10338500	0.65079500	5.92086300
C	0.72801500	0.55712900	4.68515600
C	2.01269300	1.08972700	4.48628400
C	0.09260200	-0.08536800	3.60988900
C	2.63296100	0.98695000	3.22241400
F	2.66442700	1.71156700	5.54436200
C	0.75825800	-0.15754700	2.37373500
F	-1.17206000	-0.64611200	3.78066500
C	2.03059900	0.38354200	2.09096500
F	3.91862600	1.52379100	3.15750200

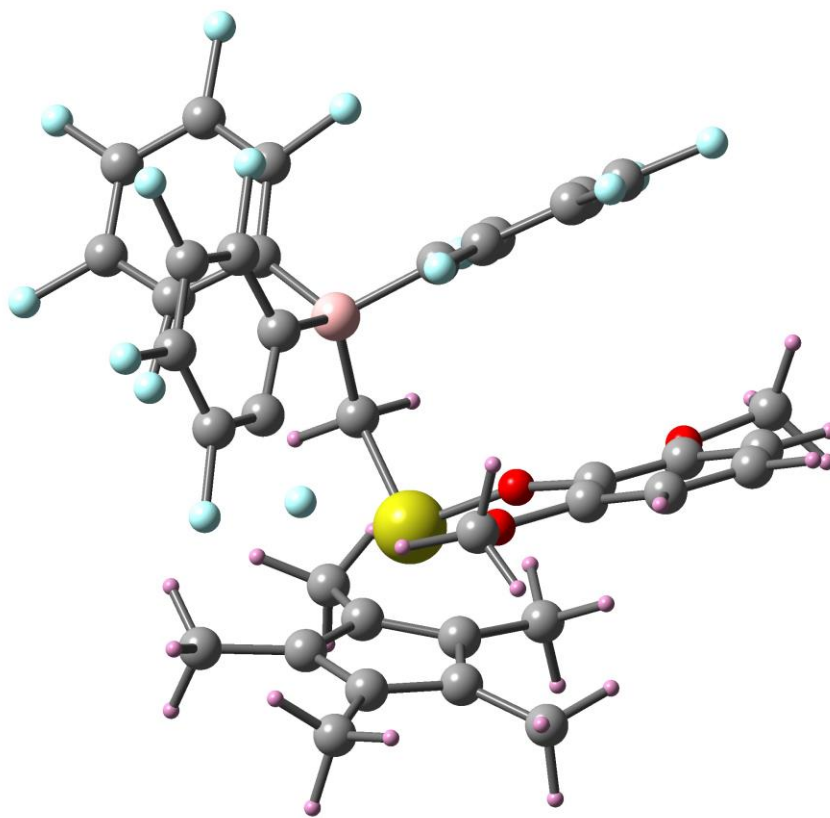
F	0.07702600	-0.86946000	1.36221900
B	2.67420500	0.19985700	0.55343600
C	3.99105700	1.17323900	0.25613700
C	3.08114800	-1.44094200	0.57229400
C	1.58216900	0.76206900	-0.63789500
C	5.16312600	0.78436400	-0.42825400
C	3.94051200	2.56727200	0.50952300
C	2.42425900	-2.49205300	-0.07235000
C	4.12780800	-1.92637600	1.40439800
H	0.93267600	1.49924000	-0.12753000
H	2.17515300	1.34298900	-1.35429100
C	6.22031100	1.65285600	-0.76926900
F	5.32943000	-0.54548400	-0.86202000
C	4.96517700	3.47695800	0.19633300
F	2.79411900	3.12862700	1.09404900
C	2.71784600	-3.86535100	0.00638500
F	1.28759000	-2.23422100	-0.94516700
C	4.48650800	-3.27938000	1.54212100
F	4.88340300	-1.02387700	2.14936300
C	6.12877500	3.01476800	-0.44398800
F	7.34296900	1.17524500	-1.44004000
F	4.83563400	4.82909300	0.49978600
C	3.77632100	-4.26735600	0.83366000
F	1.98316300	-4.80585000	-0.70755300
F	5.53413200	-3.65510300	2.36989600
F	7.15418500	3.89309000	-0.76915900
F	4.10950200	-5.60702300	0.95294800
C	1.96918000	-2.59990800	-4.08805200
H	1.46202200	-3.48423000	-3.67733000
H	2.15509900	-2.80140900	-5.15760500
H	2.95023900	-2.52083600	-3.60157000
C	3.13856100	0.36816800	-3.77475000
H	3.75743600	-0.34708400	-3.21836200
H	3.51539200	0.38730400	-4.81235900
H	3.31793200	1.36452500	-3.35311600
C	0.66287200	2.43388900	-3.84436600
H	1.47504800	2.80873100	-3.20788700
H	0.87126200	2.77523600	-4.87389000
H	-0.26327200	2.92147300	-3.51853700
C	-2.01380400	0.73741800	-4.38852600
H	-2.22553800	1.65416700	-3.82689700
H	-2.05493100	0.99132100	-5.46233200
H	-2.83075800	0.03095600	-4.18962700
C	-1.17796300	-2.38186700	-4.55971600
H	-2.24258700	-2.15769200	-4.42005400
H	-1.02692700	-2.57350400	-5.63653900
H	-0.95311200	-3.31981600	-4.03420200
C	-5.53198600	2.90583000	0.40294500
C	-6.74675400	3.19381800	-0.27272200
C	-5.05517700	3.84534800	1.35383800
C	-7.45496500	4.38816600	-0.02012600
H	-7.13467000	2.48349700	-1.00633400
C	-5.76472100	5.03591800	1.61443300
H	-4.13465800	3.63996800	1.90131600
C	-6.96616700	5.31555400	0.92599000
H	-8.38363300	4.59167100	-0.55887400
H	-5.38152800	5.74105600	2.35586500

H	-7.51398700	6.23930500	1.12641400
C	-5.84883200	-2.04747600	0.75665100
C	-6.16783100	-3.07543900	-0.16843900
C	-6.42233800	-2.11353400	2.05385700
C	-7.02449100	-4.13625100	0.19197700
H	-5.75699800	-3.03981500	-1.17809700
C	-7.27391600	-3.17744100	2.41998600
H	-6.18750300	-1.33684200	2.78473800
C	-7.57942000	-4.19477700	1.48956100
H	-7.26004400	-4.91298900	-0.53963400
H	-7.69410900	-3.21157900	3.42799500
H	-8.23995300	-5.01849000	1.77018800
C	-2.68764800	2.72265300	-0.62849700
C	-3.08715500	3.58671700	-1.68105600
C	-1.56114400	3.09530800	0.14908600
C	-2.38966100	4.78482800	-1.94366000
H	-3.96054400	3.33125500	-2.28376900
C	-0.85997400	4.29266900	-0.10832600
H	-1.24778400	2.45816200	0.97722200
C	-1.27360800	5.14454100	-1.15622500
H	-2.72549900	5.44034000	-2.75091000
H	0.00107100	4.55836000	0.50901700
H	-0.73781300	6.07646000	-1.35057800
C	-2.94801400	-2.34840400	-0.04796500
C	-2.70129800	-3.09231400	-1.22876000
C	-2.56033700	-2.91584700	1.19339300
C	-2.09329200	-4.36654600	-1.17443700
H	-3.03070100	-2.69294300	-2.18839900
C	-1.94990500	-4.18575800	1.25189200
H	-2.73347800	-2.35973700	2.11494200
C	-1.71281800	-4.91787500	0.06787000
H	-1.92978500	-4.93295900	-2.09422700
H	-1.66226300	-4.60120100	2.22047400
H	-1.24272800	-5.90259500	0.11221900
Zr	0.09003300	-0.44708700	-1.71139300

Frequencies --	9.4312	12.9964	14.3189
Frequencies --	17.3941	23.3171	26.2049
Frequencies --	29.0058	32.1582	34.0108
Frequencies --	35.3759	38.7923	43.5169
Frequencies --	44.8337	46.5805	49.4834
Frequencies --	51.0736	54.7587	57.0731
Frequencies --	60.9706	64.8195	66.3174
Frequencies --	71.1954	76.8693	78.5295
Frequencies --	100.9317	102.8066	106.3323
Frequencies --	108.9719	110.2666	118.0793
Frequencies --	120.1867	122.0459	124.2686
Frequencies --	127.6929	131.2143	134.9190
Frequencies --	135.1207	139.5154	140.4939
Frequencies --	143.4057	149.4142	150.6450
Frequencies --	155.9148	157.5324	158.2137
Frequencies --	163.1507	169.0756	169.9465
Frequencies --	175.0947	175.9763	189.6725
Frequencies --	194.9467	209.2321	210.8252
Frequencies --	212.8781	215.4408	221.6493
Frequencies --	224.2202	232.6526	235.9600
Frequencies --	247.1628	259.1850	263.1178
Frequencies --	263.9779	264.2133	265.3160
Frequencies --	273.7426	274.5847	279.4845

Frequencies --	281.7331	289.8932	297.6674
Frequencies --	300.4760	302.7369	303.4024
Frequencies --	308.5869	312.9604	325.5343
Frequencies --	327.7286	329.9692	331.6345
Frequencies --	336.1664	340.9882	357.6653
Frequencies --	374.1806	375.8077	379.9204
Frequencies --	381.1743	387.8541	390.7631
Frequencies --	398.0744	404.9889	405.8227
Frequencies --	407.3952	409.4920	411.3752
Frequencies --	415.4228	430.7896	432.5209
Frequencies --	433.3468	443.7906	451.8964
Frequencies --	458.7077	467.0575	494.9742
Frequencies --	500.8017	509.6206	523.7370
Frequencies --	537.0948	539.5265	541.1056
Frequencies --	543.0542	543.6848	548.5537
Frequencies --	550.1550	552.7594	553.6615
Frequencies --	582.7046	585.5419	594.6889
Frequencies --	603.4803	608.7775	615.8585
Frequencies --	616.9055	618.4068	621.4120
Frequencies --	625.0056	626.4864	629.4518
Frequencies --	635.2463	635.7200	637.5823
Frequencies --	640.9635	650.9461	659.4448
Frequencies --	678.8522	689.0737	692.7957
Frequencies --	705.6148	710.1719	710.5222
Frequencies --	711.0945	713.5449	716.5230
Frequencies --	721.5834	724.1216	734.8527
Frequencies --	739.9009	742.2768	748.0197
Frequencies --	763.5255	772.2806	776.2219
Frequencies --	778.8358	794.1573	800.2091
Frequencies --	801.3686	806.8190	823.2252
Frequencies --	840.6278	859.6519	860.0204
Frequencies --	860.7813	865.9316	870.2681
Frequencies --	872.0171	887.4744	903.4426
Frequencies --	908.3970	913.4266	931.5870
Frequencies --	938.1409	942.1451	945.6415
Frequencies --	957.6704	967.0456	971.0718
Frequencies --	986.6225	986.8259	987.3425
Frequencies --	994.7953	995.6633	996.8843
Frequencies --	1004.9577	1005.1483	1009.3590
Frequencies --	1010.3572	1011.3828	1014.4443
Frequencies --	1021.2317	1023.7638	1026.7672
Frequencies --	1029.8418	1039.3229	1040.4109
Frequencies --	1042.0478	1044.1828	1044.6274
Frequencies --	1045.9980	1049.3025	1049.9758
Frequencies --	1051.6329	1052.3707	1052.8473
Frequencies --	1054.7784	1055.6450	1084.0150
Frequencies --	1085.9683	1088.6067	1089.5534
Frequencies --	1091.0382	1091.8709	1096.0216
Frequencies --	1123.9078	1130.4615	1134.7357
Frequencies --	1171.3425	1176.1301	1182.5739
Frequencies --	1182.7307	1183.4922	1184.0128
Frequencies --	1201.7999	1204.3704	1205.4493
Frequencies --	1206.6580	1207.4403	1209.7010
Frequencies --	1212.3115	1232.5721	1272.4696
Frequencies --	1280.5457	1290.6398	1305.6799
Frequencies --	1319.5172	1320.8423	1325.9163
Frequencies --	1327.9338	1331.4630	1333.7475
Frequencies --	1334.8111	1339.0718	1344.4479
Frequencies --	1347.5367	1366.6102	1369.3712
Frequencies --	1369.7368	1370.5437	1381.6839
Frequencies --	1408.6803	1412.2021	1413.8974
Frequencies --	1417.2107	1417.3673	1421.6775
Frequencies --	1424.5369	1425.8839	1427.1950

Frequencies --	1430.5033	1434.6210	1441.4881
Frequencies --	1443.1974	1444.5753	1445.6184
Frequencies --	1447.4562	1454.5763	1458.1640
Frequencies --	1461.8011	1466.0936	1466.9475
Frequencies --	1470.7829	1486.1412	1492.7020
Frequencies --	1494.0830	1497.1672	1497.9501
Frequencies --	1500.4097	1502.2879	1503.7105
Frequencies --	1506.8260	1508.5612	1509.5472
Frequencies --	1511.9512	1517.2065	1520.4202
Frequencies --	1533.3947	1589.6734	1589.9823
Frequencies --	1592.8419	1594.7311	1595.3611
Frequencies --	1595.4616	1597.5979	1600.0702
Frequencies --	1618.0562	1619.3666	1622.7365
Frequencies --	1623.7870	1623.8212	1624.3691
Frequencies --	1626.7876	3008.4792	3009.0005
Frequencies --	3010.2515	3011.0121	3012.3274
Frequencies --	3014.5407	3097.7078	3102.0636
Frequencies --	3107.4990	3107.9022	3109.5695
Frequencies --	3121.6539	3139.2347	3149.1313
Frequencies --	3151.8567	3152.5084	3153.5908
Frequencies --	3154.1111	3156.2889	3157.1729
Frequencies --	3160.0198	3160.1187	3161.3325
Frequencies --	3165.0338	3165.6511	3172.6350
Frequencies --	3173.5523	3176.9367	3184.1601
Frequencies --	3184.2973	3184.7887	3184.8721
Frequencies --	3192.8644	3194.0624	3195.6603
Frequencies --	3196.7721	3197.0881	3202.5668

Catalyst 30:

vacuum	toluene-like solvent	D3 dispersion
-3230.8694117	-3230.8803179	-0.57311736

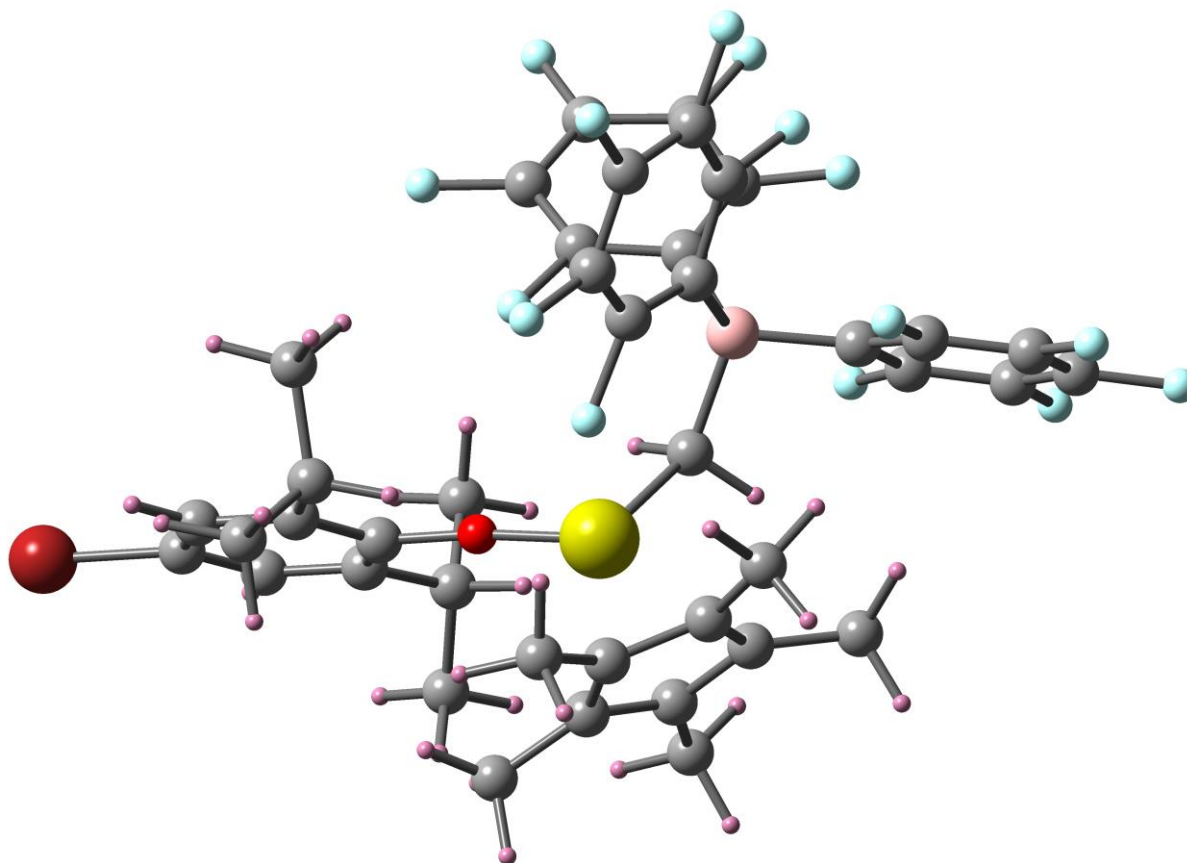
Ti	1.24348700	-1.35988300	-1.04209600
O	2.32690000	-0.11511200	-0.36349700
C	3.40014800	0.48329300	0.24710800
C	3.88092500	-0.04753900	1.48004900
C	4.00861700	1.64443400	-0.31233900
C	4.94180500	0.59082000	2.16100900
C	5.07428100	2.27341800	0.37482500
C	5.52295300	1.74596800	1.60133400
H	5.30934700	0.20844300	3.11083400
H	5.54650700	3.16681400	-0.02765500
H	6.33808300	2.24360200	2.12978100
C	0.86152700	-2.41714600	-3.21790200
C	2.18503400	-1.81534500	-3.15606700
C	0.81424400	-3.47147400	-2.24156700
C	2.97101500	-2.54747500	-2.18329200
C	2.11319800	-3.54538000	-1.59198200
F	-1.73106000	-3.00307900	4.90863900
C	-1.61974700	-2.24291100	3.75464300
C	-2.36810200	-1.06088300	3.59334000
C	-0.75023800	-2.63085700	2.72480900
C	-2.23271900	-0.30201800	2.41639700
F	-3.21937700	-0.65097000	4.60957200
C	-0.68081700	-1.82084400	1.57945400

F	0.02750200	-3.78023000	2.84803000
C	-1.38012100	-0.63895400	1.33232200
F	-2.97247900	0.87827800	2.36815100
F	0.26566400	-2.33099700	0.60153400
B	-1.31034600	0.29687300	-0.06425700
C	-2.92604800	0.44469200	-0.52026000
C	-0.54399200	1.75118600	0.20400200
C	-0.53278800	-0.42907000	-1.38086900
C	-3.70189100	1.62915400	-0.53353300
C	-3.66154100	-0.69400200	-0.93085700
C	0.17455600	2.11838900	1.36279700
C	-0.46598600	2.72927500	-0.81904700
H	-1.20801300	-1.13293900	-1.87867300
H	-0.28634000	0.36100000	-2.11291200
C	-5.03971900	1.70005300	-0.97437100
F	-3.18246700	2.83446000	-0.05374100
C	-4.99753500	-0.68091800	-1.37147000
F	-3.06634700	-1.97388200	-0.88403300
C	0.87731400	3.33031500	1.52288200
F	0.26782000	1.24862900	2.46422900
C	0.22300300	3.94846200	-0.71532800
F	-1.11218000	2.51202100	-2.04714400
C	-5.69554200	0.53694300	-1.40812600
F	-5.72395500	2.91088100	-0.96844800
F	-5.63094900	-1.85750300	-1.76526400
C	0.90449700	4.25753600	0.47263600
F	1.57219900	3.59757400	2.69959300
F	0.26584400	4.84064900	-1.78499200
F	-7.01139400	0.58505200	-1.84800200
F	1.62599200	5.44203400	0.58572000
C	4.44491500	-2.35802500	-1.91062800
H	4.71721000	-2.60401700	-0.87527900
H	5.03284700	-3.02085300	-2.56953300
H	4.77475400	-1.32958000	-2.10612600
C	2.69945000	-0.72822100	-4.07344100
H	3.42977000	-0.07548700	-3.57839200
H	3.19371100	-1.17891500	-4.95194000
H	1.88804600	-0.09009100	-4.44834200
C	-0.19946000	-2.10080400	-4.24431500
H	-0.26532500	-1.02704000	-4.46650300
H	0.03408600	-2.61833300	-5.19104700
H	-1.19526200	-2.43647500	-3.92833600
C	-0.35215200	-4.39868500	-1.98681800
H	-1.32108300	-3.89510700	-2.10122600
H	-0.33191400	-5.23732900	-2.70477400
H	-0.32141100	-4.83572400	-0.97998700
C	2.51829400	-4.56269500	-0.54838400
H	1.70763500	-4.78330100	0.15983900
H	2.79091700	-5.51508400	-1.03550900
H	3.38869300	-4.23296600	0.03426100
O	3.22508200	-1.20955100	1.90704400
O	3.47891300	2.06831400	-1.53482900
C	3.48899500	-1.70742500	3.26448600
H	3.27031400	-0.93301200	4.01688700
H	2.80486000	-2.55481200	3.39171300
H	4.53121500	-2.05198600	3.36827500
C	3.96714700	3.32937700	-2.11409200

H	3.35434600	3.47970300	-3.01056700
H	3.81978400	4.17238500	-1.42096400
H	5.03063700	3.25283800	-2.39519700

Frequencies --	7.1475	18.7093	22.3433
Frequencies --	26.3083	29.1057	31.9232
Frequencies --	32.9804	39.2043	39.8698
Frequencies --	44.8523	47.8646	53.7577
Frequencies --	60.1485	67.1658	68.0623
Frequencies --	80.3928	93.4915	95.0558
Frequencies --	99.2861	103.7514	106.4100
Frequencies --	112.3263	113.4730	117.2382
Frequencies --	119.6835	121.3669	121.8590
Frequencies --	124.9716	132.8075	137.4970
Frequencies --	144.4725	148.9534	155.5961
Frequencies --	157.8565	160.2176	163.2806
Frequencies --	165.1744	166.7022	168.5713
Frequencies --	184.7598	195.0130	197.7053
Frequencies --	211.8936	216.7141	220.9373
Frequencies --	224.1884	234.9626	251.4005
Frequencies --	257.8398	264.2252	264.4022
Frequencies --	265.0009	265.0499	275.3359
Frequencies --	276.8128	277.8404	278.9020
Frequencies --	287.8390	294.0070	296.5330
Frequencies --	300.8803	302.5113	305.9468
Frequencies --	313.5721	315.5333	324.9774
Frequencies --	331.8422	338.7431	349.2324
Frequencies --	356.1333	357.3898	365.3080
Frequencies --	375.0491	377.1524	378.2001
Frequencies --	379.9990	382.4258	391.7498
Frequencies --	399.5380	410.3345	420.5481
Frequencies --	431.3981	432.3444	442.2352
Frequencies --	452.4953	458.4941	468.0643
Frequencies --	500.3506	519.1044	535.5568
Frequencies --	537.1802	538.0183	541.2146
Frequencies --	544.3748	547.3587	557.0459
Frequencies --	564.6616	579.3782	580.7796
Frequencies --	586.9616	599.2514	604.9151
Frequencies --	605.7947	611.7009	616.0213
Frequencies --	625.4978	634.4891	636.1504
Frequencies --	640.6196	655.4668	671.6718
Frequencies --	706.9157	716.2847	721.7284
Frequencies --	726.3570	729.5477	735.8681
Frequencies --	746.0711	748.1733	759.3528
Frequencies --	766.7329	801.4362	804.2843
Frequencies --	831.2242	844.7708	848.7965
Frequencies --	851.4638	866.2107	877.5608
Frequencies --	906.2603	910.7163	919.5690
Frequencies --	951.5460	967.9705	973.8267
Frequencies --	980.2117	984.2527	1008.5563
Frequencies --	1021.8358	1029.6681	1042.2126
Frequencies --	1043.6446	1044.4882	1047.7867
Frequencies --	1049.0732	1049.7346	1052.6123
Frequencies --	1054.5886	1081.7549	1087.3859
Frequencies --	1090.8109	1098.8336	1100.5848
Frequencies --	1126.1973	1128.4278	1129.4687
Frequencies --	1167.3094	1174.5571	1174.9619
Frequencies --	1176.0034	1201.1480	1207.8903
Frequencies --	1208.0303	1209.4101	1228.6224
Frequencies --	1255.0336	1294.7749	1297.3269
Frequencies --	1313.6209	1320.2184	1338.0292
Frequencies --	1345.7679	1350.1522	1377.6514

Frequencies --	1390.3426	1410.3007	1412.7733
Frequencies --	1413.7322	1416.9768	1421.3031
Frequencies --	1424.2115	1427.6876	1427.9778
Frequencies --	1429.1280	1434.9302	1446.1508
Frequencies --	1449.4801	1452.8122	1457.1873
Frequencies --	1462.8301	1465.8999	1468.4442
Frequencies --	1470.0636	1474.4392	1478.8673
Frequencies --	1479.9022	1485.8687	1487.7022
Frequencies --	1491.5775	1492.1721	1493.6563
Frequencies --	1496.2339	1497.4511	1498.0950
Frequencies --	1504.9350	1506.2327	1511.4728
Frequencies --	1513.9648	1519.8287	1591.7491
Frequencies --	1592.2590	1593.8757	1600.3783
Frequencies --	1608.9159	1616.2878	1622.6068
Frequencies --	1629.1377	3003.5211	3005.2851
Frequencies --	3008.5305	3009.1390	3009.7087
Frequencies --	3010.5551	3012.5598	3026.7023
Frequencies --	3099.3194	3101.1549	3102.3128
Frequencies --	3103.7539	3105.3015	3105.8514
Frequencies --	3108.4721	3136.8990	3142.1146
Frequencies --	3143.0524	3145.3345	3147.5524
Frequencies --	3149.3908	3164.2655	3165.4715
Frequencies --	3178.9511	3216.2414	3224.3810

Catalyst 31:

vacuum	toluene-like solvent	D3 dispersion
-3250.2151083	-3250.2242382	-0.64786065

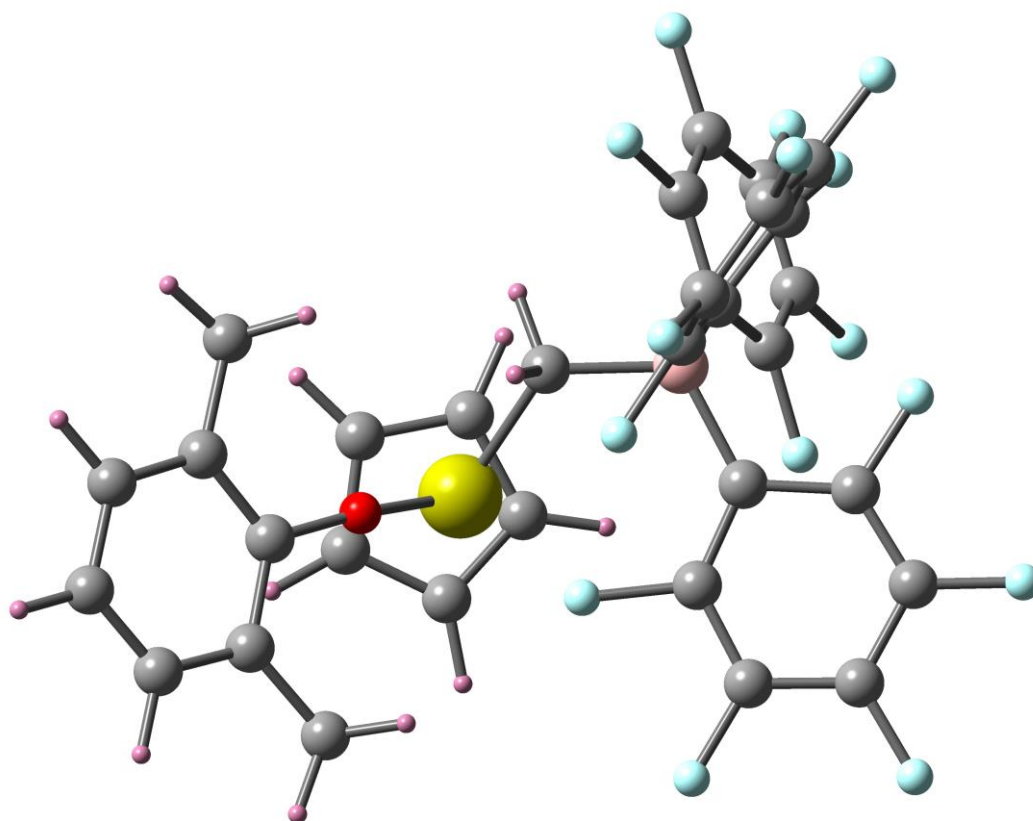
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C	-3.37955600	-0.36743500	-0.37044100
C	-3.88018200	0.29724100	-1.53381900
C	-4.15759000	-0.48995500	0.82463400
C	-5.19671800	0.81218100	-1.48756100
C	-5.46487900	0.04907200	0.82217900
C	-5.97238100	0.67947800	-0.32528200
H	-5.60332900	1.32413800	-2.35745400
H	-6.07695400	-0.01994000	1.71893700
C	-0.42558300	-3.31636000	-2.18379900
C	0.87579000	-3.43282100	-1.55570100
C	-1.43028900	-3.76459500	-1.23660400
C	0.67287600	-3.89273000	-0.20748400
C	-0.75081100	-4.09852400	-0.00834900
F	1.99607000	-0.31331000	5.87375300
C	1.98924100	-0.15907900	4.49759900
C	2.89769400	0.70987200	3.86235600
C	1.07786800	-0.86909800	3.70291300
C	2.86938500	0.85085700	2.46309000

F	3.81511200	1.41351800	4.62748500
C	1.11883300	-0.66778500	2.31260000
F	0.16204900	-1.74425100	4.27879400
C	1.97579900	0.16487400	1.59508900
F	3.81893200	1.71524300	1.92236900
F	0.12724200	-1.47541100	1.61929300
B	1.97718600	0.47484100	-0.06349200
C	1.61166500	2.11733100	-0.09538700
C	3.44401000	0.09240400	-0.75074100
C	0.83262500	-0.34542900	-1.04825500
C	2.47446800	3.19107500	-0.42621000
C	0.32225900	2.55289100	0.29110000
C	4.44115900	-0.73501400	-0.19020500
C	3.75518700	0.50820800	-2.07000500
H	0.09067100	0.39935800	-1.39156400
H	1.37025300	-0.69417100	-1.93663000
C	2.08453700	4.54715600	-0.43724700
F	3.81529100	2.96952200	-0.74512500
C	-0.11803900	3.88835800	0.30128000
F	-0.62562800	1.60661700	0.73096200
C	5.65539400	-1.07278500	-0.82385800
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C	0.77425400	4.90382000	-0.07938400
F	2.99147900	5.53926900	-0.79002300
F	-1.41821200	4.20792500	0.68328200
C	5.92032600	-0.58909800	-2.11399400
F	6.58229300	-1.89364400	-0.18827400
F	5.17527400	0.67479400	-4.03711500
F	0.37226800	6.23151100	-0.08859800
F	7.10627400	-0.90683300	-2.76060000
C	-3.03545100	0.51152600	-2.79933700
H	-2.09348200	-0.03837100	-2.67284800
C	-3.60013400	-1.11539000	2.11275300
H	-2.66771800	-1.63647100	1.85850900
C	-2.66264500	2.01458700	-2.97019400
H	-1.98008700	2.14312700	-3.82550000
H	-3.55434800	2.63352800	-3.15309200
H	-2.16498700	2.40474500	-2.07085800
C	-3.72287200	-0.03962500	-4.08133100
H	-3.99764800	-1.10024400	-3.96923100
H	-4.63959000	0.51606200	-4.32970700
H	-3.04145200	0.05058500	-4.94240000
C	-3.23277700	-0.00858500	3.14731400
H	-4.12858600	0.53337200	3.48736800
H	-2.75193500	-0.45811400	4.03069000
H	-2.54029900	0.72709900	2.71302400
C	-4.55187100	-2.17206400	2.74023400
H	-5.48379100	-1.72192300	3.11328200
H	-4.82555600	-2.95283600	2.01291500
H	-4.05863500	-2.65789700	3.59711000
C	-0.65985300	-2.97833600	-3.63888900
H	0.03037000	-2.20556800	-4.00576800
H	-0.49735100	-3.87605800	-4.26093400
H	-1.68338100	-2.63477400	-3.83140600
C	2.20133300	-3.31670000	-2.26644200

H	2.41387300	-4.26026000	-2.79912300
H	2.21193500	-2.51739200	-3.01923900
H	3.03121400	-3.14198600	-1.57342000
C	-2.89850300	-3.96818600	-1.52992900
H	-3.27304600	-3.27676300	-2.29502700
H	-3.06281500	-4.99281900	-1.90659800
H	-3.52712200	-3.84376500	-0.63868000
C	1.75717500	-4.23676500	0.78794700
H	2.12327500	-5.26156300	0.60142600
H	2.62406000	-3.56782600	0.71859100
H	1.39368600	-4.21045800	1.82365000
C	-1.38321300	-4.67696300	1.23836000
H	-2.46409200	-4.49434800	1.27937900
H	-1.23823800	-5.77100000	1.25680600
H	-0.93955800	-4.28170600	2.16374300
Br	-7.80203200	1.40740900	-0.29652300

Frequencies --	6.2435	11.1897	17.8615
Frequencies --	21.3617	25.7736	29.7887
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Frequencies --	134.5269	136.0164	137.4807
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Frequencies --	801.0053	804.3048	807.1753

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Frequencies --	1423.9227	1424.8827	1426.1062
Frequencies --	1428.5043	1431.0962	1434.8742
Frequencies --	1437.6459	1450.9719	1454.0427
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Frequencies --	1471.8855	1481.4208	1486.2765
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Frequencies --	1590.7210	1593.6459	1596.0988
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Catalyst 33:

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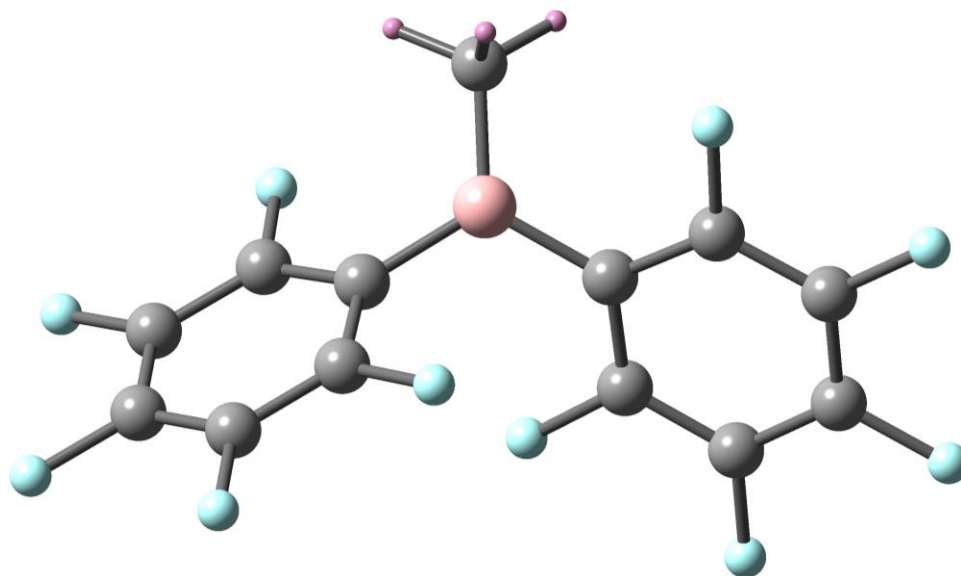
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C	-5.07039500	0.31838600	-2.20110400
C	-5.70963500	0.15379500	0.21403200
C	-6.38634200	0.74868300	-2.48821400
C	-7.00917000	0.59247100	-0.12944200
C	-7.34990000	0.88304400	-1.46690600
H	-6.65212300	0.98723100	-3.51977500
H	-7.75432100	0.71287700	0.65919400
H	-8.35882700	1.22097600	-1.71088800
H	-2.57374900	-3.31503800	-2.23653600
C	-2.24430700	-3.32476200	-1.20084600
C	-0.87651100	-3.30500900	-0.74708700
C	-3.09901400	-3.41448300	-0.04709200
H	0.00075100	-3.27573400	-1.38031400
C	-0.89063700	-3.34935800	0.68382400
H	-4.18452600	-3.44848600	-0.06017300
C	-2.26205100	-3.40953900	1.11590300
H	-0.02152500	-3.33232000	1.33324700
H	-2.60051800	-3.45358600	2.14827000
F	0.74439400	1.20399200	5.72178700

C	0.78061500	0.92308300	4.36701600
C	1.95923700	1.11811800	3.62032500
C	-0.35771400	0.43399500	3.70860000
C	1.97370100	0.82670800	2.24403800
F	3.09709600	1.58853100	4.25636400
C	-0.25275700	0.17017100	2.33252400
F	-1.54368300	0.22031200	4.39936400
C	0.86166100	0.33177800	1.51026000
F	3.18868600	1.02313700	1.59228100
F	-1.50580700	-0.33398000	1.77394300
B	0.95531000	0.10039500	-0.15559100
C	1.36844100	1.63743500	-0.70586400
C	2.04285000	-1.09114900	-0.56646600
C	-0.49362900	-0.30180700	-0.94454100
C	2.60070200	2.03715600	-1.27867100
C	0.45064400	2.70925100	-0.57466100
C	2.62362700	-2.03245700	0.31189000
C	2.41520900	-1.30563300	-1.91819500
H	-1.10276600	0.60352900	-1.12505800
H	-0.22403300	-0.70935400	-1.92851400
C	2.87611100	3.34182900	-1.73845800
F	3.66600100	1.14137100	-1.39264100
C	0.67650400	4.02708900	-1.01181200
F	-0.78861600	2.49858800	0.06545800
C	3.52233700	-3.04857500	-0.07508700
F	2.29489600	-2.03656200	1.68132600
C	3.30592800	-2.29961100	-2.36085300
F	1.88584200	-0.48338800	-2.92496500
C	1.90370000	4.34729700	-1.61529700
F	4.10926900	3.64674800	-2.30138200
F	-0.29466400	5.00959800	-0.84697300
C	3.87737900	-3.18077700	-1.42616600
F	4.04425700	-3.92807800	0.86710200
F	3.62538600	-2.42046900	-3.70793000
F	2.15514800	5.63525800	-2.06400100
F	4.75722800	-4.17179200	-1.83413600
C	-4.02952300	0.19278400	-3.29988900
H	-3.14445800	0.81210900	-3.08819800
H	-3.67853000	-0.84583400	-3.41420000
H	-4.44137700	0.51223800	-4.26664000
C	-5.33316600	-0.13053900	1.65791600
H	-5.00860100	-1.17408300	1.80095100
H	-4.50802800	0.51770600	1.99423300
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Frequencies --	33.5324	38.8360	42.0006
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Frequencies --	116.6400	121.2665	125.8919
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Frequencies --	146.7920	148.1576	155.7350
Frequencies --	158.4962	165.1752	170.0290
Frequencies --	176.7627	202.9945	211.0205
Frequencies --	216.2035	221.1267	223.4507
Frequencies --	223.9838	247.3496	260.4325

Frequencies --	263.9927	264.5722	265.0374
Frequencies --	269.3291	275.3970	278.6199
Frequencies --	283.4259	302.2460	303.8678
Frequencies --	310.4105	312.7573	324.1505
Frequencies --	330.0257	333.3186	337.2020
Frequencies --	345.7596	356.8971	361.0328
Frequencies --	374.3876	377.2310	379.6580
Frequencies --	380.8313	395.7784	427.6843
Frequencies --	431.0518	431.9687	444.7412
Frequencies --	454.3324	459.1099	468.7669
Frequencies --	489.4304	511.9924	524.4151
Frequencies --	540.8036	544.9541	546.0588
Frequencies --	549.2394	552.1305	560.5113
Frequencies --	565.8479	570.3073	580.4835
Frequencies --	588.7036	608.9024	624.7474
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Frequencies --	651.9679	675.8763	704.0600
Frequencies --	716.6415	729.9145	737.5491
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Frequencies --	822.5935	838.7292	839.7920
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Frequencies --	873.1057	891.4095	907.2124
Frequencies --	911.5146	912.8040	921.8575
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Frequencies --	1046.0115	1049.8463	1050.3624
Frequencies --	1055.1800	1057.2993	1057.4954
Frequencies --	1081.2605	1089.5614	1098.5998
Frequencies --	1107.6740	1126.1532	1193.4826
Frequencies --	1204.2886	1210.2985	1211.9536
Frequencies --	1216.1241	1278.7823	1282.4744
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Frequencies --	1348.4157	1363.2177	1391.1602
Frequencies --	1393.8316	1398.5060	1412.3326
Frequencies --	1417.3996	1420.0483	1421.0751
Frequencies --	1421.6367	1427.5840	1442.2247
Frequencies --	1452.0834	1466.8229	1469.1106
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Frequencies --	1491.1358	1500.8085	1504.4266
Frequencies --	1589.7071	1592.9088	1595.3127
Frequencies --	1604.9923	1606.9357	1616.5233
Frequencies --	1619.7912	1630.6929	3009.9705
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Frequencies --	3195.9590	3233.0860	3240.4143
Frequencies --	3258.6233	3269.0764	3299.8273

7. Product for Transfer of (C₆F₅) from Counterion to Cation
[\(return to table of contents\)](#)

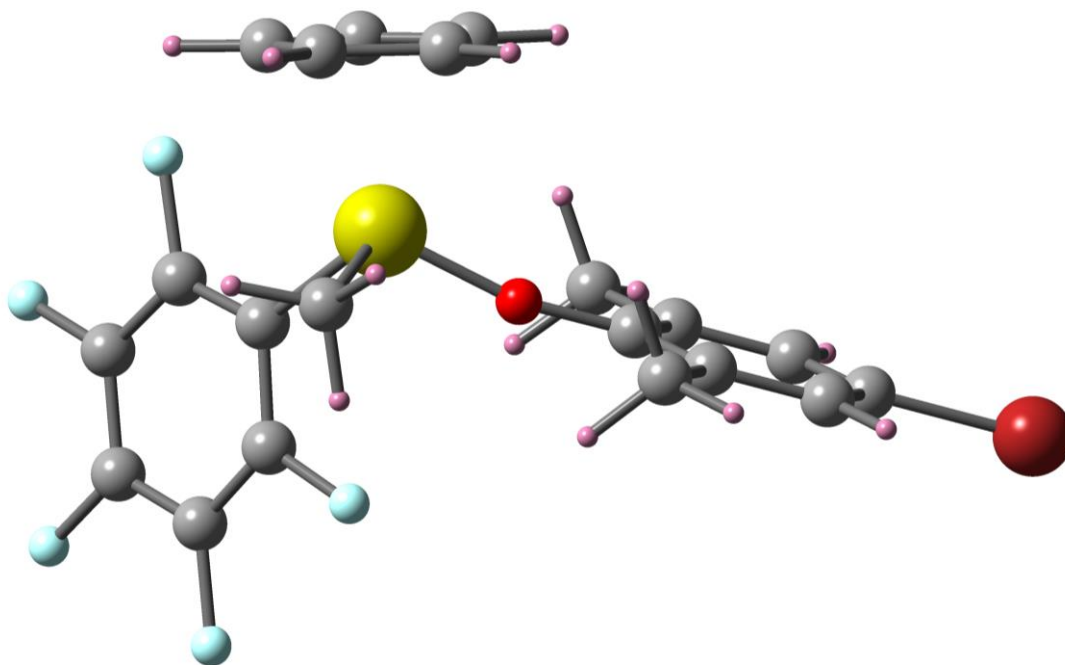
MeB(C₆F₅)₂:



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C	-1.60999100	-0.23184300	1.10488100
C	-2.43145900	0.89034200	-0.83363700
C	-2.83982000	-0.89355200	1.27616900
C	-3.67103000	0.23439200	-0.71652900
C	-3.87590500	-0.66070900	0.35121700
C	1.38014100	0.62512800	-0.13207300
C	1.49452600	-0.59792000	-0.83916500
C	2.57243500	1.06150100	0.49746000
C	2.69144800	-1.33106900	-0.93737500
C	3.78360900	0.34695500	0.44673600
C	3.84313500	-0.85603000	-0.28211100
C	0.02977500	3.02914200	-0.09351100
H	0.11096700	3.36993800	0.95840900
H	0.89043800	3.46609500	-0.61926800
H	-0.90124400	3.45200600	-0.49160200
F	5.02644400	-1.56486800	-0.35621200
F	2.74720100	-2.50892800	-1.66393700
F	0.39012300	-1.10803700	-1.52292500
F	4.91185300	0.81254900	1.10162600
F	2.57077700	2.23429500	1.25139700
F	-0.60679000	-0.47987300	2.04776700
F	-3.03886400	-1.76666900	2.33350400
F	-5.09000100	-1.30769300	0.49152000
F	-4.68391900	0.45693800	-1.63545200
F	-2.25956400	1.74704100	-1.92389700

B	0.02772600	1.45629300	-0.07372500
Frequencies --	20.3185	22.4177	33.8092
Frequencies --	69.8310	102.6646	109.7817
Frequencies --	118.9760	119.4981	139.0897
Frequencies --	148.7524	155.7366	159.8440
Frequencies --	203.9793	209.3464	243.5343
Frequencies --	264.8176	265.6732	266.9414
Frequencies --	270.6820	291.1855	296.8552
Frequencies --	305.7112	318.2450	341.0396
Frequencies --	348.3788	380.8053	381.8448
Frequencies --	421.4750	426.2756	428.6976
Frequencies --	451.5372	476.2155	487.5305
Frequencies --	538.9839	548.9824	603.9927
Frequencies --	632.1362	637.5879	639.8504
Frequencies --	645.6480	714.9270	723.6949
Frequencies --	750.5596	765.7275	800.1397
Frequencies --	871.3759	880.1244	912.2828
Frequencies --	923.7562	1004.8692	1020.6272
Frequencies --	1069.0653	1070.7835	1133.7470
Frequencies --	1138.7273	1244.3903	1257.8786
Frequencies --	1346.5666	1348.2202	1352.0650
Frequencies --	1354.9044	1361.5383	1432.8788
Frequencies --	1436.2103	1452.8787	1470.7408
Frequencies --	1472.8815	1483.9851	1593.6206
Frequencies --	1596.6725	1619.8323	1623.8456
Frequencies --	2991.9250	3097.5038	3158.7282

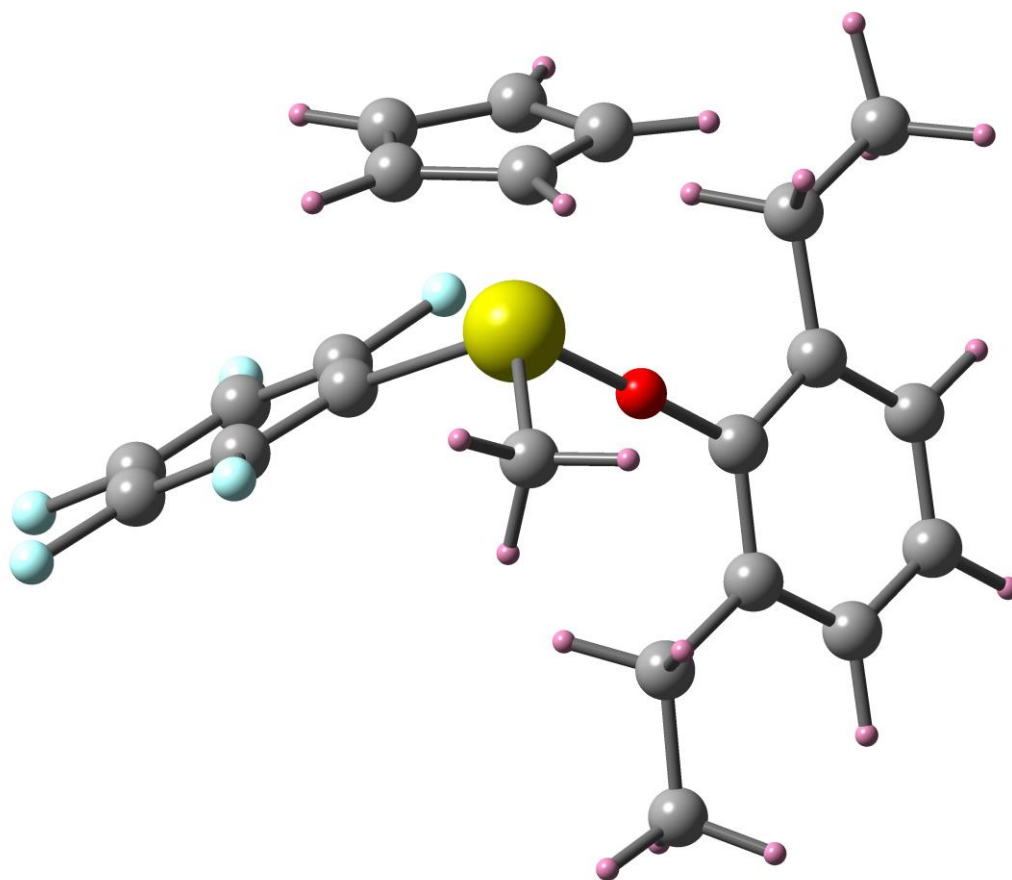
Catalyst 1:

vacuum	toluene-like solvent	D3 dispersion
-1417.0793931	-1417.0865283	-0.2890719

Ti	-1.11038400	1.55761500	0.38483100
C	-1.42942400	2.02227400	2.39743300
H	-1.19760500	1.08376600	2.92845100
H	-0.79904900	2.83239000	2.79368700
H	-2.49046600	2.28534100	2.54885900
O	0.48192600	0.75180200	0.40987600
C	1.77565100	0.30913600	0.19171300
C	2.06074400	-0.47078700	-0.96817500
C	2.77818100	0.62297300	1.15625900
C	3.38805600	-0.91983800	-1.15991300
C	4.09333300	0.15714300	0.92833800
C	4.38616100	-0.60013700	-0.22099200
H	3.62797200	-1.51922200	-2.03749500
H	4.87417300	0.38459200	1.65312500
H	-1.91161500	2.03207800	-2.57710700
C	-1.64952800	2.63958700	-1.71832400
C	-2.57627400	3.17171400	-0.75440500
C	-0.33133500	3.06289200	-1.34752100
H	-3.65097400	3.03093100	-0.76486800
C	-1.82826400	3.91814900	0.21096600
H	0.59033200	2.82479100	-1.87002500
C	-0.43937300	3.84273600	-0.14795400
H	-2.23537000	4.44221700	1.06893800
H	0.38554900	4.29518000	0.39586600
F	-4.95195000	-3.64605200	0.07123000
C	-4.15604200	-2.51145400	0.08068700
C	-4.40672300	-1.45915400	-0.81794200

C	-3.08493900	-2.39975600	0.98568100
C	-3.58433900	-0.31362800	-0.78660500
F	-5.45916400	-1.56532900	-1.72181700
C	-2.29871600	-1.23197800	0.96471100
F	-2.82357800	-3.43519100	1.87630900
C	-2.49868900	-0.13429000	0.09693700
F	-3.91605900	0.67233900	-1.73386100
F	-1.23871900	-1.20063600	1.89257400
C	0.97965400	-0.83648100	-1.97000100
H	0.14809400	-1.36636100	-1.48203700
H	0.55356400	0.05601300	-2.45386200
H	1.37963100	-1.48651900	-2.75976400
C	2.45255100	1.42079400	2.40594300
H	2.10002400	2.43440300	2.15744900
H	1.65397700	0.93598700	2.98679500
H	3.33554200	1.51950200	3.05176800
Br	6.22658300	-1.23521700	-0.51445700

Frequencies --	12.7597	13.7820	26.2258
Frequencies --	36.0799	58.4308	66.6703
Frequencies --	73.8907	83.9601	93.5320
Frequencies --	100.3043	111.4845	120.2379
Frequencies --	129.0005	133.5256	150.2068
Frequencies --	151.8927	170.0402	182.5254
Frequencies --	196.6042	201.5519	212.6616
Frequencies --	225.0265	230.4228	236.2291
Frequencies --	244.3760	248.8656	265.3550
Frequencies --	270.6756	272.5307	301.4475
Frequencies --	321.0893	341.3411	343.2672
Frequencies --	361.5855	382.1749	394.8634
Frequencies --	427.8558	430.7851	460.5328
Frequencies --	500.0446	507.7591	510.2226
Frequencies --	544.2892	561.8791	565.6397
Frequencies --	570.1391	572.4520	577.9466
Frequencies --	593.4439	599.1002	640.9069
Frequencies --	682.3833	690.5579	723.0615
Frequencies --	734.3698	743.5456	792.2832
Frequencies --	800.9952	806.6989	811.3879
Frequencies --	841.1846	842.3786	880.3019
Frequencies --	885.0216	887.5430	891.4351
Frequencies --	902.5949	929.8664	951.4331
Frequencies --	1001.5981	1012.4962	1028.2642
Frequencies --	1034.5978	1044.6095	1051.3259
Frequencies --	1054.4537	1057.8004	1089.7199
Frequencies --	1093.6467	1122.2380	1132.0851
Frequencies --	1177.9133	1193.3814	1225.7743
Frequencies --	1261.5556	1281.2686	1281.6236
Frequencies --	1289.5288	1343.0339	1355.1414
Frequencies --	1391.0764	1397.0845	1401.9659
Frequencies --	1413.8350	1422.0130	1425.9943
Frequencies --	1431.3218	1434.8056	1444.2047
Frequencies --	1446.0180	1449.4334	1458.0268
Frequencies --	1485.1992	1486.4277	1501.1204
Frequencies --	1502.7130	1588.1106	1589.2973
Frequencies --	1591.9252	1599.6309	2986.9492
Frequencies --	3018.9429	3022.9212	3105.8717
Frequencies --	3108.4796	3108.8090	3126.7023
Frequencies --	3136.2553	3136.7272	3197.8422
Frequencies --	3199.9416	3234.5038	3250.0657
Frequencies --	3261.8089	3270.0220	3288.4257

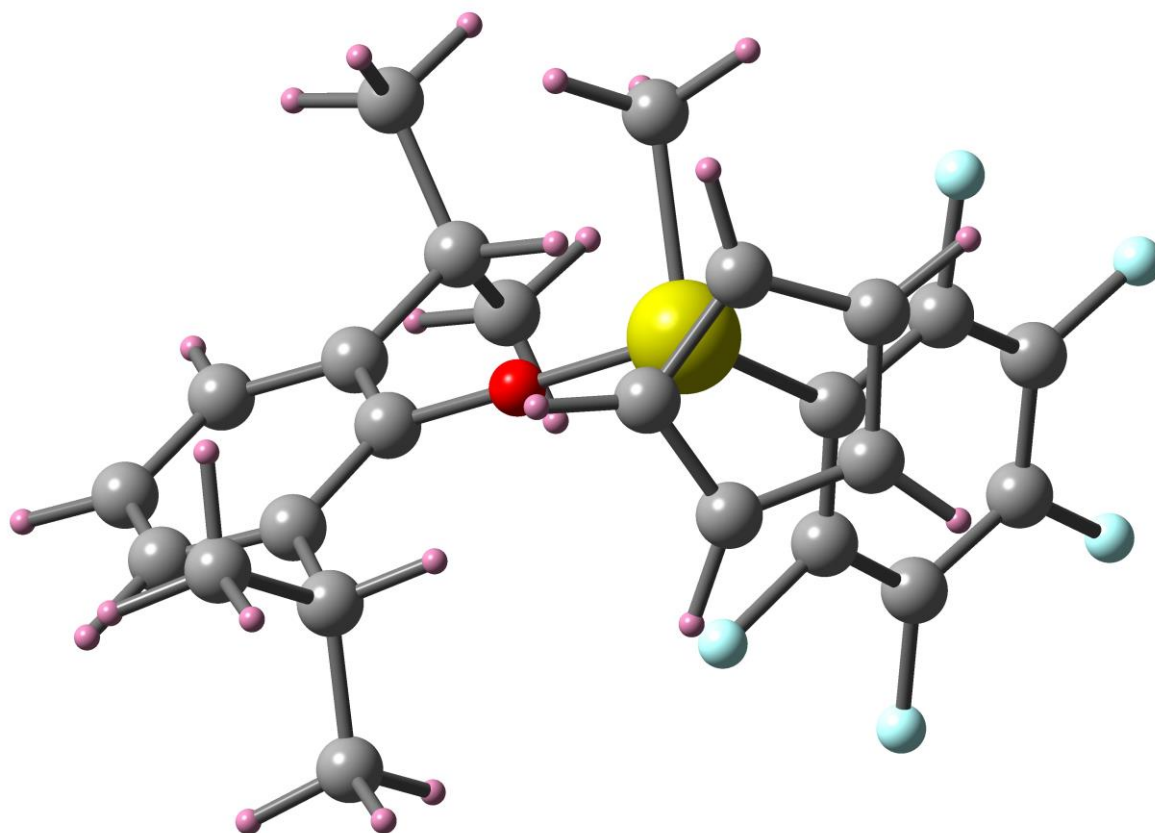
Catalyst 2:

vacuum	toluene-like solvent	D3 dispersion
-1483.0972185	-1483.10384	-0.31652233

Ti	0.01508300	1.43481300	0.63650400
C	-0.07569000	1.51760900	2.72532600
H	-0.29359700	0.47154700	3.00375500
H	0.89683700	1.80910200	3.15611200
H	-0.86783300	2.16934400	3.11697000
O	1.39703800	0.32182800	0.45170600
C	2.45372600	-0.57822700	0.30139300
C	3.39064400	-0.38269300	-0.76035400
C	2.54171300	-1.67792500	1.21123000
C	4.44861400	-1.31365900	-0.87517400
C	3.61939500	-2.57717200	1.04142200
C	4.56740000	-2.39764200	0.01574200
H	5.18429800	-1.19778100	-1.66953500
H	3.71939600	-3.42891600	1.71233400
C	0.20516000	2.99028100	-1.16088700
C	-1.18604600	3.05160100	-0.81098700
C	0.96230400	3.50118500	-0.04915100
C	-1.29032300	3.59875100	0.50953100
C	0.03286900	3.87838200	0.98081800
C	-1.58899200	0.14983900	-0.07770800

C	-2.78536100	-0.05759300	0.62859300
C	-1.47864900	-0.57854000	-1.27475500
C	-3.80198500	-0.94077900	0.21378200
F	-3.01525300	0.65230400	1.82531300
C	-2.45840500	-1.47394300	-1.74482200
F	-0.33685400	-0.41140200	-2.08336900
C	-3.63162100	-1.65760200	-0.98644500
F	-4.96395300	-1.11270600	0.95997800
F	-2.29383000	-2.17132500	-2.93777500
F	-4.61491200	-2.53455500	-1.42248000
C	3.22298500	0.78613400	-1.73033500
H	3.23009600	1.72498900	-1.15227500
C	1.49925800	-1.85853600	2.31474000
H	0.49611600	-1.79217200	1.86194700
H	5.39244900	-3.10464200	-0.09345800
C	4.26115500	0.90355100	-2.86730900
H	5.28400800	1.03884500	-2.48188000
H	4.25476400	0.01782900	-3.52152600
H	4.02472200	1.77858200	-3.49351600
C	1.57911700	-3.16099200	3.14133900
H	0.75947300	-3.17881600	3.87693200
H	1.47842300	-4.05633200	2.50792700
H	2.52469800	-3.24032200	3.70029000
H	0.60658600	2.62575600	-2.09997300
H	-2.01264400	2.73651400	-1.43908300
H	2.04129200	3.61168800	-0.00239200
H	-2.20944200	3.73567100	1.07231400
H	0.29244500	4.29321400	1.94927100
H	1.57113800	-1.00193100	3.00451900
H	2.21824200	0.71429500	-2.17641600
Frequencies --	15.3400	20.7781	26.9452
Frequencies --	41.2441	50.3814	56.0512
Frequencies --	77.1726	82.3119	85.7321
Frequencies --	95.0454	104.1028	114.8494
Frequencies --	126.4171	134.9575	145.8932
Frequencies --	154.2832	176.2590	186.8515
Frequencies --	193.9885	204.8831	206.2208
Frequencies --	216.3818	244.6917	253.2715
Frequencies --	263.6303	265.2153	267.3395
Frequencies --	279.5433	292.8430	295.3664
Frequencies --	303.7644	322.0663	324.1986
Frequencies --	341.4332	354.4693	367.0000
Frequencies --	384.9447	389.4587	426.8813
Frequencies --	463.3968	507.8751	512.3993
Frequencies --	533.2279	543.4060	548.7360
Frequencies --	563.9498	573.4752	580.2734
Frequencies --	582.9375	596.8636	603.1251
Frequencies --	635.2979	681.2263	689.8956
Frequencies --	719.7376	731.4704	732.2075
Frequencies --	738.1350	770.6552	792.0754
Frequencies --	797.2895	804.0108	807.3573
Frequencies --	829.1817	841.2500	842.7368
Frequencies --	854.9712	881.7394	887.4665
Frequencies --	908.7141	919.0161	931.7758
Frequencies --	987.7598	994.5603	997.1099
Frequencies --	1025.8694	1030.6061	1033.0076
Frequencies --	1042.9775	1057.8545	1090.0443
Frequencies --	1091.5044	1094.6786	1101.2621

Frequencies --	1105.0416	1124.4787	1129.8316
Frequencies --	1176.5929	1194.1284	1197.9105
Frequencies --	1202.3265	1264.2360	1276.8009
Frequencies --	1284.5985	1290.7971	1291.2780
Frequencies --	1294.6718	1326.0903	1347.2483
Frequencies --	1355.3359	1384.1991	1391.1185
Frequencies --	1400.5875	1403.1032	1412.6601
Frequencies --	1414.1167	1433.3185	1436.1866
Frequencies --	1438.2967	1446.4690	1449.3428
Frequencies --	1453.7040	1471.8694	1487.0645
Frequencies --	1497.4919	1500.4427	1500.8056
Frequencies --	1504.7863	1509.1167	1589.8673
Frequencies --	1600.5977	1602.4551	1610.5812
Frequencies --	2989.7769	3010.9963	3011.3636
Frequencies --	3022.0659	3026.3581	3070.2369
Frequencies --	3076.1673	3105.0977	3111.9467
Frequencies --	3113.5493	3119.2263	3119.4982
Frequencies --	3146.8014	3166.6911	3200.1211
Frequencies --	3209.3799	3239.2395	3246.7376
Frequencies --	3261.8117	3265.7337	3284.7180

Catalyst 3:

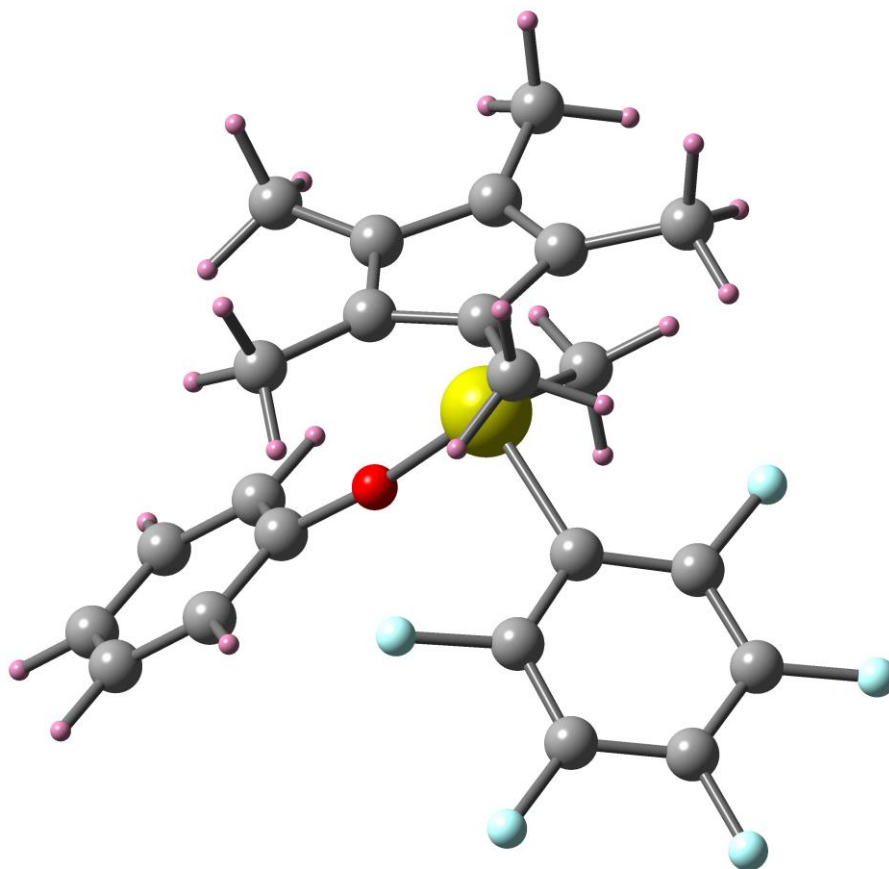
vacuum	toluene-like solvent	D3 dispersion
-1561.6739622	-1561.6801413	-0.35471845

Ti	0.00419900	1.40964200	-0.74669700
C	0.02376200	1.30918000	-2.83649700
H	0.27004100	0.25357700	-3.04829900
H	-0.97619300	1.52862300	-3.24749700
H	0.77239600	1.95942100	-3.30945100
O	-1.25842400	0.18899600	-0.44511500
C	-2.22816500	-0.79447300	-0.23019200
C	-3.36417500	-0.49707500	0.58641400
C	-2.04532600	-2.07877400	-0.83638700
C	-4.33602000	-1.51117500	0.75384700
C	-3.05403500	-3.04912600	-0.62954100
C	-4.19263100	-2.77334800	0.14935800
H	-5.21412900	-1.31104200	1.36935600
H	-2.94295700	-4.03571500	-1.08113300
C	1.05961700	3.24274900	0.55858100
C	1.14277200	3.67839900	-0.80475400
C	-0.32746900	3.09739400	0.89850200
C	-0.18940200	3.80978800	-1.31154300
C	-1.10351400	3.44725900	-0.26286600
C	1.71432300	0.35687200	0.08248400

C	2.92168000	0.17885700	-0.61143600
C	1.67082500	-0.23596400	1.35601800
C	4.01646800	-0.55339600	-0.11109800
F	3.07768700	0.76445900	-1.88559300
C	2.72990300	-0.97857300	1.91247200
F	0.51728600	-0.08339200	2.15091200
C	3.91402800	-1.13947500	1.16554100
F	5.18820600	-0.70405800	-0.84661900
F	2.63220600	-1.54927000	3.17824000
F	4.97434600	-1.86776900	1.68693600
C	-3.54332300	0.85488700	1.29086300
H	-2.69609400	1.48850500	1.01180000
C	-0.80758700	-2.43532300	-1.67316300
H	-0.13709800	-1.56841700	-1.67441200
H	-4.95744200	-3.53945300	0.29209900
C	-4.83595300	1.58957800	0.83127000
H	-4.85138200	1.71949900	-0.26272800
H	-5.74471400	1.03690500	1.11393800
H	-4.89580800	2.58672500	1.29784000
C	-3.49790000	0.70021500	2.83970100
H	-2.56129600	0.21793000	3.15938300
H	-3.55881600	1.68840200	3.32507000
H	-4.33538700	0.09217400	3.21426300
C	-0.00774100	-3.61580400	-1.04752100
H	0.91963500	-3.78859300	-1.61753900
H	0.26718900	-3.39904800	-0.00366500
H	-0.58338000	-4.55394500	-1.05493400
C	-1.17709500	-2.73168400	-3.15603700
H	-1.71211000	-1.88298800	-3.60933600
H	-0.26499200	-2.91581600	-3.74666100
H	-1.81928900	-3.62134500	-3.24575800
H	1.89784900	3.05281300	1.22058900
H	2.05805600	3.84044700	-1.36748800
H	-0.71364600	2.77889300	1.86127600
H	-0.46465500	4.11653700	-2.31524900
H	-2.18657900	3.46615100	-0.33220000

Frequencies --	14.4043	19.8655	25.1319
Frequencies --	32.5892	39.5895	50.3358
Frequencies --	57.4882	67.1004	71.7603
Frequencies --	81.1752	93.8330	112.6811
Frequencies --	120.5658	124.1197	127.1317
Frequencies --	141.6763	153.1043	164.0819
Frequencies --	175.8003	197.9345	202.2918
Frequencies --	209.7340	222.8907	225.4459
Frequencies --	236.0295	239.5447	242.3176
Frequencies --	248.6411	256.1828	263.9305
Frequencies --	264.9690	270.6872	287.6717
Frequencies --	295.0141	303.4373	314.1341
Frequencies --	317.0730	339.2190	341.9176
Frequencies --	382.6718	387.0092	424.0653
Frequencies --	426.2065	430.5950	434.7042
Frequencies --	463.5297	512.5961	541.3230
Frequencies --	543.0457	546.3775	565.9266
Frequencies --	576.5448	582.4885	597.6367
Frequencies --	602.4092	610.3857	630.2069
Frequencies --	635.9235	682.3069	690.7930
Frequencies --	726.7109	732.7358	740.2379
Frequencies --	766.0266	788.0384	797.6666

Frequencies --	798.9709	812.5665	816.9755
Frequencies --	841.1321	842.1814	878.2420
Frequencies --	882.3435	886.7079	916.5814
Frequencies --	925.2020	932.2913	932.6991
Frequencies --	935.9698	941.7880	962.7054
Frequencies --	964.6380	988.8714	996.6592
Frequencies --	1030.5783	1033.4766	1042.4809
Frequencies --	1056.6624	1073.0607	1089.8353
Frequencies --	1094.6654	1117.3603	1119.8005
Frequencies --	1121.1261	1129.6034	1166.5946
Frequencies --	1181.1352	1185.2472	1194.2781
Frequencies --	1198.5320	1204.5771	1260.9948
Frequencies --	1280.2681	1285.0697	1294.4342
Frequencies --	1307.7657	1333.2759	1334.9591
Frequencies --	1336.7314	1356.4474	1385.0863
Frequencies --	1390.3123	1398.8880	1399.7346
Frequencies --	1400.0639	1404.6185	1417.3782
Frequencies --	1418.1467	1431.7734	1437.9882
Frequencies --	1442.8690	1445.8108	1450.1426
Frequencies --	1453.0885	1475.4321	1487.7766
Frequencies --	1488.2052	1489.5236	1490.0359
Frequencies --	1500.0327	1500.9267	1506.4735
Frequencies --	1507.3753	1590.6981	1599.3677
Frequencies --	1600.7084	1608.3998	2988.9199
Frequencies --	3004.1923	3006.2269	3008.6856
Frequencies --	3010.2896	3097.2456	3102.2708
Frequencies --	3102.9072	3105.5314	3106.0523
Frequencies --	3111.2227	3114.8773	3115.6370
Frequencies --	3118.2893	3133.2478	3142.5735
Frequencies --	3146.7513	3162.1419	3180.9811
Frequencies --	3195.9152	3238.3260	3247.7609
Frequencies --	3260.6200	3264.6881	3282.0196

Catalyst 4:

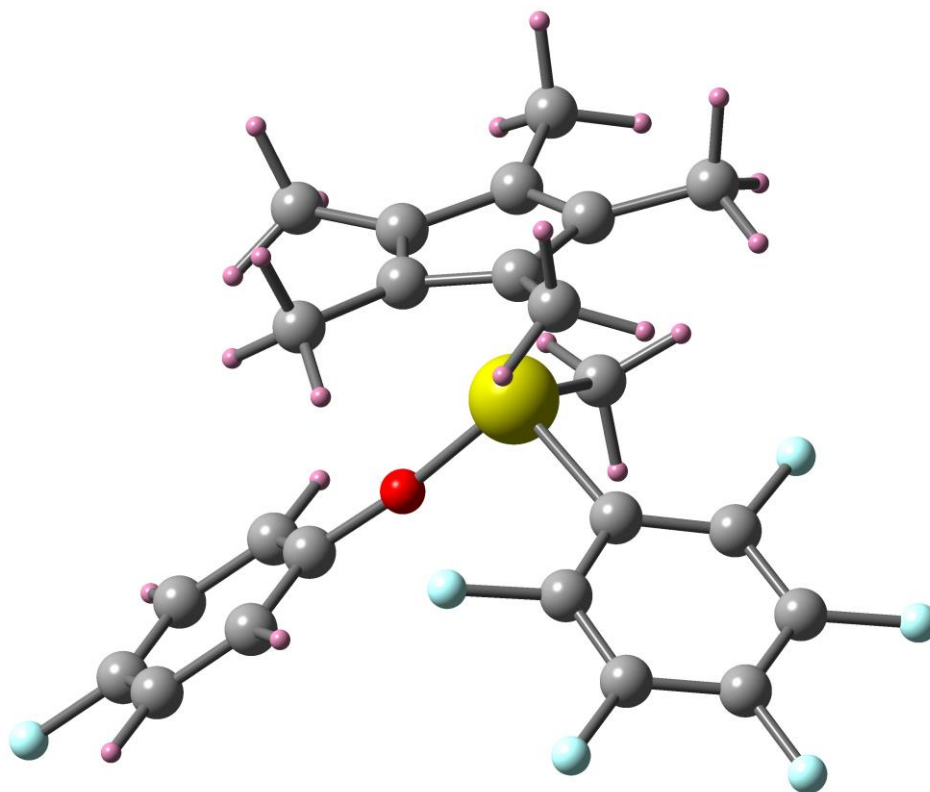
vacuum	toluene-like solvent	D3 dispersion
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Ti	-0.53826000	0.72159400	-0.40909600
C	-0.71675500	1.31311700	-2.40483900
H	-0.39110100	0.39720200	-2.93570800
H	-1.75239800	1.54161300	-2.70145000
H	-0.05766500	2.14850800	-2.67962200
O	-1.61975600	-0.69863300	-0.52052700
C	-2.56703800	-1.70289900	-0.54193300
C	-2.48483900	-2.77969300	0.37689000
C	-3.60579200	-1.66468800	-1.50715200
C	-3.44814600	-3.80806200	0.32853700
C	-4.56219400	-2.69976300	-1.54386500
C	-4.48941600	-3.77349500	-0.62711800
H	-3.38030800	-4.63860800	1.03512700
H	-5.35984000	-2.66855300	-2.28988700
C	0.16797400	2.05087200	1.54840700
C	0.10945400	2.98757400	0.45016900
C	-1.16360900	1.51961900	1.75350500
C	-1.25196700	3.04496200	-0.02318600
C	-2.04083000	2.12929400	0.77867700
C	1.43042800	-0.22886500	-0.21303000

C	2.52824100	0.10576900	-1.02437100
C	1.66384900	-1.31021700	0.65251600
C	3.76221000	-0.57512800	-1.01122200
F	2.42954900	1.19447400	-1.91640800
C	2.86982800	-2.03402500	0.71635500
F	0.64967300	-1.71593000	1.54900600
C	3.93107200	-1.66068000	-0.13076200
F	4.81194200	-0.19385600	-1.84292200
F	3.03523200	-3.09781200	1.60042200
F	5.13500700	-2.35100300	-0.09169700
C	1.35536300	1.82662200	2.45686400
H	1.36699000	2.59408300	3.25092800
H	1.32094300	0.84748300	2.95076500
H	2.31126500	1.89866500	1.92147700
C	1.25084200	3.84555900	-0.04598300
H	1.25283000	4.81680000	0.48043400
H	2.22854200	3.37821900	0.12764200
H	1.17440900	4.05923600	-1.12079000
C	-1.58850100	0.60995100	2.88472800
H	-0.80661000	-0.11109000	3.15488400
H	-1.81124000	1.20895600	3.78543200
H	-2.49496000	0.03975300	2.64173200
C	-1.79698300	4.04034600	-1.02066100
H	-2.03983500	4.98728200	-0.50709600
H	-1.07476600	4.27614000	-1.81332000
H	-2.71776200	3.68701800	-1.50337900
C	-3.54230000	1.95908200	0.70809400
H	-3.86250900	0.95900400	1.02837800
H	-4.03852500	2.69065100	1.37000000
H	-3.93298800	2.12273700	-0.30576000
H	-5.23080700	-4.57423600	-0.66013300
H	-1.67208700	-2.80446800	1.10081900
H	-3.64978100	-0.83677700	-2.21549400

Frequencies --	17.8103	22.3830	26.5543
Frequencies --	34.4749	42.4156	46.8339
Frequencies --	73.8585	79.9381	84.7706
Frequencies --	100.7680	108.4580	117.3708
Frequencies --	123.7542	128.8055	129.0616
Frequencies --	137.9208	149.0607	151.3977
Frequencies --	157.0225	163.8321	166.3964
Frequencies --	171.1841	197.6575	203.3420
Frequencies --	207.4456	224.9388	246.3325
Frequencies --	264.6370	266.9111	286.3683
Frequencies --	291.0357	293.8512	298.0051
Frequencies --	302.8341	309.0444	315.4084
Frequencies --	332.6540	347.3689	383.5872
Frequencies --	385.3582	389.8176	410.5900
Frequencies --	411.7014	427.7829	448.5847
Frequencies --	461.8218	508.4197	514.1576
Frequencies --	536.3675	540.3104	542.9378
Frequencies --	555.6452	572.2379	583.0414
Frequencies --	596.0409	603.5947	615.1675
Frequencies --	615.3523	633.7297	644.1746
Frequencies --	682.7431	689.2642	693.4600
Frequencies --	723.2268	730.1470	762.8250
Frequencies --	803.0353	804.1882	839.5077
Frequencies --	884.0121	917.9688	920.3408
Frequencies --	968.5824	970.0231	974.5401

Frequencies --	994.1337	994.7652	1011.2342
Frequencies --	1030.3970	1037.6206	1043.6963
Frequencies --	1044.2298	1048.0648	1050.4693
Frequencies --	1051.1141	1086.4784	1087.9382
Frequencies --	1088.2816	1124.0240	1172.3487
Frequencies --	1173.5040	1177.1941	1181.1676
Frequencies --	1189.4569	1191.3704	1256.4205
Frequencies --	1288.1635	1324.6916	1355.1391
Frequencies --	1373.8343	1396.8259	1411.2140
Frequencies --	1412.8646	1422.8786	1424.6997
Frequencies --	1426.6010	1429.6644	1431.1349
Frequencies --	1431.5278	1437.6681	1450.3587
Frequencies --	1453.3542	1454.0950	1457.9504
Frequencies --	1462.0758	1480.0046	1486.5373
Frequencies --	1489.8312	1491.1790	1497.3141
Frequencies --	1499.0207	1504.9614	1506.9435
Frequencies --	1511.5891	1512.9380	1515.6615
Frequencies --	1589.2849	1594.5638	1600.2533
Frequencies --	1610.0043	2974.1685	3004.0568
Frequencies --	3005.3264	3006.6297	3007.4109
Frequencies --	3008.6807	3092.9540	3097.0245
Frequencies --	3098.1258	3100.2979	3101.0213
Frequencies --	3102.4692	3135.8020	3138.8940
Frequencies --	3140.5232	3143.0241	3146.0300
Frequencies --	3148.1054	3159.2913	3168.1987
Frequencies --	3188.2505	3200.6373	3222.2991

Catalyst 5:

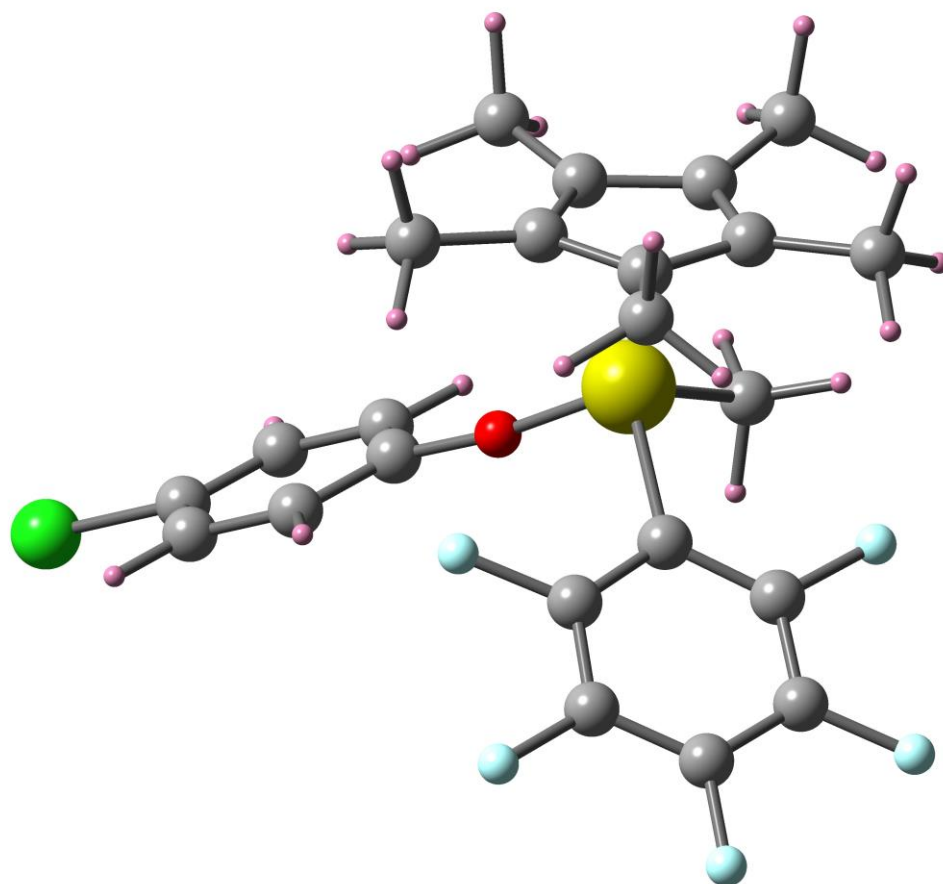
vacuum	toluene-like solvent	D3 dispersion
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Ti	-0.09611500	0.94774400	-0.40634500
C	-0.13218100	1.52898400	-2.41144000
H	-0.10516100	0.54847400	-2.92590500
H	-1.05731300	2.05193500	-2.70008400
H	0.74076700	2.12403400	-2.71410400
O	-1.54606800	-0.10467500	-0.46896200
C	-2.73412800	-0.80240400	-0.44795000
C	-2.91403900	-1.87785300	0.46011500
C	-3.76550100	-0.45738500	-1.35992200
C	-4.12286100	-2.60117600	0.46062900
C	-4.97583100	-1.17805600	-1.36238700
C	-5.12971800	-2.23509100	-0.44894300
H	-4.28187300	-3.43348800	1.14615000
H	-5.78052900	-0.93215300	-2.05514100
C	0.97782600	2.03961700	1.53248300
C	1.21165600	2.92283400	0.41332500
C	-0.45276800	1.94505900	1.73538400
C	-0.06603200	3.38530900	-0.07228300
C	-1.09890500	2.77291000	0.74088800
C	1.51211800	-0.52789200	-0.21275100
C	2.64034600	-0.55381300	-1.05102200
C	1.43409700	-1.61063800	0.67840900
C	3.61657600	-1.57051800	-1.03664600

F	2.84683800	0.49122300	-1.97549600
C	2.37169100	-2.65858200	0.74523600
F	0.36302500	-1.67762900	1.59841500
C	3.47645400	-2.63672200	-0.12791400
F	4.71109900	-1.53826900	-1.89626400
F	2.23271800	-3.70308900	1.65594200
F	4.42145700	-3.65251400	-0.08765900
C	2.03821600	1.48621300	2.45688100
H	2.27374200	2.23039600	3.23816500
H	1.71100000	0.57194100	2.96764100
H	2.97521100	1.26044800	1.93105700
C	2.56274600	3.37645800	-0.09027600
H	2.86699300	4.30564600	0.42371100
H	3.34634500	2.63022800	0.09316000
H	2.55601200	3.58824400	-1.16802400
C	-1.14044600	1.23044000	2.87720300
H	-0.59629800	0.33091600	3.19169900
H	-1.20862200	1.89891000	3.75355500
H	-2.16418300	0.92605600	2.62116300
C	-0.27680200	4.47841100	-1.09390600
H	-0.23132100	5.46456500	-0.59921400
H	0.49277300	4.47134000	-1.87686400
H	-1.25469100	4.40693300	-1.58835900
C	-2.57978400	3.07189000	0.66351500
H	-3.19439000	2.22063800	0.98500500
H	-2.82896600	3.92214900	1.32269100
H	-2.89731300	3.34720400	-0.35183500
H	-2.11051700	-2.14219200	1.14438900
H	-3.61047100	0.36351500	-2.05973900
F	-6.33897200	-2.95712900	-0.44822700

Frequencies --	17.9844	20.2330	31.2162
Frequencies --	35.2652	40.3422	43.9063
Frequencies --	79.1887	82.4325	93.2578
Frequencies --	100.3056	104.4231	111.3395
Frequencies --	116.2143	119.6844	126.0433
Frequencies --	127.4160	146.9820	150.4537
Frequencies --	155.9316	162.4661	167.3506
Frequencies --	170.2708	187.2188	200.7518
Frequencies --	205.7035	223.5248	236.5582
Frequencies --	262.6979	264.6817	269.7142
Frequencies --	284.7859	292.1234	293.8300
Frequencies --	298.8359	301.0182	306.2179
Frequencies --	323.1248	345.6287	359.6235
Frequencies --	364.1669	384.4356	391.7456
Frequencies --	398.5387	408.6517	419.3352
Frequencies --	427.7692	458.8431	463.1580
Frequencies --	507.7119	515.2500	536.6222
Frequencies --	540.2556	543.1726	555.2689
Frequencies --	560.7934	571.4644	583.0462
Frequencies --	595.7940	605.5110	614.1561
Frequencies --	633.3739	633.8991	669.0389
Frequencies --	688.0191	706.9460	723.8657
Frequencies --	730.2676	789.1212	802.8536
Frequencies --	804.2598	812.2237	837.0223
Frequencies --	884.3412	917.3986	948.8954
Frequencies --	965.8155	967.1481	970.9687
Frequencies --	994.9568	1015.9663	1037.8394
Frequencies --	1043.0031	1044.8372	1048.5670

Frequencies --	1050.6214	1050.9833	1086.4388
Frequencies --	1087.5790	1112.1201	1123.8630
Frequencies --	1168.3704	1170.4985	1173.3991
Frequencies --	1177.1379	1190.6949	1201.1896
Frequencies --	1267.4146	1288.7439	1306.4767
Frequencies --	1354.5334	1357.6107	1396.6696
Frequencies --	1411.2643	1413.2428	1421.9744
Frequencies --	1423.7235	1423.9794	1426.9424
Frequencies --	1430.1876	1431.4685	1431.6725
Frequencies --	1436.5148	1450.6957	1454.3271
Frequencies --	1457.7679	1462.6538	1479.5597
Frequencies --	1490.8102	1491.3935	1497.7066
Frequencies --	1498.5126	1499.3978	1505.0109
Frequencies --	1506.5023	1511.7946	1513.3026
Frequencies --	1515.1453	1588.6781	1599.3381
Frequencies --	1600.5439	1618.1233	2974.4905
Frequencies --	3005.4436	3005.9255	3007.2318
Frequencies --	3008.6210	3009.6921	3093.9361
Frequencies --	3096.4726	3099.8044	3101.3037
Frequencies --	3101.4737	3103.0967	3136.1660
Frequencies --	3139.1590	3141.5592	3143.2672
Frequencies --	3146.2489	3149.2778	3194.3817
Frequencies --	3203.6817	3213.9082	3232.4838

Catalyst 6:

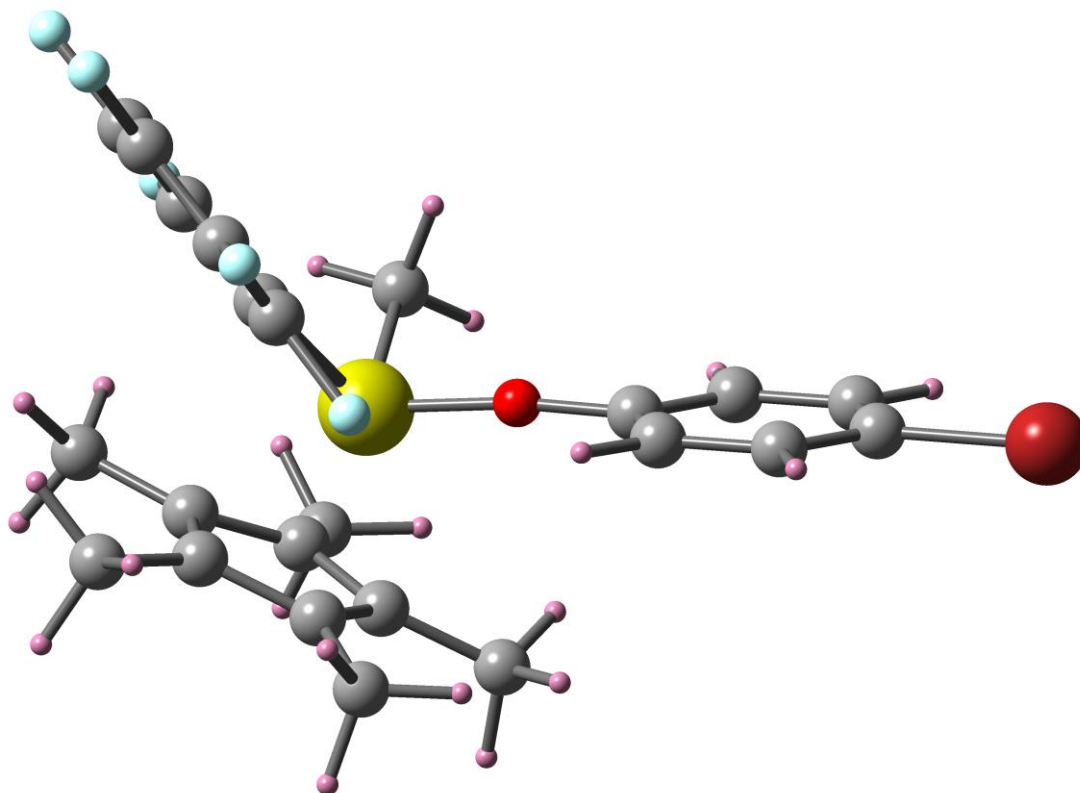
vacuum	toluene-like solvent	D3 dispersion
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Ti	0.29728500	1.00344900	-0.40213800
C	0.34109200	1.56878400	-2.41163800
H	0.19842300	0.59392800	-2.91781800
H	-0.48355700	2.23884100	-2.70061800
H	1.30070100	2.00475000	-2.72350800
O	-1.30767700	0.20371200	-0.44234300
C	-2.59906700	-0.27239600	-0.40183800
C	-2.95455800	-1.29444900	0.51493000
C	-3.56668200	0.24660600	-1.30023300
C	-4.27387000	-1.78885800	0.53529900
C	-4.88510300	-0.24947700	-1.27825700
C	-5.22861300	-1.25963900	-0.35677000
H	-4.54977500	-2.57607600	1.23686200
H	-5.63028600	0.14580200	-1.96854500
C	1.55115700	1.91327800	1.51777000
C	1.91770400	2.74313300	0.39296600
C	0.12654100	2.05648600	1.73386400
C	0.72920100	3.40436100	-0.08671300
C	-0.38338500	2.97326700	0.73833200
C	1.64968800	-0.71160700	-0.21095400

C	2.75704100	-0.90784700	-1.05412100
C	1.40808200	-1.77185700	0.67791700
C	3.56315600	-2.06390700	-1.04922900
F	3.11891600	0.09857600	-1.97368900
C	2.17230900	-2.95284300	0.73582000
F	0.34425600	-1.67530600	1.60343600
C	3.26268400	-3.09913900	-0.14355800
F	4.64529500	-2.19892600	-1.91443200
F	1.87781000	-3.96712700	1.64356400
F	4.03777700	-4.24996500	-0.11190500
C	2.51517000	1.19669000	2.43568600
H	2.89062500	1.89848300	3.20137400
H	2.04245200	0.36017400	2.96549600
H	3.38908900	0.80393200	1.89948500
C	3.32200500	2.97046000	-0.11797200
H	3.79252000	3.80821500	0.42708200
H	3.96354300	2.09082500	0.02078900
H	3.33969900	3.22608500	-1.18580200
C	-0.65711600	1.46932300	2.88621200
H	-0.27422900	0.48729800	3.19201300
H	-0.59271200	2.13648500	3.76380100
H	-1.72219800	1.34991600	2.64714400
C	0.68594300	4.51428100	-1.11063100
H	0.88171300	5.48287600	-0.61786200
H	1.44341700	4.39043400	-1.89563400
H	-0.29301200	4.59204500	-1.60201000
C	-1.79327300	3.51640100	0.66386700
H	-2.52960200	2.82560100	1.09464300
H	-1.86323700	4.46328900	1.22760100
H	-2.10369000	3.73158700	-0.36836700
H	-2.20381900	-1.69868200	1.19118900
H	-3.28433700	1.02243400	-2.01168900
Cl	-6.93927700	-1.90325900	-0.32806600

Frequencies --	17.4010	18.6230	27.1690
Frequencies --	32.6660	42.0159	47.0478
Frequencies --	76.9190	80.7869	86.7470
Frequencies --	98.1690	107.6336	112.5217
Frequencies --	120.3409	121.0529	127.7086
Frequencies --	134.0962	136.2043	148.9845
Frequencies --	155.3764	156.3020	162.8727
Frequencies --	169.4284	172.2524	202.8898
Frequencies --	205.1098	211.2825	223.7426
Frequencies --	248.5791	264.5701	266.4315
Frequencies --	271.5192	281.0360	290.6843
Frequencies --	294.0909	295.4732	297.4982
Frequencies --	302.3029	321.1834	325.9757
Frequencies --	346.1261	375.8986	386.0137
Frequencies --	388.5659	408.8274	412.1432
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Frequencies --	468.3029	484.4782	510.7251
Frequencies --	536.3386	539.8754	542.7987
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Frequencies --	627.9594	634.3639	638.2610
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Frequencies --	724.3480	731.1749	783.3129
Frequencies --	792.7834	802.4054	804.0180
Frequencies --	884.4091	915.6304	931.1406

Frequencies --	951.0158	967.3570	971.0688
Frequencies --	994.7789	1013.2217	1038.5167
Frequencies --	1042.8604	1044.0246	1048.5155
Frequencies --	1049.1647	1051.7033	1073.4860
Frequencies --	1086.4297	1088.1312	1114.6674
Frequencies --	1123.6630	1172.9238	1174.3609
Frequencies --	1176.5661	1189.2236	1191.2992
Frequencies --	1263.6555	1289.3172	1307.5595
Frequencies --	1350.6320	1355.7572	1397.9608
Frequencies --	1410.8440	1412.4429	1414.3453
Frequencies --	1423.3475	1424.3089	1427.4233
Frequencies --	1430.5730	1432.3184	1433.3116
Frequencies --	1438.4903	1450.5850	1454.5496
Frequencies --	1458.1293	1462.2407	1480.0742
Frequencies --	1486.7443	1490.3107	1491.8017
Frequencies --	1497.8595	1498.9576	1504.4728
Frequencies --	1507.2138	1510.5279	1511.5695
Frequencies --	1517.3390	1580.1538	1589.8176
Frequencies --	1600.6034	1604.7741	2974.6355
Frequencies --	3005.7421	3005.9469	3007.3787
Frequencies --	3008.2082	3009.5025	3093.7670
Frequencies --	3095.0585	3100.1492	3101.2478
Frequencies --	3101.6449	3102.9202	3135.9277
Frequencies --	3138.6233	3141.8905	3142.9613
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Catalyst 7:

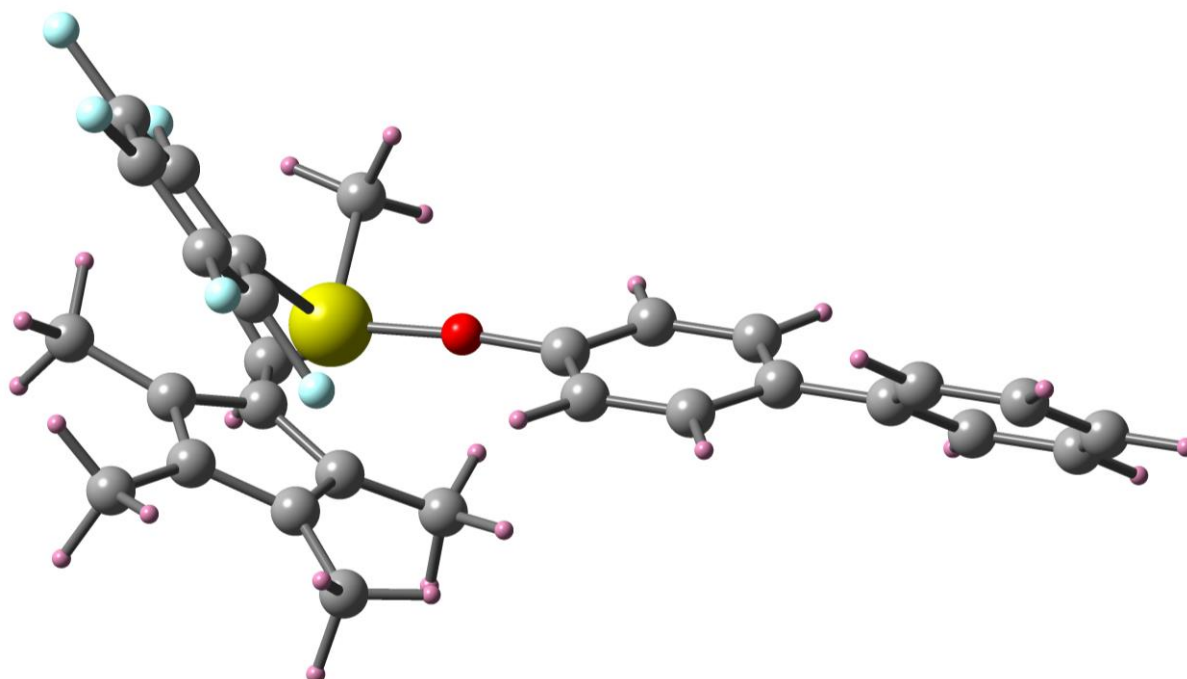
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Ti	-0.91245000	-1.02868400	-0.39678000
C	-1.00036100	-1.57015500	-2.41202600
H	-0.75109500	-0.61228000	-2.90915600
H	-0.24911300	-2.32163700	-2.70068400
H	-1.99809300	-1.90024600	-2.73398300
O	0.77840100	-0.43150200	-0.41223000
C	2.11778200	-0.11897100	-0.35290600
C	2.59442200	0.81831300	0.59833700
C	3.02151000	-0.71789600	-1.26722300
C	3.96457100	1.14523100	0.64049600
C	4.39187500	-0.39221200	-1.22613700
C	4.85388800	0.53566300	-0.26915800
H	4.32478000	1.86872600	1.37219700
H	5.08120900	-0.85544600	-1.93246900
C	-2.34275900	-1.81267600	1.45270600
C	-2.71619500	-2.61811900	0.31284700
C	-0.94915200	-2.07739600	1.74922100
C	-1.56330600	-3.38176300	-0.09744900
C	-0.46564400	-3.04302300	0.78778100
C	-2.04164200	0.84013200	-0.21130800

C	-3.11368200	1.17768300	-1.05551500
C	-1.67026400	1.86063600	0.67982900
C	-3.76684000	2.42657100	-1.05017500
F	-3.59953400	0.22783600	-1.97803500
C	-2.27777000	3.12941800	0.73769800
F	-0.63002000	1.62964900	1.60820200
C	-3.33913500	3.41455400	-0.14295500
F	-4.82219500	2.69806700	-1.91646600
F	-1.85762600	4.09691600	1.64699900
F	-3.96179200	4.65449700	-0.11137200
C	-3.28795100	-1.00639300	2.31436000
H	-3.74197800	-1.65889100	3.08092900
H	-2.77632000	-0.19188200	2.84251500
H	-4.10927500	-0.56639500	1.73378300
C	-4.10214200	-2.73145300	-0.27988000
H	-4.65795800	-3.55051000	0.21050000
H	-4.68922500	-1.81382500	-0.14764100
H	-4.07703800	-2.95478800	-1.35502600
C	-0.18362000	-1.55195200	2.94286800
H	-0.49560100	-0.53829500	3.22423800
H	-0.35511300	-2.20489100	3.81678200
H	0.89951600	-1.52672700	2.76399300
C	-1.55791700	-4.49584200	-1.11777800
H	-1.90262800	-5.43345400	-0.64723700
H	-2.22601100	-4.29290300	-1.96508200
H	-0.55471400	-4.68516500	-1.52226400
C	0.89463500	-3.70464400	0.79078100
H	1.65751200	-3.08713800	1.28202600
H	0.84827800	-4.66345700	1.33655500
H	1.25273100	-3.92752100	-0.22438500
H	1.89619700	1.29024000	1.28699400
H	2.65054900	-1.42769900	-2.00668600
Br	6.76853600	0.98915300	-0.20483800

Frequencies --	14.6932	18.3562	26.7491
Frequencies --	31.3197	39.0079	43.1723
Frequencies --	74.9261	79.2083	91.0870
Frequencies --	95.2962	107.0645	110.0804
Frequencies --	114.6690	119.2701	127.0832
Frequencies --	129.6777	138.4045	148.9807
Frequencies --	155.4610	156.5788	162.3243
Frequencies --	169.6533	174.9888	199.9041
Frequencies --	204.6765	209.9011	218.3226
Frequencies --	238.9158	251.5585	262.1198
Frequencies --	265.2205	270.7500	290.2090
Frequencies --	292.9732	294.5309	298.3094
Frequencies --	302.8773	320.2689	343.9058
Frequencies --	345.2692	375.2299	385.1011
Frequencies --	388.9442	396.0529	414.2400
Frequencies --	426.8467	433.5541	453.0282
Frequencies --	462.3089	506.9614	511.7071
Frequencies --	536.3415	540.4154	543.3144
Frequencies --	555.3498	574.8866	582.7005
Frequencies --	595.6798	605.2402	613.7921
Frequencies --	629.3091	634.1169	660.9559
Frequencies --	687.0451	695.5750	700.9978
Frequencies --	723.8539	731.1872	802.7049
Frequencies --	803.7770	823.0190	837.7360
Frequencies --	884.4162	919.0568	956.5906

Frequencies --	968.0422	970.0246	972.8235
Frequencies --	995.2193	1019.9374	1038.0611
Frequencies --	1041.8855	1044.4807	1047.6312
Frequencies --	1049.0372	1049.6108	1063.3564
Frequencies --	1085.9563	1087.5505	1114.5282
Frequencies --	1123.3531	1172.4684	1175.6079
Frequencies --	1177.1914	1190.3775	1192.2309
Frequencies --	1264.6388	1288.8360	1306.9649
Frequencies --	1347.4206	1354.2095	1396.1148
Frequencies --	1407.4365	1409.6093	1413.7126
Frequencies --	1422.4067	1424.5989	1426.2144
Frequencies --	1429.9428	1431.5281	1432.8339
Frequencies --	1438.1108	1450.4657	1454.7342
Frequencies --	1457.7944	1462.4655	1479.3236
Frequencies --	1481.9101	1490.6187	1491.4287
Frequencies --	1497.1001	1498.7545	1504.3210
Frequencies --	1505.3145	1510.9856	1512.5921
Frequencies --	1516.4529	1576.1350	1588.5630
Frequencies --	1599.2028	1600.7116	2974.9049
Frequencies --	3005.4348	3005.8059	3007.4037
Frequencies --	3008.4494	3009.5419	3093.8865
Frequencies --	3094.1610	3099.4541	3100.9739
Frequencies --	3101.8536	3103.3249	3135.2003
Frequencies --	3138.9229	3141.9486	3143.4986
Frequencies --	3146.7184	3148.6241	3188.5545
Frequencies --	3196.5137	3207.8803	3227.3594

Catalyst 8:

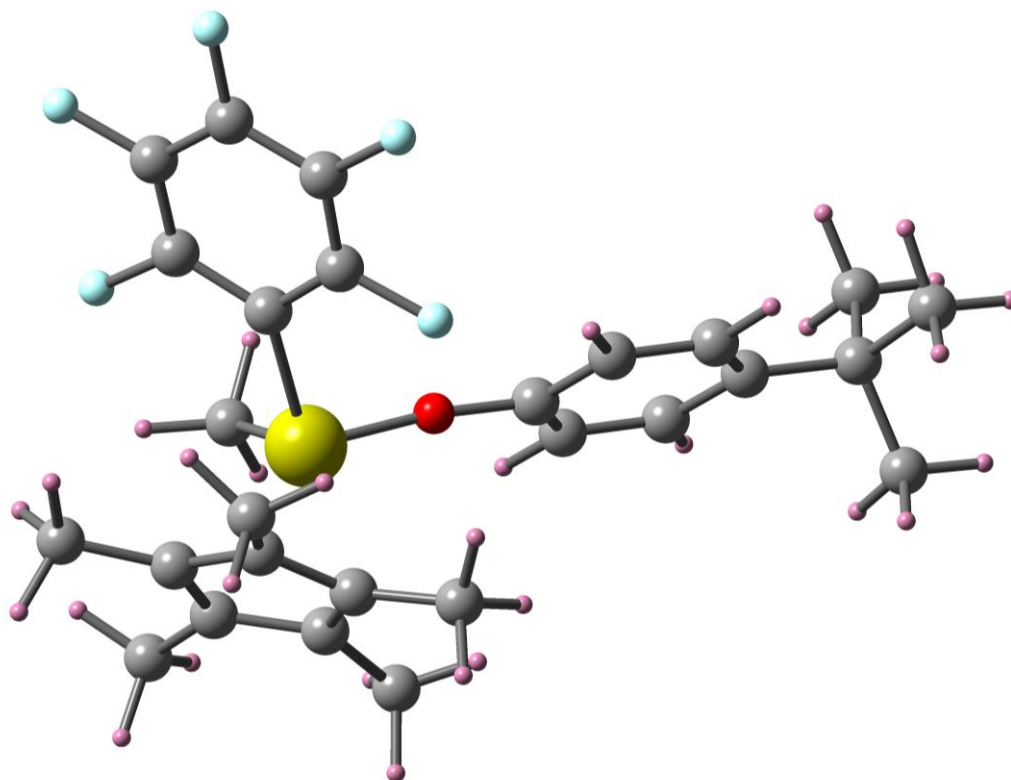
vacuum	toluene-like solvent	D3 dispersion
-1753.3602178	-1753.3674624	-0.40963283

Ti	-1.27650000	-1.02869300	-0.39746900
C	-1.38717500	-1.58719000	-2.40757100
H	-1.06158400	-0.65824400	-2.91520400
H	-0.68896100	-2.39606500	-2.67469900
H	-2.40199700	-1.84844100	-2.73887800
O	0.44457100	-0.53701100	-0.40945500
C	1.80174500	-0.30055600	-0.34892200
C	2.32872000	0.62289400	0.58798500
C	2.67729600	-0.96264600	-1.24597100
C	3.71259800	0.86929300	0.62362900
C	4.05920200	-0.70580300	-1.19649200
C	4.61246200	0.21339300	-0.26190000
H	4.09934200	1.56435800	1.37055000
H	4.71091700	-1.20321400	-1.91660700
C	-2.65876900	-1.67925200	1.54434300
C	-3.21528800	-2.39580500	0.42030700
C	-1.29228400	-2.12252800	1.72482400
C	-2.20475200	-3.28992700	-0.09091000
C	-1.00966900	-3.11564500	0.71165800
C	-2.28758800	0.91030600	-0.23127500
C	-3.32365500	1.31592500	-1.09003800
C	-1.86130900	1.90468000	0.66463700
C	-3.89602400	2.60396500	-1.09047300
F	-3.85554200	0.40084000	-2.02229300
C	-2.38734600	3.20952000	0.71679400
F	-0.84848100	1.60677400	1.60376200
C	-3.41776700	3.56175400	-0.17619600

F	-4.92056200	2.94379400	-1.97012300
F	-1.91809000	4.14853300	1.63261600
F	-3.96155500	4.83888700	-0.15008800
C	-3.42390300	-0.78107600	2.48962100
H	-3.91090500	-1.39180400	3.27022700
H	-2.77065200	-0.06200500	2.99927300
H	-4.21372500	-0.21343900	1.98030200
C	-4.64333200	-2.31411800	-0.06894600
H	-5.24152000	-3.13536500	0.36436900
H	-5.12668500	-1.37176800	0.21815000
H	-4.71492700	-2.40094200	-1.16179800
C	-0.37686800	-1.72729500	2.86195400
H	-0.53104100	-0.68710000	3.17692700
H	-0.56682400	-2.36934400	3.74018700
H	0.68362400	-1.84000800	2.60038500
C	-2.42878100	-4.36644500	-1.12707200
H	-2.81387700	-5.27925600	-0.63926700
H	-3.16516100	-4.06732100	-1.88488500
H	-1.50486800	-4.64288000	-1.65219800
C	0.25525800	-3.93832600	0.60376000
H	1.14591500	-3.37730800	0.91635500
H	0.18453400	-4.82876000	1.25323900
H	0.43119700	-4.29836800	-0.41952400
H	1.65505100	1.13351600	1.27365500
H	2.26844000	-1.65605100	-1.98157500
C	6.08246800	0.48347200	-0.21404900
C	6.58150200	1.78958200	0.04912200
C	7.03014000	-0.55588400	-0.42763500
C	7.96698800	2.04602400	0.09742500
H	5.88302200	2.61690400	0.18689700
C	8.41619400	-0.30176700	-0.37956800
H	6.68296800	-1.57593700	-0.60241000
C	8.89353900	1.00139700	-0.11630100
H	8.32177700	3.06106800	0.29187300
H	9.12155400	-1.12124500	-0.53784600
H	9.96725000	1.19925900	-0.07883500

Frequencies --	12.8645	15.9222	17.7877
Frequencies --	28.7296	38.0230	41.6724
Frequencies --	57.2168	69.0050	75.5123
Frequencies --	88.2262	96.6338	102.7331
Frequencies --	106.7046	112.7740	115.9883
Frequencies --	117.7122	125.5667	128.6702
Frequencies --	145.8282	150.1040	152.7824
Frequencies --	156.6674	159.1847	166.2831
Frequencies --	171.2752	191.1248	206.6637
Frequencies --	209.1907	229.2951	237.3185
Frequencies --	257.1564	264.8680	267.2592
Frequencies --	273.2306	288.4310	291.8453
Frequencies --	294.6917	299.2455	299.9016
Frequencies --	319.6376	334.0056	344.3548
Frequencies --	368.3040	385.5165	391.5865
Frequencies --	397.6613	406.7842	416.5169
Frequencies --	417.4268	427.0500	433.7730
Frequencies --	458.9630	464.2509	508.5160
Frequencies --	514.2681	536.4149	540.6193
Frequencies --	543.1228	555.7111	556.7429
Frequencies --	573.3926	582.8506	595.3217
Frequencies --	605.5733	615.2252	622.0894

Frequencies --	633.2779	633.9517	641.4957
Frequencies --	672.2809	688.4097	706.8996
Frequencies --	723.9032	727.3759	730.3752
Frequencies --	746.9384	774.3286	802.2220
Frequencies --	804.6315	835.3794	852.3210
Frequencies --	857.7788	884.3632	921.0768
Frequencies --	929.8374	964.4327	967.8941
Frequencies --	969.5303	978.3996	984.8351
Frequencies --	994.8393	1000.0811	1003.3428
Frequencies --	1025.0435	1037.8662	1043.3533
Frequencies --	1043.7964	1048.5459	1049.6199
Frequencies --	1050.1052	1051.1548	1060.8552
Frequencies --	1087.0113	1087.6589	1094.6485
Frequencies --	1124.0018	1128.1978	1172.1178
Frequencies --	1173.8087	1177.2391	1183.1686
Frequencies --	1190.1864	1199.4034	1212.3483
Frequencies --	1264.0226	1288.8704	1301.1733
Frequencies --	1316.3432	1324.9128	1355.1665
Frequencies --	1356.3600	1373.8445	1397.2452
Frequencies --	1410.3877	1413.3018	1422.5368
Frequencies --	1423.8438	1425.6755	1426.6791
Frequencies --	1430.3743	1431.7277	1432.6848
Frequencies --	1438.1260	1450.3829	1450.9339
Frequencies --	1454.1011	1458.5419	1462.5322
Frequencies --	1480.2469	1489.9260	1491.0532
Frequencies --	1491.9316	1496.7526	1499.7989
Frequencies --	1505.0888	1506.0542	1511.2236
Frequencies --	1513.5261	1514.8598	1520.0302
Frequencies --	1570.1367	1589.3965	1598.5510
Frequencies --	1600.3958	1620.3545	1625.1001
Frequencies --	2974.6333	3004.4909	3005.8905
Frequencies --	3006.4928	3007.8976	3009.5358
Frequencies --	3092.5700	3095.4764	3099.3659
Frequencies --	3100.4549	3100.6575	3103.3880
Frequencies --	3134.3905	3138.1627	3141.6365
Frequencies --	3142.6623	3145.7716	3149.9968
Frequencies --	3152.3145	3159.1803	3172.4574
Frequencies --	3174.8708	3179.6467	3183.1851
Frequencies --	3193.7252	3199.2726	3224.4405

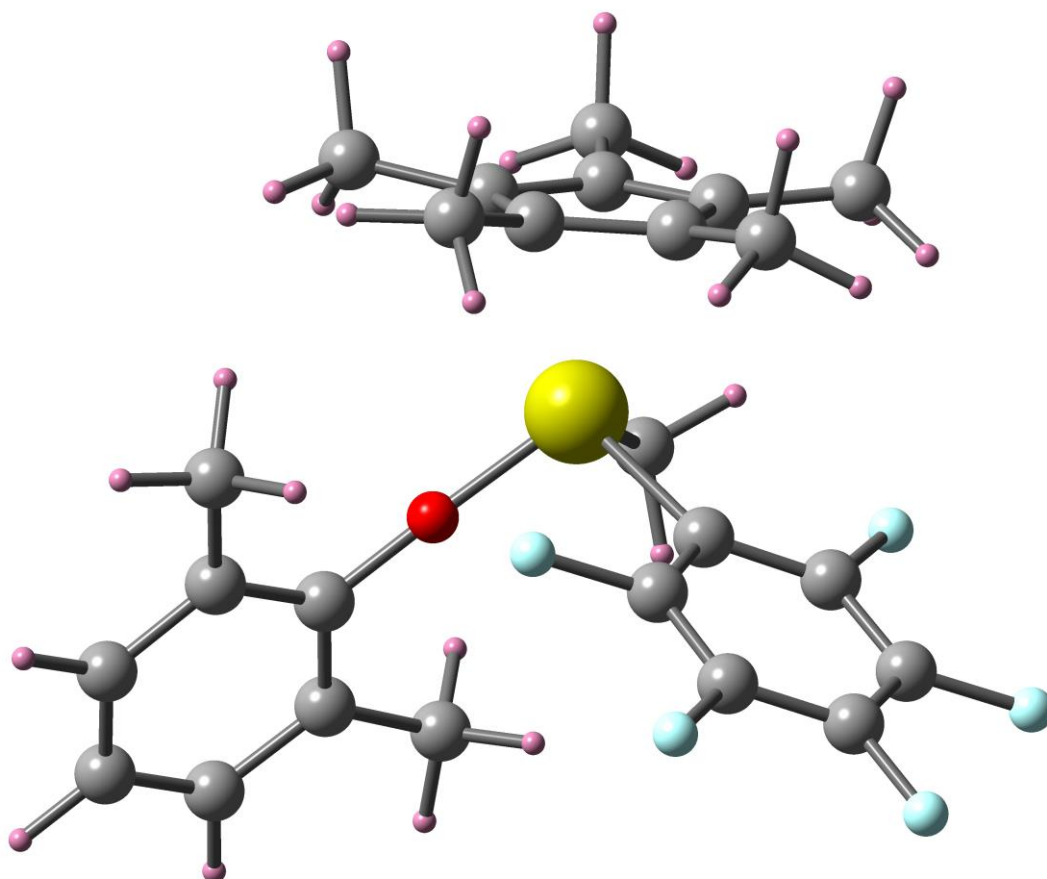
Catalyst 9:

vacuum	toluene-like solvent	D3 dispersion
-1679.5650943	-1679.5700472	-0.4058214

Ti	-0.86642300	-1.03256100	-0.40500200
C	-0.94033300	-1.57691000	-2.42161800
H	-0.68363700	-0.62075000	-2.91816800
H	-0.18409600	-2.32874300	-2.69786500
H	-1.93284000	-1.90833100	-2.75785400
O	0.81166200	-0.41914300	-0.41790300
C	2.15193000	-0.08966000	-0.35066700
C	2.59649400	0.95252300	0.49440200
C	3.09328500	-0.77978900	-1.15410800
C	3.96538600	1.28949000	0.53325200
C	4.45391700	-0.42994300	-1.09681600
C	4.93301700	0.61187900	-0.25317200
H	4.26410300	2.10119400	1.19481600
H	5.14906200	-0.98427400	-1.72892800
C	-2.16249200	-1.79866200	1.55621800
C	-2.70423200	-2.52474000	0.43119800
C	-0.76855000	-2.16443400	1.69581900
C	-1.65673200	-3.34948400	-0.12064600
C	-0.45494200	-3.12194100	0.65789500
C	-2.01997700	0.82475400	-0.21663200
C	-3.08329700	1.16002000	-1.07261500
C	-1.66948800	1.84046700	0.68803800
C	-3.75051400	2.40162900	-1.06220000

F	-3.54397400	0.21738900	-2.01533800
C	-2.29126600	3.10208300	0.75102800
F	-0.63599800	1.61251900	1.62419900
C	-3.34511300	3.38436900	-0.13934900
F	-4.79756500	2.67203100	-1.93973700
F	-1.89265100	4.06594500	1.67480500
F	-3.98194500	4.61771800	-0.10279000
C	-2.95348700	-0.96139900	2.53552800
H	-3.38413200	-1.61116800	3.31791400
H	-2.32927400	-0.21361800	3.04028000
H	-3.78827900	-0.43321400	2.05640100
C	-4.14568400	-2.51661200	-0.02511000
H	-4.68273800	-3.38671100	0.39270700
H	-4.67925100	-1.61556700	0.30309200
H	-4.23619700	-2.57236400	-1.11868400
C	0.14959900	-1.73459000	2.81830200
H	-0.05331300	-0.70798800	3.15061600
H	0.01446000	-2.39679000	3.69177800
H	1.20859400	-1.78489300	2.53230400
C	-1.84419500	-4.41756300	-1.17280300
H	-2.16559900	-5.35997700	-0.69524300
H	-2.61404400	-4.14614200	-1.90753900
H	-0.91886000	-4.63040200	-1.72427600
C	0.85290900	-3.86486400	0.49840000
H	1.71392000	-3.26643700	0.82346900
H	0.84390100	-4.78555000	1.10836900
H	1.03229400	-4.16889600	-0.54235100
H	1.87536200	1.49225700	1.10592500
H	2.75286700	-1.57582400	-1.81740600
C	6.44941100	0.95692200	-0.22169300
C	7.25600800	-0.29029700	0.26961100
H	7.11924500	-1.15544300	-0.39549300
H	8.33332000	-0.06068200	0.30348900
H	6.93819700	-0.58959900	1.28071800
C	6.92954900	1.35448000	-1.65627100
H	6.37561100	2.23166300	-2.02528000
H	8.00208400	1.60690900	-1.64327800
H	6.78757900	0.53902200	-2.38017500
C	6.77144200	2.14252400	0.73522700
H	6.25616700	3.06664500	0.43114900
H	6.49360100	1.91716600	1.77637700
H	7.85322700	2.34609200	0.71884600
Frequencies --	5.0494	16.1442	19.4783
Frequencies --	30.3574	39.1249	43.5435
Frequencies --	48.0189	70.5703	79.9328
Frequencies --	82.4716	94.7016	101.7447
Frequencies --	107.2562	109.9641	114.9125
Frequencies --	118.9544	121.6636	128.3648
Frequencies --	145.6400	154.7358	156.6236
Frequencies --	162.4629	170.0651	178.9980
Frequencies --	190.2757	199.4887	206.7530
Frequencies --	211.5673	221.7376	229.9569
Frequencies --	244.7016	254.3141	265.1517
Frequencies --	265.6403	274.6239	287.0922
Frequencies --	291.9760	294.1936	295.6313
Frequencies --	298.3215	302.5888	319.0761
Frequencies --	321.6087	323.5308	344.0554

Frequencies --	357.6318	373.1001	385.8206
Frequencies --	387.7583	393.5858	411.5915
Frequencies --	421.3191	427.4684	432.6480
Frequencies --	449.0687	461.6515	477.4659
Frequencies --	509.9624	536.4445	540.7257
Frequencies --	542.9444	554.1207	554.5046
Frequencies --	556.7210	571.7144	582.5149
Frequencies --	595.3284	605.4258	613.7035
Frequencies --	634.4038	641.0345	667.5179
Frequencies --	687.4131	715.2201	723.4319
Frequencies --	730.4806	737.3767	802.7421
Frequencies --	803.6127	831.8826	833.8552
Frequencies --	846.2903	884.0582	921.0561
Frequencies --	926.8648	933.9583	955.7219
Frequencies --	963.4864	968.4299	968.8813
Frequencies --	981.0329	994.4286	1025.8854
Frequencies --	1037.2647	1038.2472	1040.6938
Frequencies --	1043.6664	1044.0854	1049.0234
Frequencies --	1050.9233	1051.8517	1086.3572
Frequencies --	1087.9490	1123.2678	1123.9872
Frequencies --	1132.1440	1172.5065	1173.9048
Frequencies --	1177.0640	1189.6537	1206.0783
Frequencies --	1215.0989	1222.9091	1262.8601
Frequencies --	1275.6110	1288.1461	1326.7582
Frequencies --	1349.6186	1354.3908	1395.8900
Frequencies --	1396.1826	1398.7692	1410.4503
Frequencies --	1412.7660	1421.6347	1423.3624
Frequencies --	1424.2956	1425.5507	1426.3482
Frequencies --	1430.4098	1432.0497	1432.5035
Frequencies --	1437.7495	1450.4482	1453.9467
Frequencies --	1458.3502	1462.3711	1480.2012
Frequencies --	1482.1618	1487.3035	1490.1421
Frequencies --	1491.0626	1491.3293	1497.2139
Frequencies --	1499.4334	1499.5666	1504.4418
Frequencies --	1505.9721	1509.7161	1510.7799
Frequencies --	1511.5027	1514.4852	1515.1320
Frequencies --	1520.1274	1578.0992	1588.8896
Frequencies --	1600.2037	1622.1725	2974.1433
Frequencies --	3004.3573	3005.0332	3006.0113
Frequencies --	3006.2706	3007.2278	3007.8202
Frequencies --	3008.9467	3014.7839	3091.2910
Frequencies --	3095.0151	3098.0906	3099.3000
Frequencies --	3100.4245	3103.3116	3105.7426
Frequencies --	3108.9507	3114.2030	3121.0735
Frequencies --	3123.0159	3125.5667	3134.8528
Frequencies --	3137.5583	3140.9959	3141.7644
Frequencies --	3144.4897	3149.9022	3169.4027
Frequencies --	3194.3259	3198.1929	3222.0708

Catalyst 10:

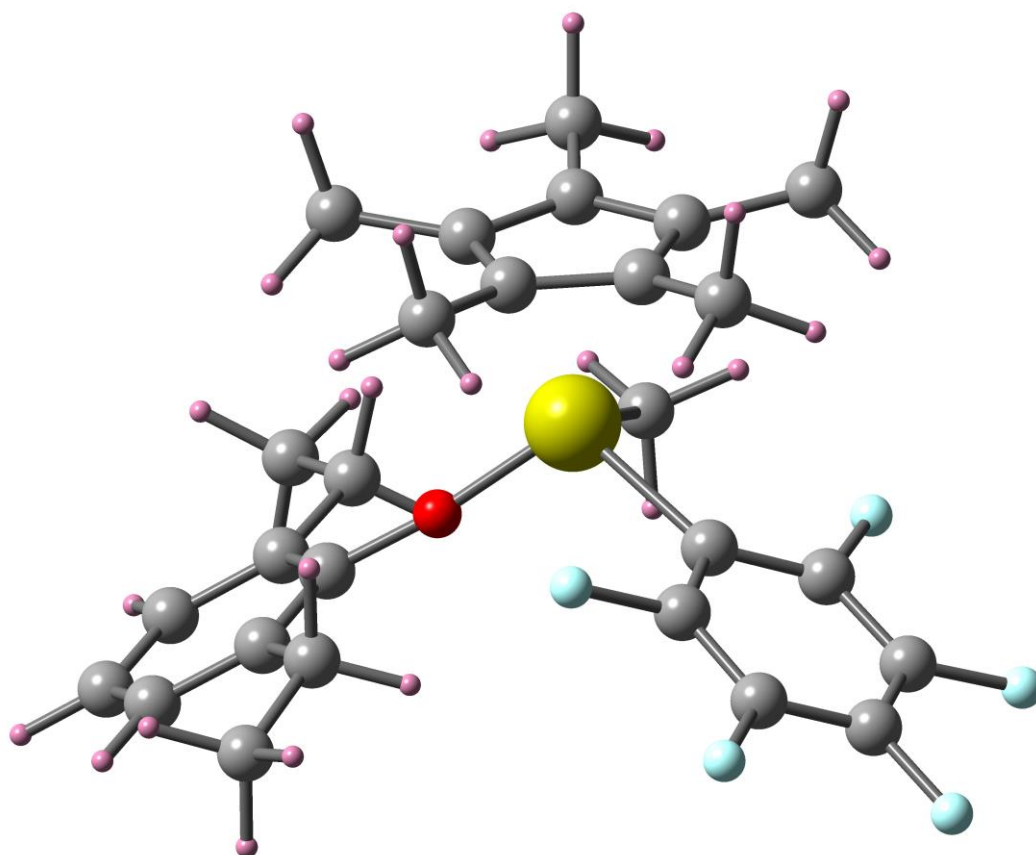
vacuum	toluene-like solvent	D3 dispersion
-1600.9846181	-1600.98987	-0.37649573

Ti	-0.33198200	0.91652200	-0.38028400
C	-0.32688600	1.28261400	-2.44156600
H	-0.06936700	0.30283300	-2.87415400
H	-1.33265700	1.57359400	-2.78578800
H	0.40866400	2.02333000	-2.77500600
O	-1.63069900	-0.33785500	-0.36299600
C	-2.62163100	-1.32121900	-0.39469000
C	-3.36376600	-1.62746700	0.78848800
C	-2.85602400	-2.03300400	-1.61394800
C	-4.36342800	-2.62600400	0.71536300
C	-3.86406600	-3.02596100	-1.62886000
C	-4.62246400	-3.32223000	-0.48040500
H	-4.93524900	-2.86177300	1.61525000
H	-4.04704400	-3.57320500	-2.55593400
C	-0.41036500	2.23433900	1.64608500
C	0.93668200	2.43349200	1.15337300
C	-1.32453800	2.81068900	0.68339300
C	0.85663800	3.16134500	-0.08966700
C	-0.53398800	3.39400700	-0.38376300
C	1.40179400	-0.40165400	-0.08384400

C	2.51881500	-0.45939300	-0.93655400
C	1.41435800	-1.36699900	0.93723600
C	3.55919800	-1.40390100	-0.81977200
F	2.65195300	0.47121600	-1.98767700
C	2.42091700	-2.33548100	1.11244000
F	0.36761100	-1.38687300	1.88380500
C	3.50689300	-2.35446700	0.21686000
F	4.63529100	-1.40945400	-1.70426300
F	2.36684500	-3.26272600	2.15033300
F	4.51845600	-3.29483500	0.35936400
C	-3.09942700	-0.93704300	2.11096300
H	-2.07589900	-1.12900000	2.45879000
H	-3.21878600	0.14985700	2.02918300
H	-3.79480000	-1.29666600	2.88188600
C	-2.05457900	-1.77471000	-2.87633100
H	-2.22129400	-0.76005300	-3.26408400
H	-0.97425200	-1.88140600	-2.69702600
H	-2.33663800	-2.48644100	-3.66456100
C	-0.73905800	1.74183500	3.03841700
H	-0.38027800	2.47847700	3.77803000
H	-1.81644800	1.62713100	3.19822000
H	-0.25929200	0.78318000	3.27653500
C	2.20098400	2.15002000	1.93295000
H	2.46352700	3.02649400	2.55200300
H	2.08700500	1.29518100	2.61191100
H	3.05861500	1.94649600	1.27860000
C	-2.82013500	2.99628800	0.83277600
H	-3.25585600	2.33627400	1.59132000
H	-3.04275500	4.03425800	1.13573300
H	-3.35985300	2.81261300	-0.10852000
C	2.03219000	3.68839300	-0.87918700
H	2.32608100	4.68307900	-0.49906800
H	2.91095900	3.03556400	-0.80281300
H	1.80029800	3.80639200	-1.94593000
C	-1.07818900	4.27568300	-1.48388200
H	-2.09225600	3.98379200	-1.78922300
H	-1.13251900	5.32067000	-1.13029100
H	-0.44482600	4.26874500	-2.38010600
H	-5.39686600	-4.09106000	-0.51407700

Frequencies --	10.3217	19.6704	24.3621
Frequencies --	32.2415	36.9103	42.9185
Frequencies --	72.3133	85.2280	92.0905
Frequencies --	102.0399	108.4495	112.9090
Frequencies --	118.3423	119.5282	128.1131
Frequencies --	133.9143	134.5375	141.7361
Frequencies --	153.0138	153.8769	156.1180
Frequencies --	176.6403	182.2952	185.6543
Frequencies --	200.1836	205.1968	208.8458
Frequencies --	220.1639	229.5758	249.9526
Frequencies --	260.5000	264.8284	269.6574
Frequencies --	281.7410	284.4272	288.4369
Frequencies --	294.6965	296.8633	297.6170
Frequencies --	317.0822	319.8822	345.1730
Frequencies --	350.0039	355.9262	380.6731
Frequencies --	384.1351	385.7221	409.6894
Frequencies --	428.5545	461.0542	496.1922
Frequencies --	509.0126	516.0387	532.6642

Frequencies --	539.9716	543.7508	551.1670
Frequencies --	554.6765	555.9715	559.8053
Frequencies --	566.4934	584.8576	596.2899
Frequencies --	601.9742	618.8781	632.7985
Frequencies --	679.4740	687.6933	721.0212
Frequencies --	727.7001	740.5898	744.3674
Frequencies --	780.5177	799.9484	804.4640
Frequencies --	885.5058	904.7135	912.1600
Frequencies --	926.6762	966.8056	968.7268
Frequencies --	980.5544	994.8764	1009.1047
Frequencies --	1038.6552	1040.2604	1043.8597
Frequencies --	1048.0310	1049.1274	1051.7203
Frequencies --	1051.9710	1059.1575	1065.6479
Frequencies --	1084.7600	1086.0584	1115.7347
Frequencies --	1121.5041	1172.3780	1175.8993
Frequencies --	1176.7222	1189.7471	1191.0519
Frequencies --	1203.0619	1279.2952	1285.7280
Frequencies --	1288.4118	1354.0352	1357.3833
Frequencies --	1396.0137	1409.4323	1411.9771
Frequencies --	1420.3176	1420.9181	1423.1090
Frequencies --	1424.3471	1426.0799	1427.8110
Frequencies --	1428.5688	1434.3532	1437.2022
Frequencies --	1448.3720	1450.3467	1454.6443
Frequencies --	1459.7158	1464.8703	1472.4816
Frequencies --	1481.4538	1486.3724	1487.8459
Frequencies --	1490.8530	1493.0624	1497.0791
Frequencies --	1498.9585	1501.3056	1505.4138
Frequencies --	1509.8678	1511.4191	1513.2670
Frequencies --	1517.0390	1520.5539	1589.0841
Frequencies --	1600.4683	1603.9568	1609.8852
Frequencies --	3003.2346	3004.8533	3005.3360
Frequencies --	3006.2994	3008.2315	3015.1680
Frequencies --	3023.1594	3042.1704	3087.9276
Frequencies --	3097.3024	3099.8488	3100.9573
Frequencies --	3105.9263	3113.5089	3119.5625
Frequencies --	3130.2310	3138.4866	3139.6046
Frequencies --	3142.7827	3143.5844	3146.9504
Frequencies --	3151.9200	3157.9618	3165.3819
Frequencies --	3166.2204	3168.7611	3191.1230

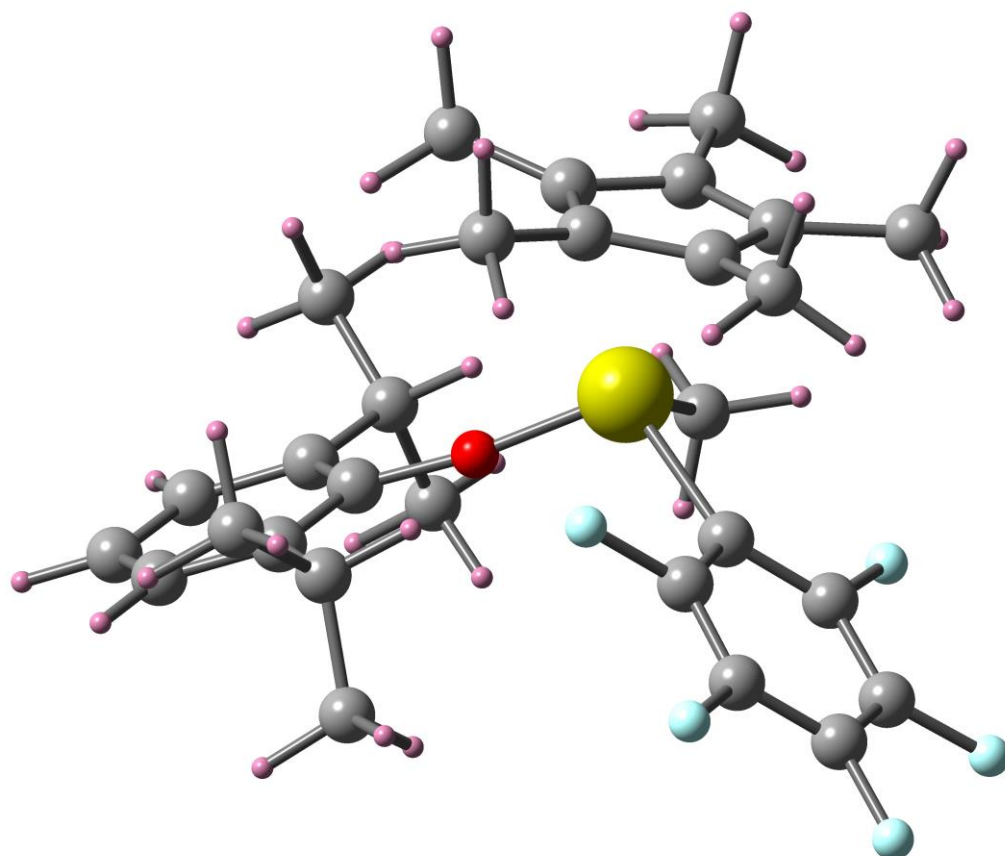
Catalyst 11:

vacuum	toluene-like solvent	D3 dispersion
-1679.5574157	-1679.5622716	-0.41287598

Ti	-0.15600900	0.88197500	-0.08264500
C	-0.38430600	1.84888800	-1.92035000
H	-0.30211000	1.01491800	-2.64101700
H	-1.34832100	2.35107000	-2.06125300
H	0.43148800	2.56093200	-2.09559500
O	-1.47513800	-0.34543600	-0.27325700
C	-2.60427400	-1.16607300	-0.39584400
C	-2.64525100	-2.40760000	0.31867600
C	-3.68241100	-0.75980300	-1.24983800
C	-3.78656200	-3.22772200	0.16017800
C	-4.79899400	-1.62066500	-1.36058800
C	-4.85729900	-2.84350200	-0.66694000
H	-3.83694800	-4.17845800	0.68809800
H	-5.63219600	-1.33554800	-2.00068600
C	1.09579200	1.99343800	1.77947300
C	0.80997100	3.04223000	0.83146400
C	-0.16545200	1.46471600	2.25412900
C	-0.62222500	3.17281200	0.72032600
C	-1.23018300	2.18677000	1.59248400
C	1.79126100	-0.15975900	-0.39788300

C	2.70031300	0.12611700	-1.43758200
C	2.19074400	-1.24731100	0.39905800
C	3.87184900	-0.61484200	-1.70136700
F	2.49231100	1.22763700	-2.28983000
C	3.34179300	-2.03069400	0.19182400
F	1.41610900	-1.59591500	1.52795300
C	4.19285400	-1.71182100	-0.88199000
F	4.71966700	-0.27239500	-2.75204600
F	3.65804100	-3.09615200	1.03237900
F	5.33991800	-2.45710700	-1.11803100
C	-1.49210500	-2.81748500	1.22979300
H	-0.55131800	-2.70597800	0.67680700
H	-1.43860600	-2.08947600	2.05501300
C	-3.61458100	0.55208300	-2.03015700
H	-3.36592500	1.36415700	-1.33037800
H	-2.76461600	0.49424800	-2.72726600
C	2.46162800	1.67868700	2.34571800
H	2.69832600	2.39005700	3.15698100
H	2.51537100	0.66992800	2.77207600
H	3.25633900	1.77006800	1.59324000
C	1.84199600	3.92155000	0.16331400
H	2.15159300	4.73236500	0.84657600
H	2.74860000	3.36437000	-0.11014400
H	1.45762900	4.39575100	-0.74905600
C	-0.34145400	0.49305600	3.39934500
H	-1.25321000	-0.10772300	3.29392900
H	0.50272900	-0.19946700	3.49345700
H	-0.42567700	1.04930000	4.34971300
C	-1.35247200	4.28306700	0.00043400
H	-1.40075300	5.17552800	0.64897200
H	-0.85052400	4.58311900	-0.92841900
H	-2.38624800	4.01078100	-0.25093000
C	-2.70414600	2.07096800	1.91402200
H	-2.99560300	1.04336700	2.17013200
H	-2.95395700	2.70919400	2.78002700
H	-3.34005700	2.39463500	1.07924500
H	-5.72912600	-3.49245000	-0.77352400
C	-4.87270400	0.96094200	-2.82813600
H	-5.11707300	0.23292700	-3.61728300
H	-5.75611400	1.07275000	-2.17938700
H	-4.69479400	1.93035300	-3.32094000
C	-1.54310300	-4.23708900	1.83539600
H	-0.63601500	-4.40760900	2.43642200
H	-2.41087200	-4.37817300	2.49937500
H	-1.57719900	-5.01525100	1.05646400
Frequencies --	12.3365	21.0216	24.5461
Frequencies --	33.1583	35.0563	45.5783
Frequencies --	56.2658	70.5087	77.6002
Frequencies --	85.5921	93.0229	94.9492
Frequencies --	107.5575	115.7775	121.4034
Frequencies --	124.9531	127.6033	134.0437
Frequencies --	144.2454	155.0328	157.6336
Frequencies --	166.6901	171.7803	179.1483
Frequencies --	184.6436	190.7469	197.0253
Frequencies --	204.8620	210.0579	224.5201
Frequencies --	249.3093	264.0621	265.7809
Frequencies --	270.8137	283.0797	287.6573

Frequencies --	290.9089	291.7671	299.2803
Frequencies --	301.1589	301.8725	304.2654
Frequencies --	320.8812	322.7868	326.4271
Frequencies --	339.3657	349.2490	368.5528
Frequencies --	378.1683	382.3639	393.3772
Frequencies --	405.6562	430.3291	459.5545
Frequencies --	499.4277	509.8422	533.0539
Frequencies --	533.8001	539.4408	545.0381
Frequencies --	551.8278	554.9402	569.9945
Frequencies --	581.0694	585.3619	591.5340
Frequencies --	598.9045	606.2823	616.0614
Frequencies --	632.9064	676.2089	686.4941
Frequencies --	715.1745	716.4012	723.7672
Frequencies --	728.3382	770.8113	786.3487
Frequencies --	801.1168	805.5004	824.7366
Frequencies --	855.2779	886.7574	907.9642
Frequencies --	919.6061	967.1935	971.7717
Frequencies --	987.2965	993.1048	995.1490
Frequencies --	1025.2638	1038.1688	1042.2761
Frequencies --	1045.8396	1048.7320	1049.1199
Frequencies --	1050.8166	1058.3720	1086.9337
Frequencies --	1087.5668	1091.7995	1097.7843
Frequencies --	1101.7361	1124.3106	1126.3296
Frequencies --	1173.7936	1176.1669	1179.0169
Frequencies --	1187.6245	1188.9516	1202.2207
Frequencies --	1262.9784	1278.6006	1284.0105
Frequencies --	1287.5960	1290.4416	1319.9976
Frequencies --	1347.2799	1348.0730	1383.1587
Frequencies --	1389.7705	1410.6463	1411.3527
Frequencies --	1412.4284	1413.3239	1422.1636
Frequencies --	1423.4832	1427.6362	1430.3204
Frequencies --	1431.0538	1433.2504	1440.6470
Frequencies --	1444.5121	1450.6798	1456.3860
Frequencies --	1458.9552	1463.4603	1467.9724
Frequencies --	1479.4827	1480.9734	1491.6131
Frequencies --	1492.9653	1494.0561	1499.4380
Frequencies --	1500.4864	1501.7282	1502.2555
Frequencies --	1506.0930	1507.3588	1507.5059
Frequencies --	1508.4147	1513.7314	1514.9147
Frequencies --	1517.0893	1586.7535	1599.7293
Frequencies --	1600.8219	1612.0874	2995.9786
Frequencies --	3004.8026	3005.6118	3006.8812
Frequencies --	3008.4221	3008.9098	3009.0254
Frequencies --	3009.7937	3036.0439	3043.3354
Frequencies --	3084.2258	3096.8747	3097.6204
Frequencies --	3099.8669	3101.2758	3101.4672
Frequencies --	3109.1322	3110.5456	3114.1383
Frequencies --	3119.3101	3128.0028	3129.7400
Frequencies --	3135.7321	3139.0495	3143.1324
Frequencies --	3151.1948	3160.3681	3165.2814
Frequencies --	3171.2534	3201.8486	3212.1362

Catalyst 12:

vacuum	toluene-like solvent	D3 dispersion
-1758.1339877	-1758.1388286	-0.45251006

Ti	-0.06011700	0.97504400	-0.03534300
C	-0.37047700	1.98397500	-1.84015400
H	-0.31550500	1.16834700	-2.58370800
H	-1.33257300	2.49992100	-1.94758300
H	0.44292400	2.69774400	-2.02469400
O	-1.33244700	-0.30219700	-0.22143000
C	-2.43294900	-1.16976900	-0.30739600
C	-2.35558800	-2.46493100	0.30559400
C	-3.60483200	-0.76707300	-1.03386500
C	-3.46463400	-3.33366000	0.17405300
C	-4.67895900	-1.68397900	-1.12573600
C	-4.62054800	-2.95548900	-0.52974100
H	-3.41687800	-4.32401800	0.62769900
H	-5.57385400	-1.39790600	-1.67912200
C	1.14417400	2.00455800	1.90274000
C	0.92120600	3.08032000	0.96769600
C	-0.14663400	1.49245900	2.31046300
C	-0.50174400	3.25658400	0.81118400
C	-1.16597100	2.26423000	1.63332900
C	1.91732700	-0.00363600	-0.40278200

C	2.76884900	0.29979800	-1.48576000
C	2.39191700	-1.06564500	0.38731100
C	3.95392700	-0.40196200	-1.79290900
F	2.48255700	1.37997700	-2.34200600
C	3.55858700	-1.81174800	0.13661900
F	1.68413500	-1.43016600	1.55422000
C	4.34951700	-1.47695400	-0.97716500
F	4.74119500	-0.04333500	-2.88441500
F	3.94557000	-2.85768200	0.97213500
F	5.50983000	-2.18569100	-1.25706600
C	-1.10664800	-2.95635600	1.04513200
H	-0.44115500	-2.10260400	1.18085200
C	-3.72066000	0.58174600	-1.75762100
H	-2.89879700	1.21439600	-1.41254600
C	2.47811700	1.65407500	2.52127000
H	2.69847200	2.36144100	3.34055900
H	2.48865800	0.64552900	2.94925800
H	3.30511000	1.72528800	1.80209600
C	1.99996800	3.94052700	0.35055200
H	2.29360900	4.74532600	1.04780800
H	2.90687800	3.36469300	0.12026300
H	1.66788000	4.42107500	-0.57892800
C	-0.39821000	0.48025500	3.40505200
H	0.39578300	-0.27296400	3.46815700
H	-0.44707700	0.99202700	4.38273100
H	-1.35081700	-0.04850400	3.26983500
C	-1.17224500	4.41282600	0.10652500
H	-1.21433500	5.28338200	0.78459400
H	-0.62935900	4.72839000	-0.79387100
H	-2.20439000	4.18256500	-0.18891700
C	-2.65179400	2.18650300	1.90579700
H	-2.98683900	1.16035400	2.10885200
H	-2.90343900	2.79515800	2.79243300
H	-3.24924400	2.57017300	1.06935800
H	-5.46319000	-3.64438700	-0.61781100
C	-1.41838200	-3.51622000	2.46226400
H	-1.98021300	-2.78707700	3.06707500
H	-2.00663600	-4.44583600	2.42548600
H	-0.47685700	-3.74206200	2.98820900
C	-0.33548200	-4.00822900	0.19206700
H	-0.06456800	-3.59747800	-0.79320600
H	0.59198500	-4.30949800	0.70437200
H	-0.94095900	-4.91262600	0.02348900
C	-3.55018100	0.39742700	-3.29576800
H	-3.56619400	1.37392900	-3.80695400
H	-2.59568200	-0.09525700	-3.53311500
H	-4.36048000	-0.21895500	-3.71546300
C	-5.04225100	1.33834600	-1.43944500
H	-5.19310800	1.44619500	-0.35441300
H	-5.01335900	2.34664300	-1.88465800
H	-5.92562600	0.82741200	-1.85080000

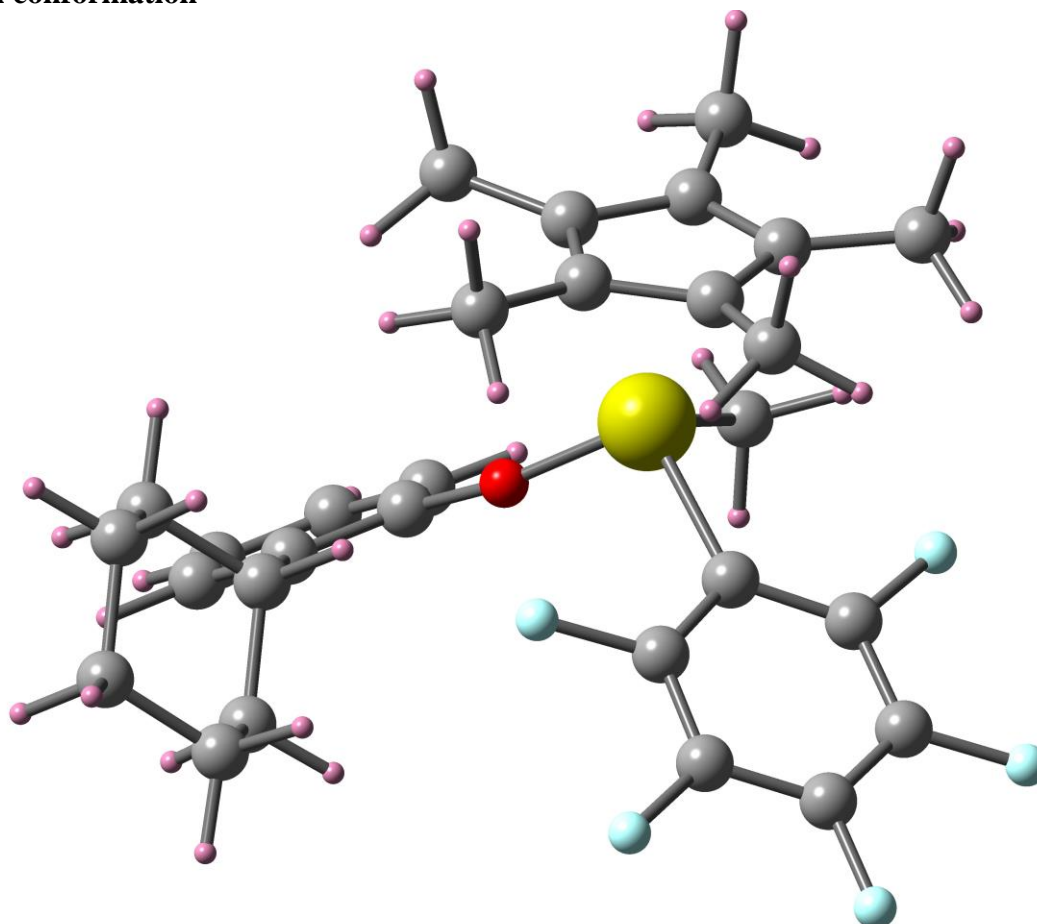
Frequencies --	15.0226	21.2909	25.4241
Frequencies --	28.9263	37.5092	50.2039
Frequencies --	57.4009	63.3107	72.3406
Frequencies --	76.7645	93.3563	101.9928
Frequencies --	111.2893	120.2893	122.2552

Frequencies --	125.9899	126.4986	131.0204
Frequencies --	135.6510	148.4825	152.7681
Frequencies --	153.2846	159.9174	165.7608
Frequencies --	172.8260	185.4552	189.4980
Frequencies --	204.4391	208.7141	212.0351
Frequencies --	224.0238	224.8871	237.2596
Frequencies --	238.6426	253.3733	255.2672
Frequencies --	263.9606	269.1688	277.0489
Frequencies --	284.7897	288.3313	291.0816
Frequencies --	295.7748	297.2488	302.0398
Frequencies --	302.5828	311.8416	322.1986
Frequencies --	330.3547	331.9646	349.1897
Frequencies --	373.8439	382.6111	393.0550
Frequencies --	407.0860	421.4898	428.1771
Frequencies --	431.3735	435.6660	459.4945
Frequencies --	501.4589	533.7279	539.5324
Frequencies --	540.2652	545.2116	547.9062
Frequencies --	555.1588	580.5523	586.2726
Frequencies --	592.8698	595.4041	605.3598
Frequencies --	610.8309	617.4916	630.2814
Frequencies --	634.0284	684.1102	688.2640
Frequencies --	716.1769	721.3155	726.2776
Frequencies --	763.3821	797.6182	801.3356
Frequencies --	807.1478	813.5796	873.3356
Frequencies --	887.4787	912.6840	918.8208
Frequencies --	928.7487	930.2817	942.2836
Frequencies --	962.1934	963.1276	968.9268
Frequencies --	971.7063	985.5254	995.2727
Frequencies --	1038.7826	1042.1944	1046.3627
Frequencies --	1049.2578	1049.8145	1051.4350
Frequencies --	1057.7863	1074.2915	1087.4161
Frequencies --	1088.4130	1112.9799	1116.8964
Frequencies --	1121.5899	1124.7524	1165.6098
Frequencies --	1174.3416	1176.5374	1181.0390
Frequencies --	1184.6306	1188.4210	1191.8337
Frequencies --	1204.1871	1260.5663	1279.7970
Frequencies --	1285.0157	1302.1837	1324.6207
Frequencies --	1334.5051	1345.8547	1348.8073
Frequencies --	1385.3925	1392.0512	1394.9581
Frequencies --	1399.5457	1411.2535	1412.0335
Frequencies --	1413.8483	1417.6808	1422.4858
Frequencies --	1424.8715	1428.5104	1430.8274
Frequencies --	1432.0600	1439.4748	1441.7398
Frequencies --	1451.1242	1455.1679	1457.6001
Frequencies --	1460.1061	1463.6507	1473.5526
Frequencies --	1481.0434	1485.4807	1488.2891
Frequencies --	1489.7481	1490.2072	1492.7988
Frequencies --	1493.7909	1499.7531	1500.4554
Frequencies --	1501.7695	1504.3578	1505.2790
Frequencies --	1506.7230	1509.2076	1510.0608
Frequencies --	1513.2556	1515.5228	1516.5034
Frequencies --	1588.5114	1597.0659	1602.3108
Frequencies --	1609.2376	2997.2295	3004.4510
Frequencies --	3004.6637	3005.6084	3006.3647
Frequencies --	3006.8965	3007.7816	3008.9985
Frequencies --	3010.5679	3011.2619	3097.2523
Frequencies --	3098.9683	3100.7978	3101.8118
Frequencies --	3103.2715	3105.3876	3105.7568
Frequencies --	3106.8955	3108.8109	3113.2183
Frequencies --	3115.1314	3117.8417	3119.0020
Frequencies --	3125.0924	3137.6594	3142.0348
Frequencies --	3146.0396	3149.2359	3154.7119
Frequencies --	3159.4139	3160.7171	3161.9633

Frequencies -- 3175.5036

3182.9074

3196.4149

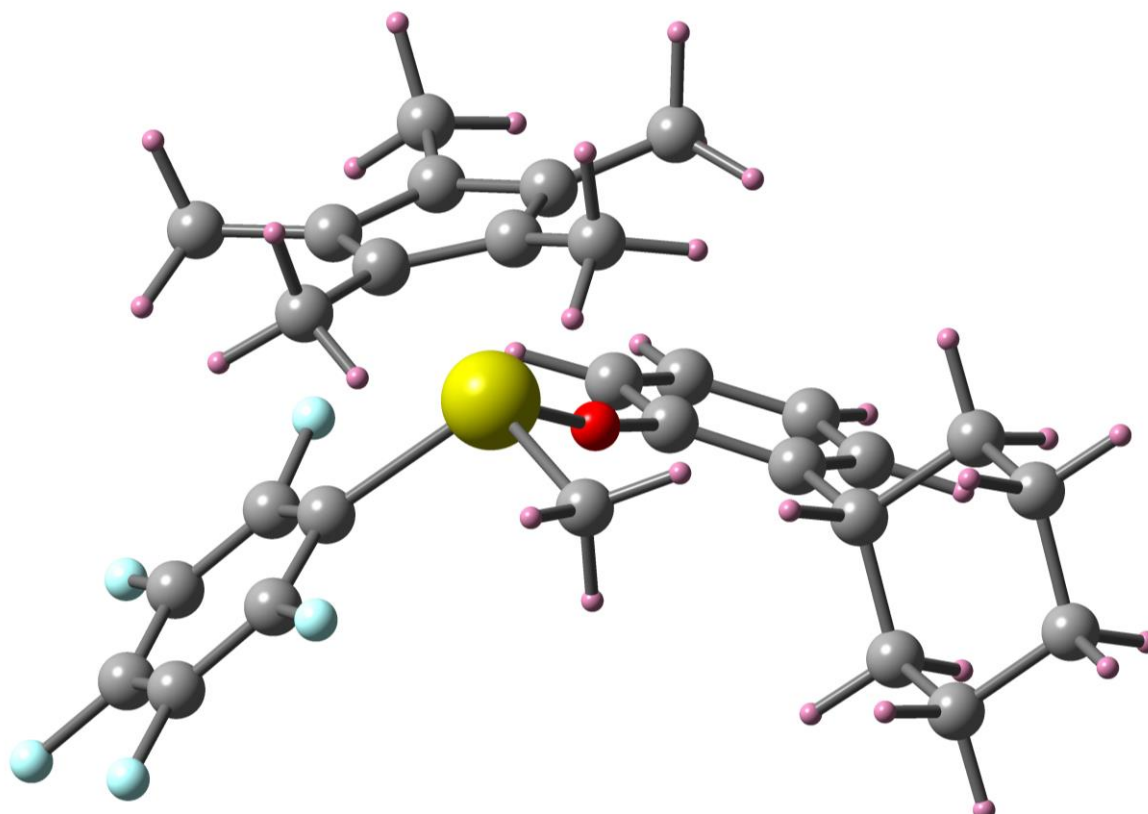
Catalyst 13:**distal conformation**

vacuum	toluene-like solvent	D3 dispersion
-1756.9449824	-1756.9501881	-0.44199992

Ti	0.70442800	-1.21981200	0.21943000
C	1.32273300	-2.24493800	1.93704300
H	1.16560400	-1.49508600	2.73541700
H	0.72625200	-3.14000200	2.16593000
H	2.38651700	-2.51536800	1.89559700
O	-0.95416300	-0.84124900	0.81037400
C	-2.18228900	-0.93283700	1.46169000
C	-3.30727000	-0.14339000	1.06987600
C	-2.26963600	-1.83282600	2.55780700
C	-4.49581900	-0.30592100	1.83104200
C	-3.46484800	-1.96877100	3.28398900
C	-4.58908500	-1.19719000	2.91688800
H	-5.37255700	0.28622800	1.56528800
H	-3.51431200	-2.66279200	4.12606200
C	0.45571600	-1.59278000	-2.12450500
C	1.88653800	-1.44651700	-1.95388700
C	0.04138400	-2.79157000	-1.42779100
C	2.35457400	-2.55770300	-1.16183300

C	1.22116000	-3.39016000	-0.83667000
C	1.78635900	0.69333400	0.34905800
C	3.02199000	0.85851900	1.00047500
C	1.23320500	1.89146900	-0.13153600
C	3.65699600	2.10173900	1.19707500
F	3.71356200	-0.26679200	1.49381700
C	1.81136000	3.16479000	0.02997900
F	0.01767100	1.85043400	-0.84893500
C	3.04058500	3.26905900	0.70825900
F	4.88084600	2.19481000	1.85515500
F	1.19984600	4.31138000	-0.47256500
F	3.64285100	4.50749100	0.88393500
C	-0.41555700	-0.74810200	-3.02611600
H	-0.35290400	-1.12424000	-4.06274800
H	-1.47228200	-0.78204500	-2.73307200
H	-0.10873800	0.30521300	-3.04076900
C	2.76026400	-0.43495900	-2.66084000
H	3.11343700	-0.85071200	-3.62120300
H	2.21981800	0.49292000	-2.88773200
H	3.65028500	-0.16830600	-2.07536800
C	-1.34904900	-3.38790400	-1.45206800
H	-2.11910800	-2.60659800	-1.48690600
H	-1.47823400	-4.02447700	-2.34477900
H	-1.55291700	-4.01213900	-0.57149200
C	3.79813500	-2.86106600	-0.83324900
H	4.25372900	-3.45489200	-1.64577300
H	4.40085000	-1.95099600	-0.71714400
H	3.90106000	-3.44558300	0.09070600
C	1.28267400	-4.74756400	-0.17568300
H	0.33174400	-5.02269800	0.30025000
H	1.50436000	-5.52122800	-0.93174900
H	2.06808100	-4.80555900	0.58914400
H	-1.39157300	-2.41151000	2.83487700
H	-5.52538600	-1.28655400	3.47161000
C	-3.26613600	0.85777300	-0.08861100
C	-4.35922600	0.57137700	-1.16646400
C	-3.38919100	2.33000700	0.42239900
H	-2.28876700	0.77037600	-0.57888000
C	-4.30316300	1.59508500	-2.32940300
H	-5.36112100	0.61463300	-0.70692900
H	-4.24087000	-0.45427400	-1.55741300
C	-3.34899600	3.35531500	-0.73910000
H	-4.33414900	2.44904600	0.98060100
H	-2.57335300	2.53834900	1.13389600
C	-4.42174500	3.05074200	-1.81372100
H	-5.11199100	1.37993600	-3.04942100
H	-3.35122600	1.48069000	-2.87894000
H	-3.49697500	4.37189900	-0.33556200
H	-2.34839500	3.34302200	-1.20340600
H	-4.32550100	3.75862800	-2.65488100
H	-5.42845900	3.20401900	-1.38292200
Frequencies --	-11.7539	20.2504	22.7602
Frequencies --	32.8343	44.5048	50.4669
Frequencies --	55.3457	70.1067	76.7742
Frequencies --	78.2852	90.8342	100.2318
Frequencies --	113.1487	116.2057	125.1524

Frequencies --	127.9831	135.1110	139.8427
Frequencies --	141.9366	144.2349	153.5452
Frequencies --	158.1993	169.0868	172.2227
Frequencies --	177.6779	183.1970	203.6954
Frequencies --	206.1885	222.4110	232.6132
Frequencies --	240.1997	264.0563	264.6245
Frequencies --	271.4577	274.0848	278.5680
Frequencies --	283.5263	289.8235	292.3684
Frequencies --	297.4872	300.2659	312.0537
Frequencies --	324.2497	335.3038	344.7265
Frequencies --	357.4509	381.6294	384.2651
Frequencies --	391.2320	411.8480	428.7189
Frequencies --	436.8009	442.3547	461.2146
Frequencies --	494.5519	496.5094	504.4612
Frequencies --	519.4485	535.3665	539.0999
Frequencies --	544.0582	552.9130	556.3809
Frequencies --	576.8216	583.8467	594.7821
Frequencies --	605.2826	616.9480	618.7142
Frequencies --	633.4841	650.4789	685.0046
Frequencies --	690.0998	721.3645	728.2664
Frequencies --	745.0736	765.8746	768.9304
Frequencies --	791.0750	801.0404	802.3692
Frequencies --	819.5926	866.9431	867.5066
Frequencies --	885.0765	887.2069	902.9422
Frequencies --	923.9781	927.2416	957.0149
Frequencies --	965.7669	969.4284	988.7205
Frequencies --	994.6797	999.9506	1038.0201
Frequencies --	1042.6887	1045.3536	1047.7554
Frequencies --	1049.3039	1050.2861	1055.4122
Frequencies --	1056.5612	1059.2556	1086.5245
Frequencies --	1087.6616	1088.0984	1096.7655
Frequencies --	1116.7067	1123.3420	1153.6004
Frequencies --	1173.0844	1176.7248	1177.9586
Frequencies --	1183.9079	1189.5770	1191.4511
Frequencies --	1200.9255	1224.3126	1251.5051
Frequencies --	1279.1934	1282.2331	1287.4643
Frequencies --	1296.0776	1320.3982	1331.6667
Frequencies --	1353.7525	1355.7139	1357.6816
Frequencies --	1360.6336	1363.5343	1370.5217
Frequencies --	1391.8755	1394.7383	1409.7681
Frequencies --	1411.4300	1422.3275	1423.1449
Frequencies --	1427.0079	1430.2869	1431.4402
Frequencies --	1437.2682	1446.2132	1450.2903
Frequencies --	1451.7032	1454.8303	1459.5678
Frequencies --	1462.4837	1479.3659	1480.2126
Frequencies --	1482.0159	1486.1380	1486.5137
Frequencies --	1490.4825	1491.0233	1492.2058
Frequencies --	1496.6078	1497.6185	1499.7553
Frequencies --	1505.4304	1507.7337	1510.1199
Frequencies --	1513.2412	1515.4396	1586.2268
Frequencies --	1588.4980	1600.4735	1614.5470
Frequencies --	2983.6386	2997.6399	3001.5594
Frequencies --	3004.3238	3006.0524	3007.0071
Frequencies --	3007.2115	3009.1178	3009.3649
Frequencies --	3013.1999	3020.2027	3058.2586
Frequencies --	3062.3519	3071.0021	3076.5297
Frequencies --	3086.9830	3097.0987	3098.2158
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Frequencies --	3106.7048	3116.8188	3136.3798
Frequencies --	3140.1272	3141.4387	3144.3210
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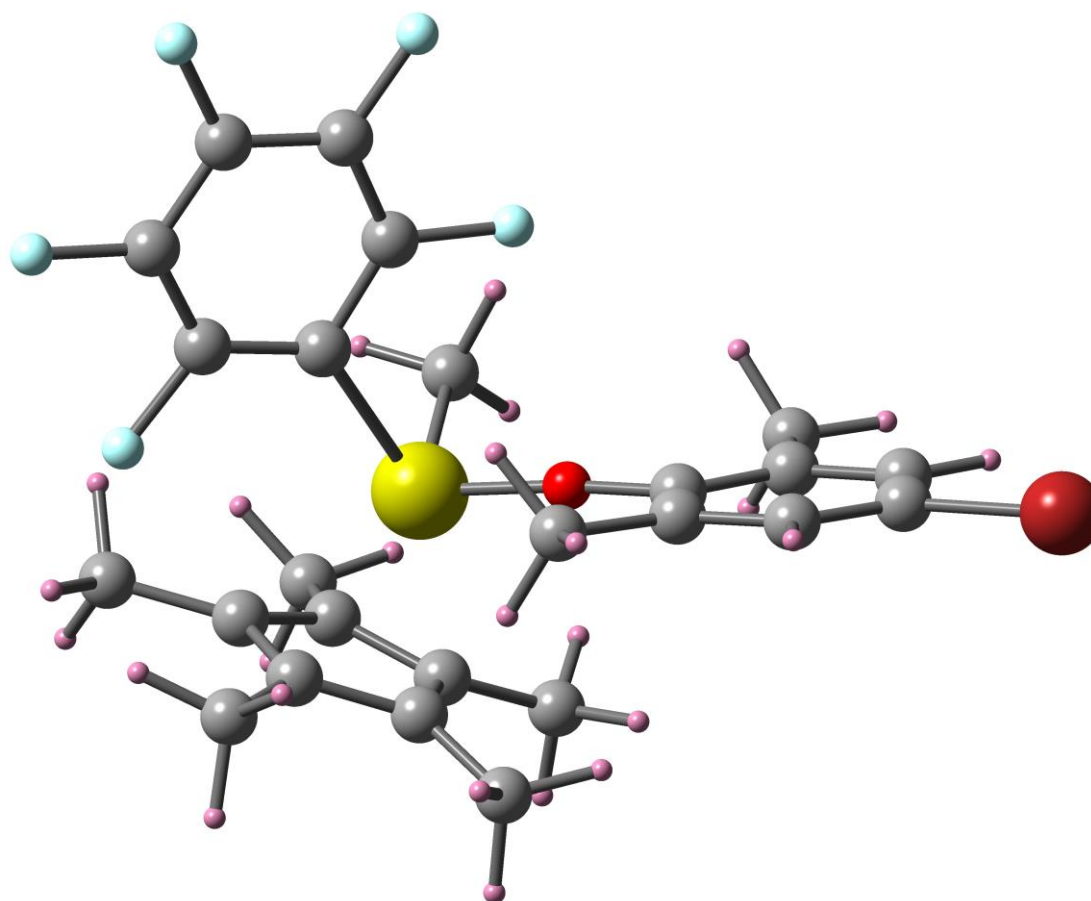
proximal conformation

vacuum	toluene-like solvent	D3 dispersion
-1756.94686556	-1756.9522621	-0.44110865

Ti	-0.27344067	0.85631843	-0.01691334
C	0.50660402	1.29285660	1.87316560
H	0.54119052	0.29471180	2.34983308
H	1.52402785	1.70991126	1.84452941
H	-0.14699005	1.95249094	2.45995875
O	0.91812622	-0.38877941	-0.51985797
C	1.79657354	-1.26831034	-1.14515020
C	1.34552751	-1.94384779	-2.30919105
C	3.10461941	-1.50209894	-0.61820526
C	2.18791380	-2.84624222	-2.98179590
C	3.92651075	-2.41731864	-1.32637995
C	3.49092928	-3.08084616	-2.49005827
H	1.82680924	-3.36360721	-3.87336917
H	4.93153356	-2.61945072	-0.95254515
C	-1.81987081	2.27082096	-1.34074051
C	-1.44767055	3.07811854	-0.20271845
C	-0.61943965	1.98773046	-2.09955448
C	-0.02392771	3.30218241	-0.25416314
C	0.49290350	2.61841538	-1.42409371
C	-2.07081469	-0.35198531	0.38634486
C	-2.78322982	-0.30322624	1.59836642
C	-2.53597838	-1.33258478	-0.50618542
C	-3.85142276	-1.16217935	1.92864300

F	-2.44948852	0.65928084	2.57311400
C	-3.59429191	-2.22223232	-0.24087033
F	-1.93969991	-1.45020530	-1.78144583
C	-4.25767652	-2.13644486	0.99797245
F	-4.51157901	-1.06146735	3.15091225
F	-4.00008376	-3.17159358	-1.17604327
F	-5.30696845	-2.99611830	1.29363840
C	-3.23282714	1.96292902	-1.78164584
H	-3.63328097	2.81011151	-2.36624347
H	-3.28268201	1.07327069	-2.42148033
H	-3.91149721	1.80452465	-0.93328226
C	-2.39819677	3.68385094	0.80451600
H	-2.69048173	4.70065400	0.48664857
H	-3.32035477	3.09836442	0.91130021
H	-1.94707034	3.77331436	1.80203860
C	-0.56832538	1.32020995	-3.45553593
H	-1.30654126	0.51415726	-3.55358707
H	-0.78542704	2.06186689	-4.24456250
H	0.42017427	0.89613838	-3.67278243
C	0.74827255	4.25930099	0.62358652
H	0.66353463	5.28396724	0.22078331
H	0.36832628	4.28286250	1.65349588
H	1.81806674	4.01567835	0.66898367
C	1.91279359	2.69891471	-1.94049361
H	2.20644274	1.79821421	-2.49583651
H	2.01666752	3.55678031	-2.62830984
H	2.64250302	2.84333411	-1.13203066
H	4.15635381	-3.77915885	-3.00189579
H	0.33292685	-1.76571545	-2.66081825
C	3.60830547	-0.82983690	0.66182999
C	3.87338086	-1.86741940	1.79922935
C	4.87965766	0.04401978	0.42359976
H	2.81703394	-0.15944260	1.01896840
C	4.35930351	-1.18477030	3.10252830
H	4.63303432	-2.59608175	1.46763564
H	2.95128592	-2.44009068	1.99452016
C	5.35948262	0.72753598	1.72894691
H	5.69637760	-0.58198870	0.02515621
H	4.66426611	0.80481942	-0.34572841
C	5.60906738	-0.30263166	2.85874855
H	4.58193685	-1.95520059	3.86086385
H	3.54667116	-0.56079948	3.51657302
H	6.28130616	1.30120038	1.52938311
H	4.59943550	1.45669683	2.06487199
H	5.89246947	0.21815939	3.78946230
H	6.46397259	-0.94699304	2.58266908
Frequencies --	16.1595	17.4747	23.1795
Frequencies --	33.7819	39.4064	47.9913
Frequencies --	57.1961	69.0601	83.1218
Frequencies --	85.1165	100.7441	109.7461
Frequencies --	113.6826	114.5582	119.0302
Frequencies --	121.5502	128.4413	140.4363
Frequencies --	145.6196	153.1692	154.1831
Frequencies --	156.2656	158.2117	168.0425
Frequencies --	173.0419	192.6408	204.8136
Frequencies --	215.8043	224.4880	225.9396
Frequencies --	234.7042	244.2656	264.9768

Frequencies --	266.2907	269.4953	279.6535
Frequencies --	286.4587	291.0036	296.1003
Frequencies --	298.5199	301.8343	313.4829
Frequencies --	322.6256	338.5224	344.6491
Frequencies --	355.8226	381.8268	384.4446
Frequencies --	389.1360	411.5177	428.3395
Frequencies --	437.9154	440.4892	460.7307
Frequencies --	496.6028	500.0070	503.8447
Frequencies --	522.8683	535.0389	540.0468
Frequencies --	543.5661	554.0909	557.3164
Frequencies --	570.0847	584.0774	594.7147
Frequencies --	605.1581	613.7584	618.6212
Frequencies --	633.1358	647.5199	683.0754
Frequencies --	687.9299	720.9678	726.8803
Frequencies --	746.4958	768.9421	770.4275
Frequencies --	792.1116	801.9444	804.0477
Frequencies --	820.5065	865.2662	872.2331
Frequencies --	884.9907	888.0762	905.9712
Frequencies --	925.2327	932.6759	959.5393
Frequencies --	968.6274	970.0282	989.7055
Frequencies --	994.6571	998.8366	1037.5101
Frequencies --	1043.5154	1044.7756	1048.6227
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Frequencies --	1055.1691	1062.5714	1084.7523
Frequencies --	1086.5187	1087.7491	1095.8765
Frequencies --	1115.0873	1123.6684	1154.3377
Frequencies --	1171.4517	1173.5550	1177.2181
Frequencies --	1184.7435	1189.4191	1192.8009
Frequencies --	1201.3020	1231.2704	1249.0441
Frequencies --	1279.9492	1280.4089	1286.4128
Frequencies --	1295.8647	1315.4087	1330.7852
Frequencies --	1352.5566	1354.6043	1359.5691
Frequencies --	1360.5360	1364.0560	1369.3493
Frequencies --	1387.0920	1394.1293	1410.7941
Frequencies --	1412.4547	1423.0959	1423.7373
Frequencies --	1427.0414	1430.3015	1431.6462
Frequencies --	1435.0318	1440.6113	1448.3119
Frequencies --	1450.8857	1454.5725	1458.6400
Frequencies --	1463.4824	1480.3865	1482.5342
Frequencies --	1482.8241	1486.6010	1486.9807
Frequencies --	1491.5835	1492.1989	1492.9996
Frequencies --	1498.4997	1499.6599	1500.2590
Frequencies --	1504.8071	1507.9467	1512.0377
Frequencies --	1513.4055	1516.0274	1586.2376
Frequencies --	1588.2266	1600.0862	1614.7073
Frequencies --	2981.9558	2997.9587	3001.0871
Frequencies --	3004.2647	3004.4967	3005.1399
Frequencies --	3006.6291	3007.7617	3008.9102
Frequencies --	3011.4147	3016.0529	3058.7561
Frequencies --	3061.6443	3067.9468	3075.9155
Frequencies --	3080.5679	3096.6619	3098.0548
Frequencies --	3098.9982	3101.7516	3104.0899
Frequencies --	3105.2913	3113.3042	3136.2234
Frequencies --	3140.3021	3141.8409	3146.0661
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Frequencies --	3172.8304	3190.8193	3242.9616

Catalyst 14:

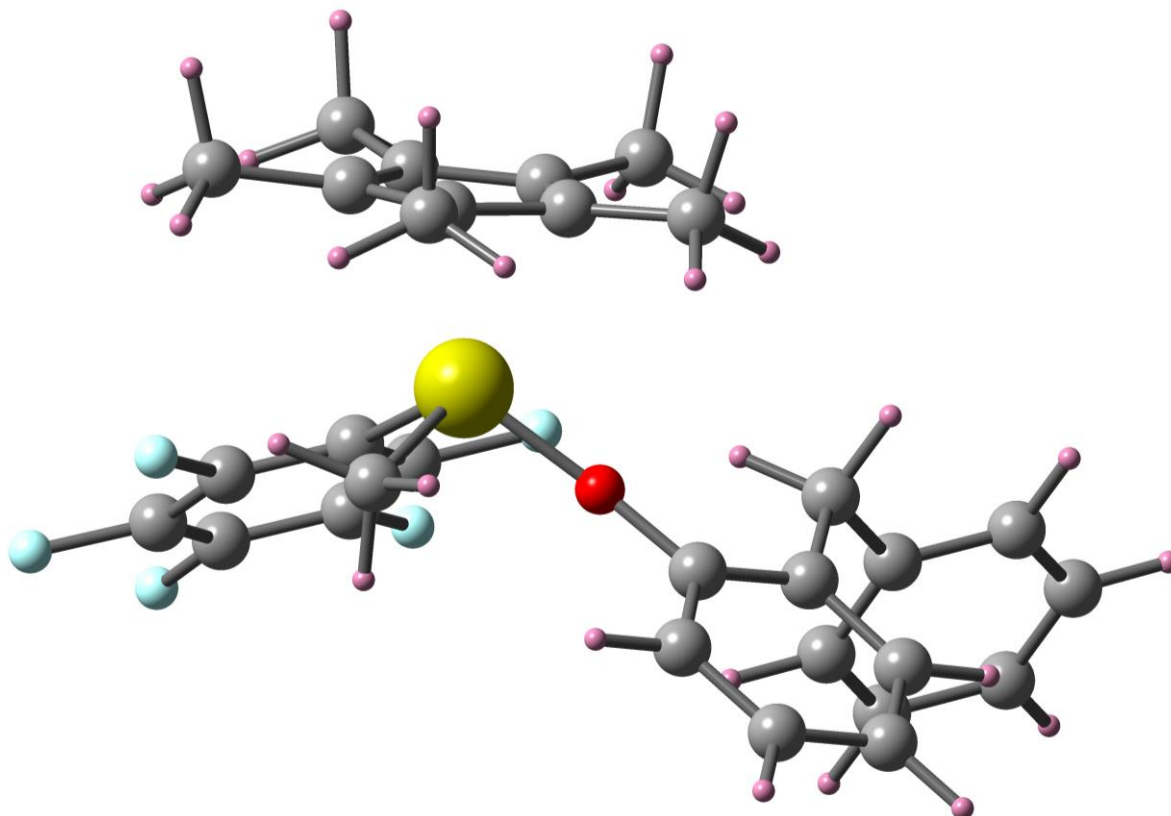
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Ti	-1.15453700	-0.99148000	-0.41963100
C	-1.45430300	-1.10020500	-2.48821400
H	-0.99802500	-0.18242900	-2.88906600
H	-0.99930600	-1.97261000	-2.97913800
H	-2.53717200	-1.09503900	-2.69611400
O	0.57422000	-0.53213500	-0.32859500
C	1.91111900	-0.22374700	-0.14964300
C	2.31577300	0.48579800	1.02148300
C	2.84772300	-0.58639900	-1.16383300
C	3.68785600	0.78802200	1.18404500
C	4.21148100	-0.27023700	-0.96304300
C	4.61899200	0.40031800	0.20403600
H	4.01412700	1.32900500	2.07172100
H	4.93993200	-0.54257100	-1.72607200
C	-2.08431500	-2.21966600	1.49789800
C	-3.03745300	-2.43551100	0.43066000
C	-0.83327100	-2.83922900	1.10948100
C	-2.37314600	-3.18549800	-0.61089400
C	-1.01509200	-3.43536800	-0.19092900
F	-3.39603000	5.14181500	-0.20929400

C	-2.95415200	3.82700400	-0.20115600
C	-3.60226600	2.86035400	0.58598800
C	-1.84724500	3.43930000	-0.97654200
C	-3.12955400	1.53167000	0.56908100
F	-4.69526300	3.22816100	1.36747900
C	-1.42431400	2.09489100	-0.94469700
F	-1.19085400	4.38614400	-1.75809500
C	-2.03389000	1.06667300	-0.18616500
F	-3.84434700	0.65203500	1.40239800
F	-0.30067500	1.81971400	-1.74796800
C	1.31558500	0.93934300	2.07008800
H	0.52076100	1.55317900	1.62274200
H	0.82711600	0.08533200	2.56135400
H	1.80840700	1.53654700	2.84925200
C	2.41099200	-1.26359200	-2.45036900
H	1.91270200	-2.22453400	-2.25894700
H	1.69588900	-0.63330400	-2.99924700
H	3.27232500	-1.45214900	-3.10554100
Br	6.52684700	0.82030200	0.46228300
C	-2.36254900	-1.66446700	2.87854200
H	-3.33415300	-1.16639300	2.93703400
H	-2.36081900	-2.48779500	3.61395100
H	-1.60368300	-0.93905000	3.20845200
C	-4.52545400	-2.15578900	0.44010300
H	-4.84059500	-1.61069600	1.33434100
H	-4.85416400	-1.57075400	-0.43265300
H	-5.07965700	-3.10972700	0.41481400
C	0.37758600	-3.02313500	1.99693100
H	0.41374000	-2.28432000	2.80712500
H	0.34560400	-4.01998800	2.47092400
H	1.32360400	-2.95786800	1.44237700
C	-3.05813000	-3.79912400	-1.80901700
H	-3.47517800	-4.78472500	-1.53550900
H	-3.89219200	-3.18317300	-2.17138500
H	-2.37097900	-3.96010400	-2.64994600
C	-0.00830900	-4.29691000	-0.91828700
H	-0.17630600	-5.36033700	-0.67157100
H	-0.08773000	-4.20567500	-2.01084500
H	1.02469800	-4.05953700	-0.63126600

Frequencies --	13.7534	16.3666	28.5943
Frequencies --	32.6628	41.7769	63.6783
Frequencies --	65.8404	77.7178	84.8571
Frequencies --	89.6134	99.2107	102.6269
Frequencies --	110.8285	114.7300	126.0833
Frequencies --	133.7553	136.5582	139.3952
Frequencies --	144.5354	149.0037	152.9004
Frequencies --	160.5809	169.1973	172.0837
Frequencies --	179.0295	181.0908	190.6457
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Frequencies --	228.4915	240.4881	246.3266
Frequencies --	258.9240	261.7473	264.9133
Frequencies --	274.3217	282.7730	284.7402
Frequencies --	293.3081	296.0883	305.6131
Frequencies --	323.2103	339.3161	346.6904
Frequencies --	355.7873	380.2268	383.7868
Frequencies --	390.9505	398.5795	424.4354
Frequencies --	431.0283	457.9560	501.8079

Frequencies --	504.7365	508.3759	533.4090
Frequencies --	538.6602	546.4088	555.3641
Frequencies --	560.5683	565.6947	572.2808
Frequencies --	585.1199	591.8672	595.9892
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Frequencies --	681.5462	687.8664	713.5782
Frequencies --	734.8643	736.0319	795.2720
Frequencies --	798.5297	808.3229	883.4621
Frequencies --	885.5822	891.2010	924.8758
Frequencies --	950.1387	965.3185	972.1945
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Frequencies --	1054.7569	1057.3188	1085.8814
Frequencies --	1086.5079	1122.5269	1126.2689
Frequencies --	1173.3249	1176.4844	1180.7500
Frequencies --	1188.9822	1226.1346	1264.3495
Frequencies --	1277.2309	1289.7359	1340.3651
Frequencies --	1353.4365	1386.0872	1409.4635
Frequencies --	1413.1497	1413.9296	1419.7177
Frequencies --	1422.2069	1423.6560	1424.6194
Frequencies --	1426.2392	1431.9550	1433.0263
Frequencies --	1433.5052	1439.2067	1450.5331
Frequencies --	1452.0556	1457.4193	1462.2212
Frequencies --	1465.2375	1481.0800	1485.5102
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Frequencies --	1496.5879	1500.2996	1501.7940
Frequencies --	1502.1680	1505.0371	1506.1890
Frequencies --	1510.5913	1513.6407	1521.0817
Frequencies --	1587.7493	1588.0002	1592.3010
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Frequencies --	3085.6665	3090.5267	3091.2308
Frequencies --	3096.7058	3098.9437	3119.6994
Frequencies --	3120.9111	3121.6146	3133.8929
Frequencies --	3135.3442	3136.8398	3137.3092
Frequencies --	3141.5691	3145.5810	3171.0110
Frequencies --	3178.8494	3197.6296	3199.9327

Catalyst 15:**distal conformation**

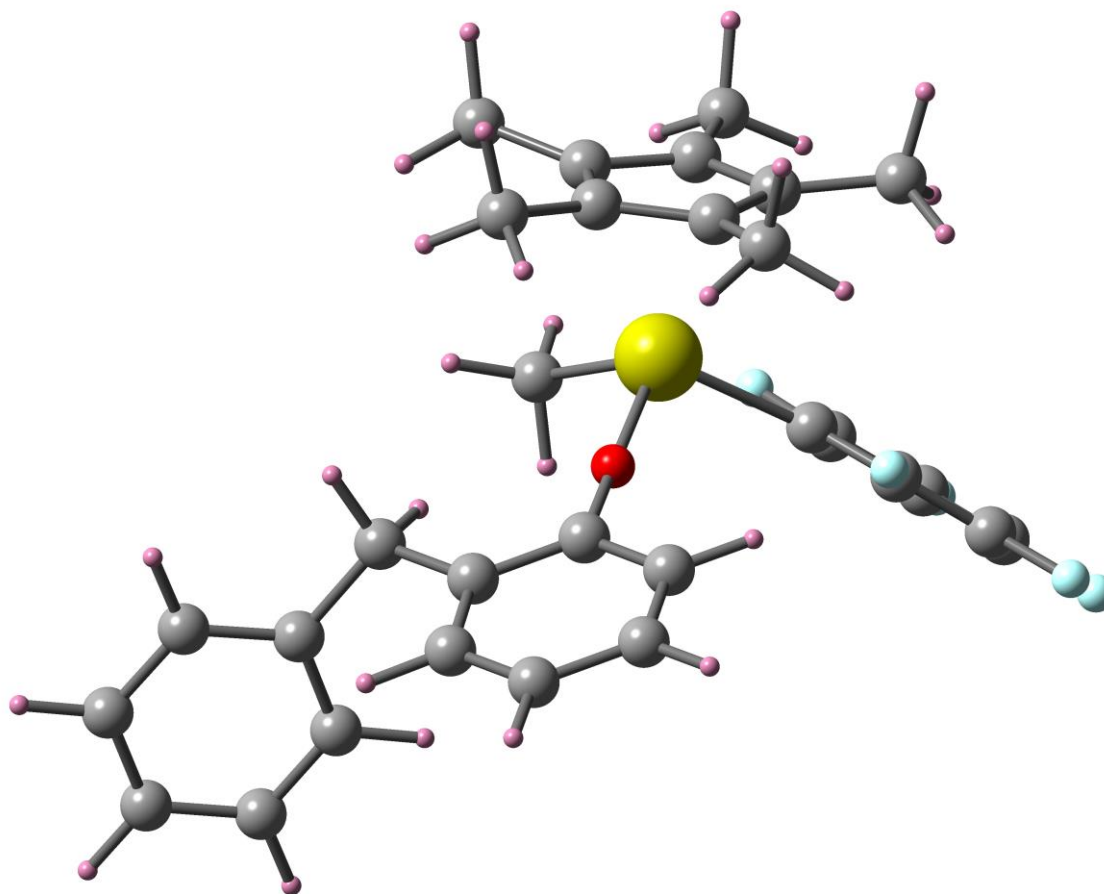
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H	1.67059500	-1.02028100	2.75409800
H	1.77962900	-2.74670300	2.27096800
H	3.18531900	-1.65626200	2.02304100
O	-0.45845200	-1.20755900	0.73319300
C	-1.63773100	-1.62687600	1.33820900
C	-2.91382400	-1.35359500	0.76029300
C	-1.53394700	-2.32431300	2.57083100
C	-4.05702100	-1.81311500	1.46193500
C	-2.68747100	-2.76746600	3.24093700
C	-3.95911500	-2.51157400	2.68154000
H	-5.04280100	-1.60523600	1.04341800
H	-2.59302300	-3.30146700	4.18914500
C	2.51917000	-0.92605600	-1.92037100
C	3.32139600	-1.75810700	-1.05719100
C	1.23997200	-1.58013900	-2.10761500
C	2.54491300	-2.92148600	-0.70197900
C	1.25208700	-2.81203600	-1.34895600
C	1.61331200	1.13869400	0.28884600

C	2.70047000	1.73009200	0.95687800
C	0.69603700	2.06412400	-0.23639400
C	2.86864900	3.11918900	1.12711600
F	3.71757200	0.91777400	1.49927800
C	0.80179900	3.46176700	-0.10264000
F	-0.41639500	1.59502600	-0.96821100
C	1.90400300	3.99424400	0.59300800
F	3.96858100	3.63898300	1.80487700
F	-0.15080400	4.31966700	-0.64639100
F	2.04241100	5.36740600	0.74306100
C	-3.06009400	-0.63822800	-0.58705200
H	-2.11721500	-0.13308900	-0.81986100
H	-3.20682600	-1.40515800	-1.36779200
C	3.00078600	0.29430900	-2.67161100
H	3.48510300	-0.01386100	-3.61523400
H	2.17833900	0.97189200	-2.93514400
H	3.74006000	0.87141100	-2.10078700
C	4.76452700	-1.51194500	-0.68263100
H	5.43358600	-1.96671200	-1.43487000
H	5.00503000	-0.44250000	-0.63394000
H	5.02306600	-1.95326700	0.28926300
C	0.16212500	-1.14095800	-3.07262900
H	0.05472900	-0.04949500	-3.11825100
H	0.41030500	-1.48901500	-4.09100500
H	-0.81930300	-1.55980000	-2.81832500
C	3.05970700	-4.13690800	0.03348000
H	3.56540300	-4.81520200	-0.67622500
H	3.78949400	-3.87808000	0.81164200
H	2.25188400	-4.70884700	0.50934900
C	0.17819200	-3.87758600	-1.35875200
H	-0.82036700	-3.45781200	-1.53669700
H	0.37573900	-4.61031000	-2.16097400
H	0.13476500	-4.43491300	-0.41253300
H	-4.86403800	-2.84744100	3.19198200
H	-0.54730700	-2.50667100	2.99147900
C	-4.20664900	0.37172800	-0.67758200
C	-5.33239600	0.12866100	-1.50263800
C	-4.15520700	1.59436200	0.04082300
C	-6.37993600	1.07182900	-1.60629000
H	-5.39181300	-0.80259100	-2.07256300
C	-5.19720000	2.53916100	-0.05752900
H	-3.29466300	1.80848600	0.67886000
C	-6.31622300	2.28152900	-0.88225000
H	-7.23763400	0.86290100	-2.25056100
H	-5.13352600	3.47634900	0.50083400
H	-7.12252300	3.01465000	-0.96134400

Frequencies --	7.3910	13.4609	19.6637
Frequencies --	24.9957	29.6187	34.0073
Frequencies --	43.5264	53.2533	67.4313
Frequencies --	79.3217	94.5516	100.1748
Frequencies --	109.2516	112.2353	118.0392
Frequencies --	120.1864	122.6581	126.2616
Frequencies --	132.5257	151.4509	156.7900
Frequencies --	159.0649	163.4282	164.8107
Frequencies --	171.5462	180.1436	187.1453
Frequencies --	203.1342	213.7291	225.3622
Frequencies --	246.3856	262.2200	264.5922

Frequencies --	273.7099	279.9567	290.7259
Frequencies --	292.5015	297.0124	301.3926
Frequencies --	306.5740	311.2884	318.1191
Frequencies --	328.1018	344.1461	353.8705
Frequencies --	380.2484	383.6005	390.0860
Frequencies --	407.2184	413.7520	428.4749
Frequencies --	448.3543	460.7411	465.4697
Frequencies --	484.8346	504.0298	534.6636
Frequencies --	535.3860	540.2983	543.7081
Frequencies --	555.4002	572.0553	576.6764
Frequencies --	583.9761	594.7921	605.6846
Frequencies --	616.9078	618.0429	624.5430
Frequencies --	633.4703	644.8396	678.9677
Frequencies --	688.5507	708.0622	721.7255
Frequencies --	722.8723	729.0198	746.1342
Frequencies --	767.2828	802.8540	804.2049
Frequencies --	812.5688	826.6196	860.6900
Frequencies --	871.8625	885.4674	923.4544
Frequencies --	928.2569	945.5640	965.9705
Frequencies --	969.4941	971.5034	986.9936
Frequencies --	993.5320	995.2342	1003.2904
Frequencies --	1021.5205	1038.8321	1042.3034
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Frequencies --	1050.4194	1052.1749	1053.0375
Frequencies --	1086.4882	1087.9673	1089.7552
Frequencies --	1110.5317	1123.8524	1172.6274
Frequencies --	1174.2931	1177.5121	1180.8848
Frequencies --	1181.8080	1190.2236	1193.2863
Frequencies --	1202.5861	1208.5743	1221.2229
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Frequencies --	1322.0175	1351.4278	1354.6574
Frequencies --	1375.1332	1380.5442	1395.9759
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Frequencies --	1424.7540	1426.2835	1429.9782
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Frequencies --	1455.2199	1458.7260	1463.4178
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Frequencies --	1627.0137	2982.3079	3005.4806
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Frequencies --	3147.0742	3148.2367	3151.2422
Frequencies --	3151.3480	3153.5854	3160.7027
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proximal conformation

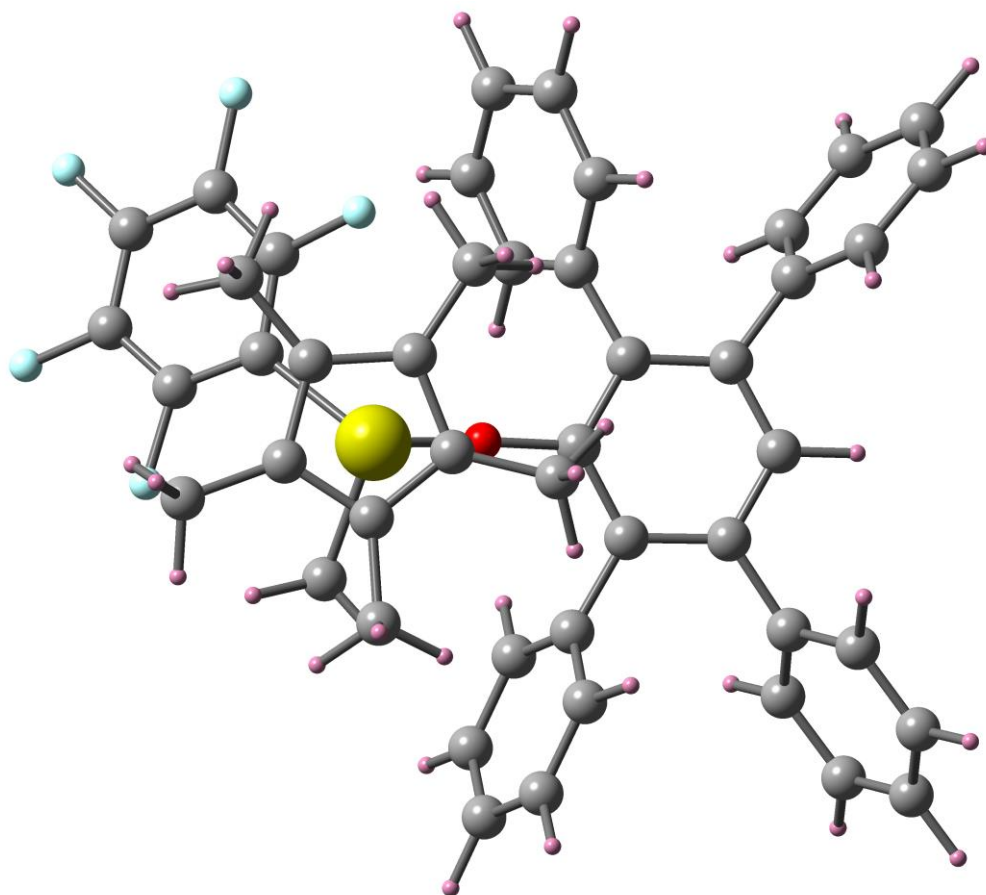
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H	-0.49044500	-0.19015000	-2.30847400
H	-1.19432200	1.46046900	-2.25534200
H	0.44119600	1.20652100	-2.95117400
O	-0.75081300	0.12378200	0.63717700
C	-1.72273300	-0.32752100	1.52169100
C	-1.30454500	-0.84429600	2.77533500
C	-3.10582900	-0.29263800	1.16887800
C	-2.25339300	-1.31041200	3.70294400
C	-4.03570100	-0.76570000	2.12777200
C	-3.62802800	-1.26579500	3.38067000
H	-1.91981400	-1.70930400	4.66348000
H	-5.09754700	-0.75246500	1.87663600
C	2.45594900	2.34102900	0.51032100
C	2.12094100	2.82405100	-0.80943400
C	1.29693000	2.52069600	1.35972600
C	0.76236300	3.30634700	-0.78188200
C	0.24651600	3.10959500	0.55925500
C	2.12815800	-0.67507100	-0.31485700

C	2.73148900	-1.13116700	-1.50112000
C	2.50608200	-1.39800800	0.82879100
C	3.61664000	-2.22626000	-1.57284300
F	2.47128600	-0.47304000	-2.72044300
C	3.38115400	-2.50061200	0.82875800
F	2.01183900	-1.00444200	2.09296400
C	3.94039800	-2.92164500	-0.39280300
F	4.17800100	-2.62686100	-2.78268500
F	3.70958200	-3.17024900	2.00520500
F	4.81074100	-4.00246900	-0.43081900
C	-3.58129800	0.27156000	-0.17387700
H	-3.90314000	1.31632000	-0.01865700
H	-2.72436000	0.31182800	-0.85564600
C	3.83552600	1.93386300	0.97601500
H	4.41250500	2.83281300	1.25654700
H	3.80142600	1.28094500	1.85682000
H	4.40494700	1.41385400	0.19445300
C	3.06661100	2.91578900	-1.98533100
H	3.56610500	3.90106400	-1.99430400
H	3.85407800	2.15214000	-1.94668000
H	2.54814600	2.80638900	-2.94749100
C	1.25262200	2.29559700	2.85445000
H	1.88417300	1.45526800	3.16833600
H	1.61756600	3.19619900	3.37929700
H	0.23532400	2.09905600	3.21691700
C	0.07689900	4.08052100	-1.88338000
H	0.34236700	5.14977300	-1.80736900
H	0.37708000	3.74139100	-2.88355200
H	-1.01754200	4.01277500	-1.82321800
C	-1.09391100	3.59503300	1.06538200
H	-1.41687400	3.05762400	1.96628100
H	-1.03426000	4.66654400	1.32593000
H	-1.88736000	3.48920300	0.31224900
H	-4.37327000	-1.62520100	4.09321900
H	-0.24163900	-0.88324700	3.00009500
C	-4.72061600	-0.49336000	-0.85281600
C	-5.97151200	0.12523900	-1.09611300
C	-4.53752700	-1.82907900	-1.29598000
C	-7.01159700	-0.56502100	-1.75897700
H	-6.13628400	1.15495100	-0.76735200
C	-5.57103100	-2.52321200	-1.95787800
H	-3.58225900	-2.32943500	-1.11821800
C	-6.81480300	-1.89321500	-2.19300900
H	-7.96787800	-0.06647100	-1.93574700
H	-5.40671600	-3.55055700	-2.29217700
H	-7.61563100	-2.42978500	-2.70726300

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Frequencies --	103.9856	113.0493	118.8080
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Frequencies --	141.1452	151.2067	155.4273
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Frequencies --	205.6739	215.6707	217.2194
Frequencies --	237.8963	248.6652	262.1941

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Frequencies --	1086.4037	1088.2943	1090.1532
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Frequencies --	1491.5124	1495.1465	1498.5082
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Frequencies --	1508.0915	1511.0034	1514.4594
Frequencies --	1518.6695	1587.4380	1588.3396
Frequencies --	1600.6446	1604.5120	1614.6757
Frequencies --	1626.7528	2977.4785	3004.6666
Frequencies --	3005.2858	3007.4001	3008.2933
Frequencies --	3009.8481	3019.6142	3095.2238
Frequencies --	3097.6335	3098.8591	3102.3924
Frequencies --	3103.5059	3105.2000	3133.1614
Frequencies --	3137.0592	3140.5047	3142.3418
Frequencies --	3146.3855	3147.4264	3148.8413
Frequencies --	3151.3481	3152.7321	3161.4819
Frequencies --	3163.7317	3173.4203	3175.2520
Frequencies --	3190.3914	3192.6708	3236.6285

Catalyst 16:

vacuum	toluene-like solvent	D3 dispersion
-2446.1612696	-2446.1719709	-0.66977625

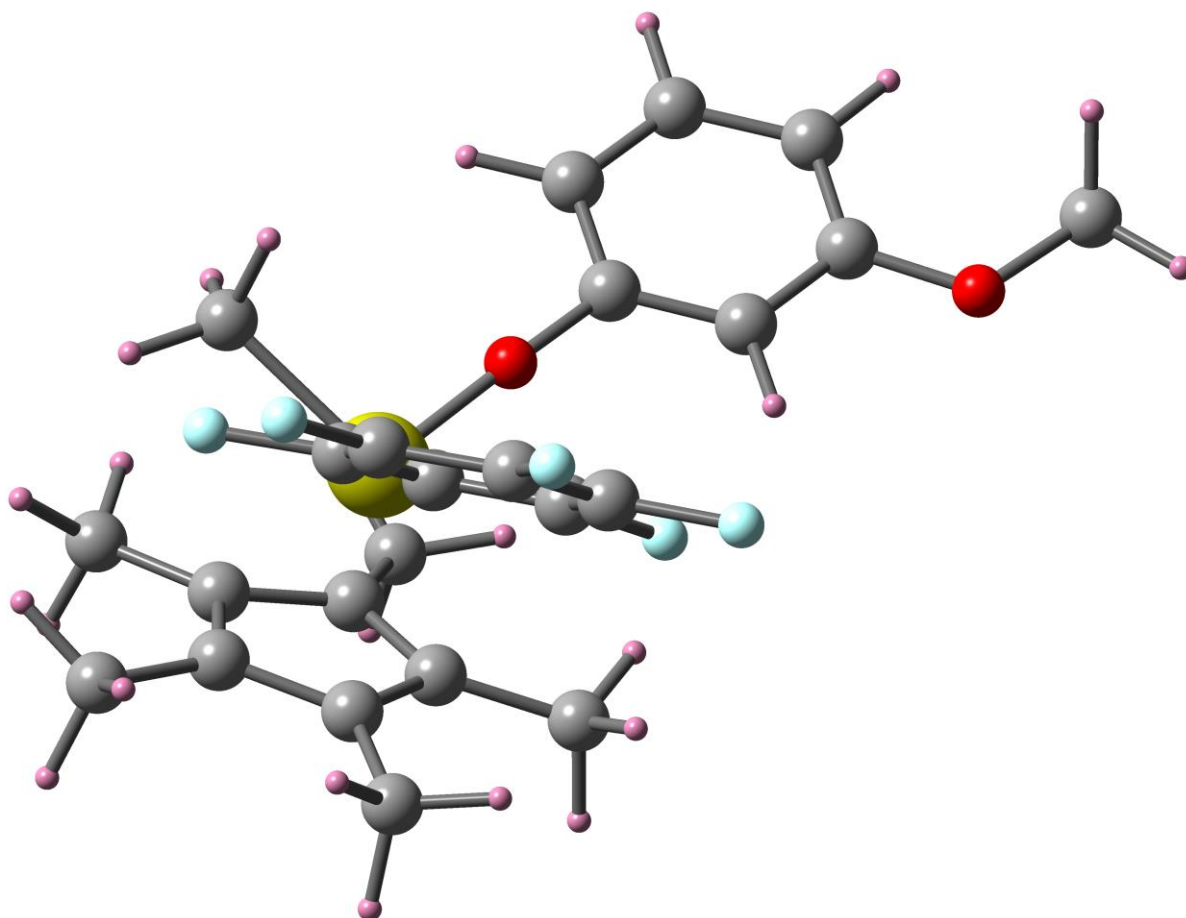
Ti	-1.50925200	-1.22596900	0.49873000
C	-1.37110700	-2.96755700	-0.61473800
H	-1.35404800	-2.57508300	-1.64646700
H	-0.44362800	-3.52086400	-0.43327000
H	-2.23787900	-3.62756900	-0.48848200
O	-0.01845900	-0.38377000	-0.15298500
C	1.27445100	0.12461400	-0.25930000
C	1.49115400	1.53825700	-0.11341600
C	2.36928500	-0.78159500	-0.47674900
C	2.83356000	2.00057100	0.05172200
C	3.69876900	-0.29169400	-0.30105800
C	3.89432300	1.06845500	0.02205300
C	-2.94720300	-1.16065300	2.55455600
C	-2.77047700	-2.55807800	2.23674700
C	-1.64428100	-0.60013700	2.83618900
C	-1.36730500	-2.87159500	2.33460600
C	-0.66537600	-1.65411700	2.69025800
C	-3.30205000	-0.31665100	-0.44779800
C	-4.17938900	-0.93553900	-1.36088700
C	-3.60261300	1.03660600	-0.21156400

C	-5.23836900	-0.27287900	-2.01787900
F	-4.05620500	-2.30384300	-1.66792800
C	-4.64557600	1.75349000	-0.82612400
F	-2.83414600	1.74358600	0.73053800
C	-5.46965900	1.08834200	-1.75236200
F	-6.06246100	-0.94569800	-2.91854600
F	-4.88546000	3.09505900	-0.53261000
F	-6.50606000	1.76360300	-2.38500600
C	-4.28417100	-0.49460700	2.78757900
H	-4.65157400	-0.75290200	3.79686100
H	-4.22459400	0.59811100	2.73195300
H	-5.04710900	-0.82874500	2.07158700
C	-3.89355100	-3.53233200	1.96474200
H	-4.41860700	-3.77987900	2.90413800
H	-4.64347500	-3.12032300	1.27435100
H	-3.53050000	-4.47489600	1.53648400
C	-1.35401300	0.77579300	3.39100400
H	-0.50144800	1.25715900	2.89562500
H	-2.21014800	1.45108000	3.28724400
H	-1.11252500	0.70002600	4.46587400
C	-0.76153400	-4.25503600	2.29204000
H	-0.81462900	-4.71285100	3.29582300
H	-1.28915100	-4.92320500	1.59953400
H	0.29407400	-4.23692200	1.99445400
C	0.79068800	-1.54699900	3.08420000
H	1.19261400	-0.54059000	2.90902200
H	0.90353900	-1.76283100	4.16177300
H	1.42503400	-2.25803900	2.54176600
H	4.91340200	1.43477500	0.13781700
C	3.22375700	3.44979000	0.20330800
C	3.02485800	4.38990600	-0.84048000
C	3.89788500	3.88269500	1.37495100
C	3.47665500	5.71986700	-0.71323500
H	2.52083600	4.07987100	-1.75648600
C	4.34483900	5.21486900	1.50893200
H	4.06598100	3.17448900	2.18962700
C	4.13607100	6.14054700	0.46327000
H	3.31483900	6.42505700	-1.53209900
H	4.85427300	5.52627700	2.42421900
H	4.48347600	7.17172400	0.56193700
C	4.94062400	-1.12846600	-0.48532900
C	5.32211500	-1.62971500	-1.75652800
C	5.80973200	-1.35683100	0.61309700
C	6.52775900	-2.34313600	-1.92182200
H	4.67906000	-1.45578500	-2.62006600
C	7.01338800	-2.07689700	0.45312600
H	5.53820500	-0.97440500	1.59979700
C	7.37782800	-2.57397000	-0.81734900
H	6.80284700	-2.71565000	-2.91159100
H	7.66256000	-2.24599600	1.31578500
H	8.31015700	-3.12891900	-0.94590200
C	0.37307800	2.53719000	-0.22873000
C	-0.33927400	2.64510900	-1.45260300
C	0.10091900	3.48609100	0.78836100
C	-1.27092300	3.68224100	-1.66100100
H	-0.14221300	1.92955700	-2.25362500
C	-0.83737500	4.51822400	0.58726200

H	0.63885600	3.42955500	1.73579200
C	-1.52093600	4.62765700	-0.64235200
H	-1.79821200	3.75380600	-2.61544200
H	-1.02878800	5.23834100	1.38626600
H	-2.24463400	5.42997900	-0.80157300
C	2.16517900	-2.18968000	-0.96825000
C	1.66306900	-2.40154500	-2.27924400
C	2.59169300	-3.32018800	-0.22681900
C	1.59878300	-3.69649500	-2.83331600
H	1.33901900	-1.54549800	-2.87421400
C	2.52002200	-4.61873600	-0.77294700
H	3.00621600	-3.18296400	0.77276200
C	2.02809400	-4.81284100	-2.08210200
H	1.21534300	-3.83311300	-3.84715900
H	2.86088100	-5.47331000	-0.18343400
H	1.98175200	-5.81642300	-2.51101800

Frequencies --	13.2686	15.4961	18.3307
Frequencies --	22.4255	27.6766	35.6528
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Frequencies --	52.4478	53.5805	60.3637
Frequencies --	64.5014	65.4613	71.0492
Frequencies --	75.8018	85.4683	88.3179
Frequencies --	91.1318	99.6232	104.9233
Frequencies --	112.4049	118.0266	123.8326
Frequencies --	125.7103	132.8223	137.9883
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Frequencies --	1050.3262	1052.6248	1053.2123
Frequencies --	1053.6071	1054.0874	1088.0694
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Frequencies --	1090.1628	1090.9104	1122.0899
Frequencies --	1124.9987	1126.9185	1174.9539
Frequencies --	1177.8247	1181.7478	1181.7623
Frequencies --	1182.8711	1183.0310	1183.9862
Frequencies --	1188.0191	1203.3864	1204.6267
Frequencies --	1205.7091	1206.4444	1225.5919
Frequencies --	1262.7342	1279.0183	1288.9731
Frequencies --	1298.0905	1315.4374	1325.1781
Frequencies --	1330.1564	1332.3340	1333.9004
Frequencies --	1349.5292	1364.6565	1368.0624
Frequencies --	1370.0710	1370.9201	1378.6209
Frequencies --	1392.8260	1411.8477	1414.4930
Frequencies --	1422.9144	1425.5882	1428.4298
Frequencies --	1431.6755	1433.5305	1435.8332
Frequencies --	1437.3323	1441.9985	1443.2207
Frequencies --	1445.3847	1447.3513	1452.2324
Frequencies --	1452.9384	1454.8733	1460.5761
Frequencies --	1464.4057	1481.6820	1492.8007
Frequencies --	1493.3942	1496.3247	1496.3675
Frequencies --	1498.5492	1501.1800	1501.7884
Frequencies --	1504.6730	1506.4920	1506.6505
Frequencies --	1512.8668	1515.8273	1520.4088
Frequencies --	1525.3614	1584.4794	1588.1025
Frequencies --	1593.9350	1595.6242	1596.6260
Frequencies --	1597.9022	1600.9916	1622.8667
Frequencies --	1623.2755	1623.7356	1624.8784
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Frequencies --	3095.0131	3101.3064	3104.8622
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Frequencies --	3150.5886	3152.2001	3153.1540
Frequencies --	3153.8538	3155.6754	3157.3912
Frequencies --	3157.9432	3158.4298	3160.2244
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Frequencies --	3173.1181	3174.5093	3179.9232
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Catalyst 17:**distal conformation**

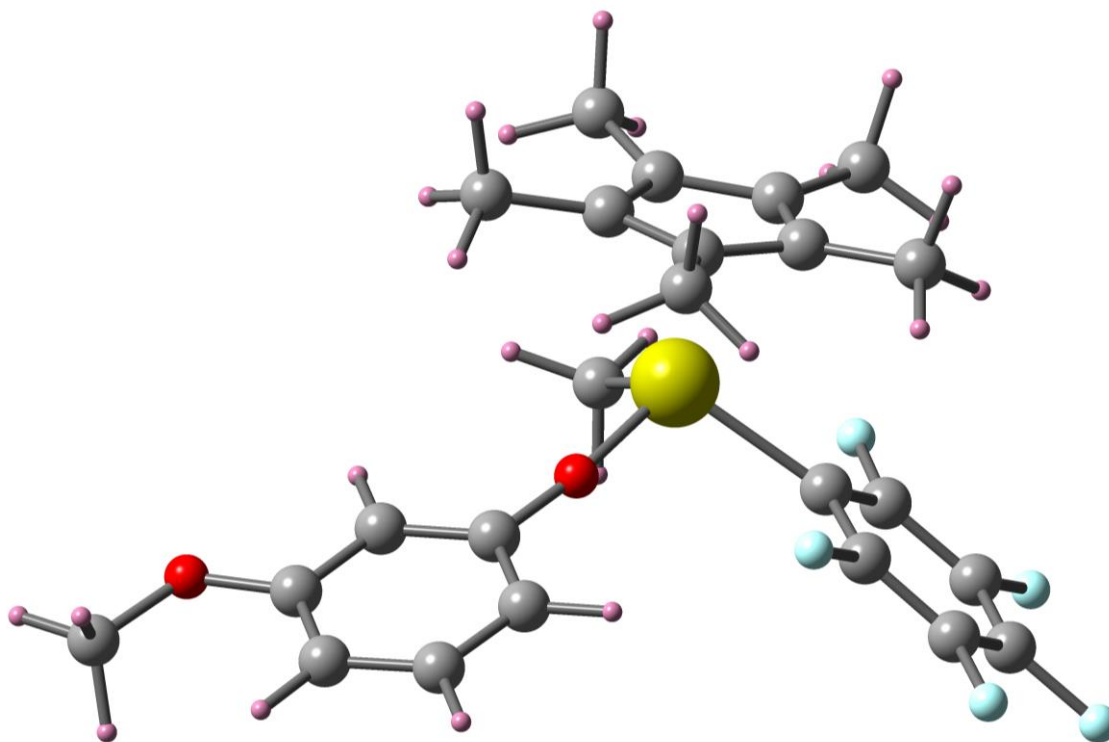
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C	-0.65565200	-1.78407800	-2.35263100
H	-0.54142400	-0.85384100	-2.94301900
H	0.10504200	-2.50690900	-2.68682000
H	-1.65994500	-2.19934300	-2.51629500
O	1.29973200	-0.42407900	-0.68490200
C	2.62359300	-0.06209000	-0.83636800
C	3.19658000	0.88343300	0.03913400
C	3.38470500	-0.63091400	-1.89276800
C	4.54886500	1.26303000	-0.13492800
C	4.72577400	-0.23889800	-2.05029900
C	5.32325200	0.70299000	-1.18191800
H	5.31911500	-0.66797500	-2.86106100
C	-1.49636100	-1.77491000	1.65881100
C	-1.95831800	-2.68864000	0.63927400
C	-0.06557700	-1.95059300	1.80091500
C	-0.82222600	-3.42981500	0.14910800

C	0.35302900	-2.96828300	0.86292500
C	-1.52763300	0.74976200	-0.21687400
C	-2.70913100	0.97551400	-0.94379000
C	-1.09948000	1.85208600	0.54182100
C	-3.41403300	2.19582200	-0.95525300
F	-3.26090800	-0.06680700	-1.71882800
C	-1.75436900	3.09819800	0.57463800
F	0.05031500	1.73421300	1.35246400
C	-2.92549900	3.27059000	-0.18842400
F	-4.57915900	2.35588100	-1.70144400
F	-1.27483900	4.15324500	1.34715700
F	-3.59635900	4.48629500	-0.17690200
C	-2.37733000	-0.94288000	2.56310800
H	-2.70894700	-1.55042900	3.42376600
H	-1.85150000	-0.06803800	2.96602300
H	-3.28003700	-0.58529100	2.05048300
C	-3.39770700	-2.91061200	0.23397700
H	-3.86252900	-3.67148300	0.88621100
H	-4.00049200	-1.99709200	0.31660000
H	-3.48647300	-3.27126100	-0.79961800
C	0.80480000	-1.29871900	2.85173000
H	0.47490400	-0.28035800	3.09234000
H	0.76932100	-1.88721300	3.78563300
H	1.85718500	-1.24049400	2.54448200
C	-0.87527700	-4.62170800	-0.77785100
H	-1.09710400	-5.53516900	-0.19833800
H	-1.65655600	-4.52409000	-1.54315000
H	0.07866400	-4.78880300	-1.29582600
C	1.74046600	-3.55967000	0.74773200
H	2.51926900	-2.85678200	1.07023800
H	1.82405100	-4.45840400	1.38401700
H	1.97863400	-3.86667300	-0.28043500
H	6.36356600	0.98489100	-1.33197200
H	2.60790000	1.33549800	0.83326600
H	2.92183000	-1.35136900	-2.56583100
O	5.01279400	2.20554700	0.79427800
C	6.38795100	2.69599400	0.67774100
H	6.49899600	3.41837800	1.49563700
H	7.12054500	1.88024500	0.80271000
H	6.55513500	3.20219000	-0.28819400

Frequencies --	12.6890	18.7643	20.8901
Frequencies --	30.1269	40.7202	43.1906
Frequencies --	75.0963	78.8870	99.0055
Frequencies --	100.5326	104.5864	109.6778
Frequencies --	114.4332	120.6688	124.7126
Frequencies --	127.7250	132.1224	142.2709
Frequencies --	151.0200	157.5701	162.1958
Frequencies --	168.9724	176.9650	189.9526
Frequencies --	197.1601	204.2814	207.8853
Frequencies --	226.0491	235.9415	248.4906
Frequencies --	260.5512	265.1901	266.9366
Frequencies --	286.6183	291.0192	294.1138
Frequencies --	298.8153	300.5514	308.4642
Frequencies --	312.0693	329.6071	348.1663
Frequencies --	380.4682	384.8269	389.0102
Frequencies --	397.2860	416.8259	427.5596
Frequencies --	456.3738	461.7501	474.8488

Frequencies --	508.9217	536.5033	540.5060
Frequencies --	543.0075	555.7891	558.5789
Frequencies --	572.6822	582.6574	595.2644
Frequencies --	604.9806	605.4252	613.5814
Frequencies --	633.7465	642.1022	676.2436
Frequencies --	681.2964	688.1916	723.3511
Frequencies --	729.9285	761.0870	780.4237
Frequencies --	803.1240	804.3372	851.0696
Frequencies --	865.8060	884.6129	949.9162
Frequencies --	958.4301	968.3109	969.9817
Frequencies --	988.7159	994.7162	1027.1964
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Frequencies --	1124.0052	1126.2720	1165.7365
Frequencies --	1171.7385	1173.5902	1174.7682
Frequencies --	1177.1405	1189.9240	1200.5969
Frequencies --	1278.8892	1289.4256	1302.9061
Frequencies --	1354.7984	1385.3230	1396.4738
Frequencies --	1411.7649	1412.8808	1423.8173
Frequencies --	1424.3733	1426.9530	1430.0631
Frequencies --	1431.5609	1432.4716	1438.9308
Frequencies --	1446.0828	1450.8715	1453.8439
Frequencies --	1457.3976	1457.9044	1462.5358
Frequencies --	1479.9748	1483.7594	1485.2724
Frequencies --	1489.9534	1490.4490	1491.4660
Frequencies --	1497.4974	1499.4999	1505.3561
Frequencies --	1506.7119	1510.6437	1513.1627
Frequencies --	1516.6576	1589.0570	1589.8394
Frequencies --	1600.0230	1618.6539	2974.1478
Frequencies --	2991.7392	3004.6407	3005.2489
Frequencies --	3007.0252	3007.9455	3009.0977
Frequencies --	3089.0858	3093.0560	3095.4781
Frequencies --	3099.1171	3100.7556	3102.0572
Frequencies --	3103.6888	3136.3052	3139.2018
Frequencies --	3141.2673	3144.0625	3146.9393
Frequencies --	3149.5510	3155.5521	3166.8617
Frequencies --	3207.4308	3217.0298	3239.2576

proximal conformation

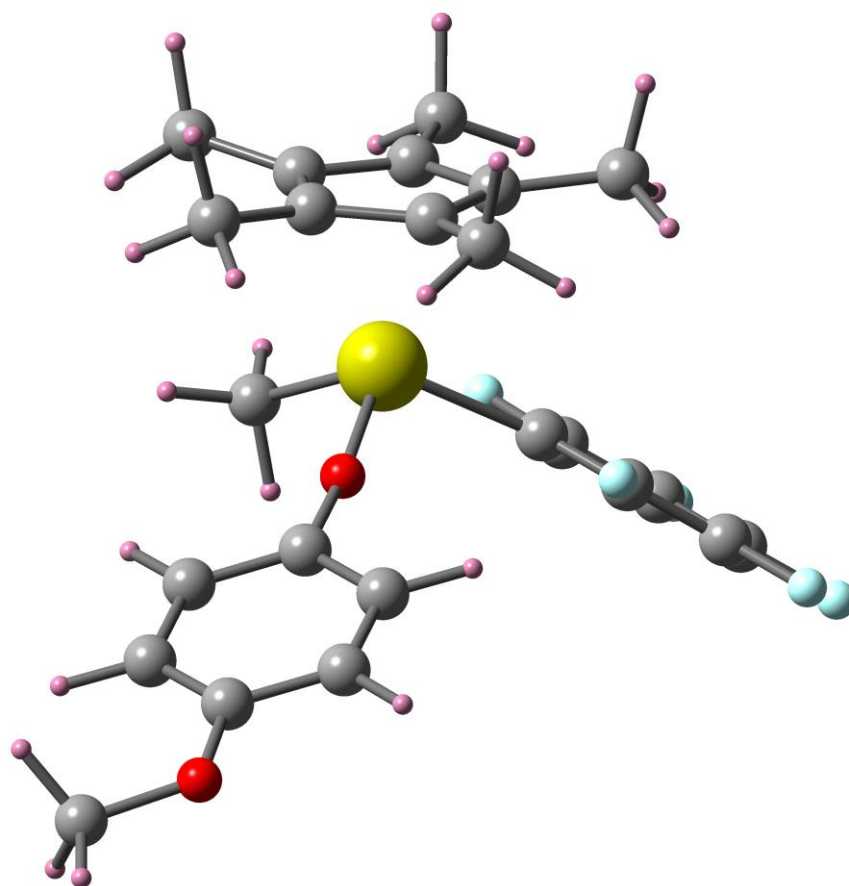
vacuum	toluene-like solvent	D3 dispersion
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Ti	0.06728900	0.88586000	-0.32010400
C	-0.20289700	1.36285400	-2.33547900
H	-0.20022300	0.35871900	-2.80271200
H	-1.17035500	1.84455200	-2.54652700
H	0.61305000	1.96582600	-2.75833900
O	-1.34232100	-0.20475400	-0.17257900
C	-2.51303500	-0.91352700	0.01181900
C	-2.55912300	-1.97903000	0.94966200
C	-3.64660200	-0.58207200	-0.76077000
C	-3.76038800	-2.69477900	1.09958200
C	-4.84583500	-1.31392400	-0.59391500
C	-4.91027900	-2.37689400	0.34129800
H	-3.80569100	-3.51834700	1.81588700
C	1.25810200	2.08272500	1.48562500
C	1.40965800	2.91234200	0.31256800
C	-0.15483400	1.98630400	1.78537900
C	0.09832900	3.34009900	-0.11128100
C	-0.87249600	2.76156900	0.79729100
C	1.75249200	-0.51617400	-0.24975900
C	2.78589100	-0.52145300	-1.20304000
C	1.82005200	-1.57167600	0.67487800
C	3.80469000	-1.49355200	-1.26511900
F	2.84493800	0.49852200	-2.17545900
C	2.80782900	-2.57512700	0.66953300
F	0.85748600	-1.65692600	1.70565300

C	3.81175900	-2.53421600	-0.31719600
F	4.79972700	-1.44244000	-2.23818700
F	2.81576900	-3.59491300	1.61874500
F	4.80230400	-3.50660100	-0.34994700
C	2.38034700	1.57632100	2.36291800
H	2.65081300	2.34986100	3.10337400
H	2.09753500	0.67590600	2.92259900
H	3.28764900	1.34426500	1.78982500
C	2.72158400	3.35499900	-0.29407400
H	3.05303100	4.30208700	0.16799900
H	3.52068000	2.61893500	-0.13793800
H	2.64333000	3.53018400	-1.37542400
C	-0.76015500	1.31529300	2.99803900
H	-0.18069700	0.44026200	3.31978300
H	-0.78961700	2.02197700	3.84619000
H	-1.79010700	0.98032100	2.81653300
C	-0.19129000	4.37966600	-1.16848200
H	-0.14195200	5.38885200	-0.72293100
H	0.53475200	4.35123400	-1.99158900
H	-1.19215800	4.26492600	-1.60521900
C	-2.35855200	3.04432700	0.80078700
H	-2.94264800	2.20210100	1.19431700
H	-2.57539300	3.92003600	1.43790500
H	-2.74158600	3.27283100	-0.20338200
H	-5.82226500	-2.95324300	0.48430200
H	-1.67235100	-2.23073600	1.52675800
H	-3.60800200	0.22515200	-1.48953300
O	-5.90563900	-0.89381300	-1.41238100
C	-7.17998400	-1.61252400	-1.33959000
H	-7.63093000	-1.53577000	-0.33542000
H	-7.82676900	-1.11392600	-2.07194500
H	-7.06037100	-2.67445800	-1.61381800

Frequencies --	7.8992	17.8557	27.2304
Frequencies --	33.4459	39.9864	48.1866
Frequencies --	76.9851	79.0337	81.6755
Frequencies --	92.4829	96.8691	101.6571
Frequencies --	111.7955	119.1146	123.1085
Frequencies --	124.8592	130.3948	143.2862
Frequencies --	149.0861	156.6316	157.4441
Frequencies --	161.6341	168.9390	192.3307
Frequencies --	193.8580	200.4974	209.5363
Frequencies --	219.8979	234.7130	254.9794
Frequencies --	260.3057	265.1564	268.4181
Frequencies --	282.1904	290.7563	293.9714
Frequencies --	294.8754	301.3484	307.4767
Frequencies --	313.5099	324.6485	346.8174
Frequencies --	378.1327	386.6543	392.0523
Frequencies --	396.8558	415.0070	427.4695
Frequencies --	456.1105	461.5391	475.7709
Frequencies --	508.9894	536.6113	539.8512
Frequencies --	543.0745	553.9287	560.2329
Frequencies --	566.8534	582.9718	596.5265
Frequencies --	605.5885	606.5720	615.6707
Frequencies --	634.8640	641.8285	677.6194
Frequencies --	682.3140	687.0855	723.7613
Frequencies --	730.7322	764.2622	779.9702
Frequencies --	801.8038	802.9799	840.5466
Frequencies --	872.4080	884.3919	949.4258

Frequencies --	964.5654	964.7103	971.8223
Frequencies --	989.4603	994.7787	1025.4669
Frequencies --	1037.3259	1043.3021	1044.9215
Frequencies --	1047.9946	1050.3426	1051.2475
Frequencies --	1085.7944	1087.2479	1101.9518
Frequencies --	1122.8226	1126.5481	1163.3976
Frequencies --	1170.7739	1172.9741	1175.1319
Frequencies --	1177.3597	1189.8780	1201.9861
Frequencies --	1278.1656	1289.4657	1302.2732
Frequencies --	1353.4843	1384.9269	1394.9908
Frequencies --	1409.6803	1411.8591	1422.6326
Frequencies --	1423.1814	1426.8539	1429.1587
Frequencies --	1431.1934	1431.6863	1436.9731
Frequencies --	1447.0228	1450.8191	1453.5965
Frequencies --	1457.0497	1457.9271	1462.2946
Frequencies --	1479.0386	1482.5042	1485.5781
Frequencies --	1489.8297	1491.0251	1491.3252
Frequencies --	1497.1212	1497.6663	1504.4352
Frequencies --	1506.3971	1510.5163	1513.6412
Frequencies --	1514.1299	1588.1727	1590.9947
Frequencies --	1599.6929	1618.9424	2974.8542
Frequencies --	2992.0932	3004.0860	3004.4787
Frequencies --	3006.3815	3007.8622	3008.9161
Frequencies --	3089.7690	3093.8429	3095.4477
Frequencies --	3099.0007	3100.9132	3101.2307
Frequencies --	3102.9120	3135.4161	3138.7125
Frequencies --	3141.2410	3142.8706	3145.7571
Frequencies --	3148.7786	3154.6075	3169.1316
Frequencies --	3212.4733	3219.2534	3233.0275

Catalyst 18:

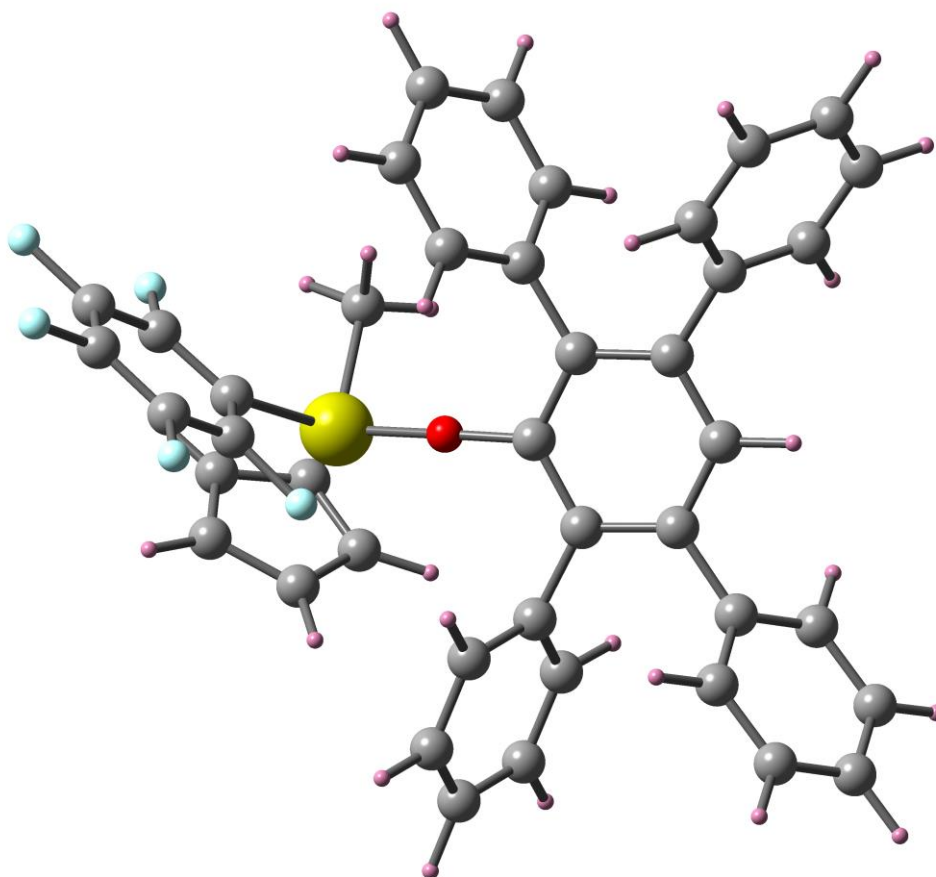
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Ti	0.26821300	0.98106600	-0.39028800
C	0.23495400	1.52014000	-2.41050600
H	0.11993800	0.53492600	-2.90320400
H	-0.62647100	2.15048900	-2.68156600
H	1.16530100	1.99397000	-2.75422400
O	-1.30261300	0.13188200	-0.37586000
C	-2.58526700	-0.37371400	-0.29441200
C	-2.91787700	-1.32857100	0.70287800
C	-3.56726800	0.04040500	-1.22420200
C	-4.21922100	-1.84860800	0.76562300
C	-4.87560800	-0.48235900	-1.16205100
C	-5.20805600	-1.42941100	-0.16166600
H	-4.49027900	-2.58509600	1.52216700
H	-5.61094500	-0.14768900	-1.89227500
C	1.56585100	1.96648500	1.46889500
C	1.85013000	2.79998100	0.32392300
C	0.14603400	2.05082600	1.74184200
C	0.61544600	3.40414300	-0.11201400
C	-0.44330400	2.93512500	0.76104600
C	1.68016700	-0.69190000	-0.21991800

C	2.77266900	-0.85969600	-1.08779600
C	1.49436200	-1.75161700	0.68285400
C	3.61566400	-1.98913100	-1.09378500
F	3.08048600	0.15017300	-2.02388700
C	2.29807300	-2.90664100	0.73166900
F	0.45194700	-1.68103400	1.63400000
C	3.37099500	-3.02545100	-0.17281200
F	4.68107400	-2.09717500	-1.98442900
F	2.05959700	-3.92241700	1.65486700
F	4.18437100	-4.15067400	-0.15075600
C	2.59518500	1.29547200	2.35011300
H	2.97775900	2.01725500	3.09334600
H	2.17650800	0.44691500	2.90575500
H	3.45841800	0.92880900	1.77898400
C	3.21938600	3.08532700	-0.24995300
H	3.63931700	3.99965300	0.20623200
H	3.92908500	2.27021900	-0.05939600
H	3.18999800	3.24874900	-1.33594900
C	-0.56432100	1.44286400	2.93081700
H	-0.13164600	0.47805200	3.22483600
H	-0.48824700	2.11811400	3.80142300
H	-1.63302800	1.28061300	2.73791500
C	0.48598000	4.49785700	-1.14651400
H	0.65117600	5.48149000	-0.67238000
H	1.22378900	4.39812800	-1.95346500
H	-0.51059200	4.52265600	-1.60742300
C	-1.87703200	3.41734900	0.74080100
H	-2.56756900	2.69096100	1.18860300
H	-1.96911000	4.35559100	1.31604400
H	-2.23146800	3.62665000	-0.27841500
H	-2.15467300	-1.65929600	1.40518200
H	-3.30345700	0.76434900	-1.99581500
O	-6.46910800	-2.02012500	0.00788000
C	-7.54743200	-1.65745900	-0.91392800
H	-7.29850600	-1.92949700	-1.95395600
H	-8.41366900	-2.24108500	-0.57900900
H	-7.78289300	-0.58078100	-0.85681500

Frequencies --	16.6872	17.6406	23.5011
Frequencies --	31.9579	41.1046	47.7103
Frequencies --	72.7553	80.3192	95.3432
Frequencies --	97.2964	104.1388	114.5990
Frequencies --	117.0214	118.9808	124.0974
Frequencies --	125.3210	127.9882	148.2372
Frequencies --	148.6484	155.5865	157.6085
Frequencies --	163.4429	171.4319	185.0414
Frequencies --	203.6759	204.9395	212.2022
Frequencies --	221.6520	229.0886	241.9482
Frequencies --	264.4018	264.9851	272.5847
Frequencies --	285.9964	290.4219	294.6283
Frequencies --	296.9146	299.1249	305.7330
Frequencies --	325.5503	346.0536	363.2983
Frequencies --	386.0324	390.4522	404.0466
Frequencies --	409.1983	419.5464	427.6343
Frequencies --	433.1134	461.5060	479.8710
Frequencies --	508.5199	520.5799	536.6921
Frequencies --	540.7891	542.7314	556.2393
Frequencies --	567.1544	576.9638	583.3587
Frequencies --	596.3680	608.7604	614.3377

Frequencies --	634.0756	638.2468	671.4668
Frequencies --	689.7666	716.3250	723.4007
Frequencies --	729.8655	766.6461	802.6944
Frequencies --	804.4021	805.2119	832.0880
Frequencies --	884.3243	921.4834	943.0283
Frequencies --	968.0039	971.3014	973.6009
Frequencies --	993.9402	996.3344	1013.4620
Frequencies --	1037.8887	1043.5747	1045.0565
Frequencies --	1049.4502	1050.8172	1052.5335
Frequencies --	1087.1991	1087.9244	1121.1925
Frequencies --	1124.3253	1126.8220	1171.2761
Frequencies --	1172.3043	1173.8424	1176.8428
Frequencies --	1187.8243	1189.5587	1229.1798
Frequencies --	1267.8834	1288.9488	1316.6659
Frequencies --	1356.9138	1358.7154	1398.4441
Frequencies --	1411.8519	1413.4005	1423.9985
Frequencies --	1424.5622	1427.4294	1430.7398
Frequencies --	1432.4016	1433.9427	1435.1640
Frequencies --	1438.0759	1450.4989	1453.9876
Frequencies --	1455.6844	1458.5704	1463.3056
Frequencies --	1480.9963	1482.5210	1488.1332
Frequencies --	1490.9710	1491.1338	1497.7751
Frequencies --	1499.4674	1504.6671	1505.1749
Frequencies --	1507.1108	1510.6290	1512.0251
Frequencies --	1517.4160	1582.7430	1590.4021
Frequencies --	1600.5226	1626.8014	2974.7128
Frequencies --	2990.3939	3003.4203	3004.5604
Frequencies --	3006.2237	3007.2317	3008.5478
Frequencies --	3087.4529	3092.9850	3094.7650
Frequencies --	3096.9660	3099.4668	3100.7580
Frequencies --	3102.0732	3135.6396	3137.7273
Frequencies --	3140.0348	3142.5035	3145.1782
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Frequencies --	3197.3784	3210.2649	3225.1528

Catalyst 19:

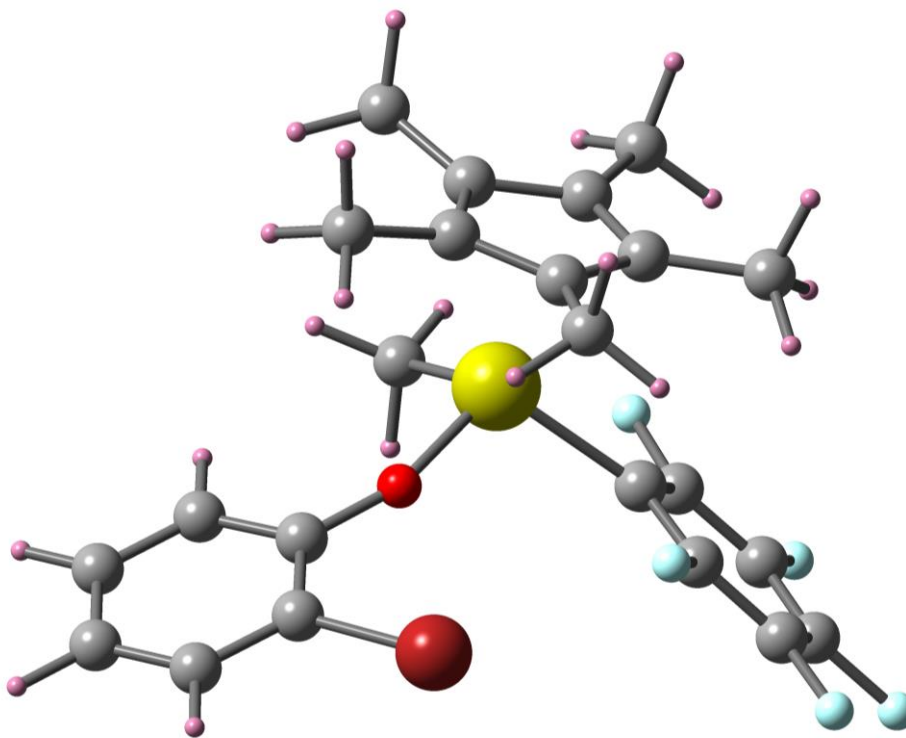
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Ti	-1.78628300	-0.90030800	-1.37902300
C	-1.98243600	0.55598300	-2.85894200
H	-2.06335500	1.47914500	-2.26025300
H	-1.07356600	0.61505100	-3.47962900
H	-2.86764000	0.44614200	-3.49891300
O	-0.23441000	-0.32627700	-0.67963700
C	1.03897700	0.07898200	-0.29360800
C	2.04806700	-0.89618000	-0.00888100
C	1.30390400	1.48810300	-0.25564200
C	3.38194900	-0.43632000	0.21221600
C	2.64323700	1.91900300	-0.01826300
C	3.65258700	0.94863100	0.17079600
C	-3.12415500	-2.98729400	-1.41663300
C	-3.35383200	-2.38788700	-2.69814900
C	-1.72164800	-3.27028700	-1.30013500
C	-2.09710800	-2.29873900	-3.37920900
C	-1.08409300	-2.84320300	-2.51752500
C	-3.26614700	-0.44223900	0.16013400
C	-4.52763700	0.10301900	-0.13541300
C	-3.01764200	-0.62542800	1.53067100

C	-5.47800700	0.46958700	0.83772000
F	-4.90009500	0.30498800	-1.47944200
C	-3.92606500	-0.28411700	2.55173100
F	-1.79463300	-1.18929900	1.94495400
C	-5.17017400	0.27239200	2.19765000
F	-6.70895400	1.01468600	0.48308500
F	-3.61930600	-0.48722600	3.89532000
F	-6.08619400	0.62184300	3.18091800
H	4.66906500	1.28598200	0.36891300
C	4.54067000	-1.35121600	0.52038700
C	4.60975000	-2.08781000	1.73079700
C	5.63901000	-1.42813500	-0.37513300
C	5.73520100	-2.88375500	2.03097600
H	3.78775800	-2.03102500	2.44533900
C	6.76350600	-2.22904900	-0.08117600
H	5.60923800	-0.86510900	-1.31079300
C	6.81597000	-2.96181800	1.12481800
H	5.76808900	-3.43872800	2.97164400
H	7.59374400	-2.27878300	-0.78994600
H	7.68611000	-3.58049300	1.35667700
C	3.05426500	3.36527000	0.07785100
C	2.52890800	4.22721000	1.07509600
C	4.05176900	3.87809500	-0.79273900
C	2.98018300	5.55834700	1.19298100
H	1.77286700	3.85469600	1.76700400
C	4.49960600	5.21180300	-0.68276800
H	4.47074100	3.23280500	-1.56807700
C	3.96504700	6.05900300	0.31260400
H	2.56430100	6.20148500	1.97226800
H	5.26159200	5.58613600	-1.37074900
H	4.31143400	7.09122900	0.40271500
C	1.75314600	-2.37025900	0.08193000
C	1.06036800	-2.89338500	1.20367000
C	2.26181000	-3.28036100	-0.87900300
C	0.89769500	-4.28544400	1.36927900
H	0.66562000	-2.21248100	1.95808700
C	2.09150300	-4.67228800	-0.72290400
H	2.81173000	-2.89872500	-1.74154700
C	1.41376100	-5.18166100	0.40675700
H	0.37566400	-4.66631600	2.25030900
H	2.49825800	-5.35571500	-1.47196100
H	1.29358500	-6.25955700	0.53706000
C	0.20761700	2.49719200	-0.46493800
C	-0.84193600	2.63361000	0.47946500
C	0.23030500	3.37964100	-1.57479900
C	-1.83129900	3.62756000	0.32581400
H	-0.87324900	1.97276100	1.34751000
C	-0.76011500	4.37040700	-1.73573800
H	1.02794300	3.29312500	-2.31429000
C	-1.79470500	4.50141200	-0.78323500
H	-2.62479700	3.72137000	1.07110000
H	-0.72215100	5.03852700	-2.59922900
H	-2.55994700	5.27160800	-0.90273400
H	-3.87791100	-3.19246100	-0.66365600
H	-4.30554500	-2.01633200	-3.06597700
H	-1.23088000	-3.73369400	-0.45376200
H	-1.93451800	-1.88353300	-4.36832500

H	-0.02889600	-2.93529200	-2.74777300
Frequencies --	10.5432	15.2403	20.1806
Frequencies --	24.6008	33.0255	41.3445
Frequencies --	43.3171	46.4612	47.1654
Frequencies --	50.1327	56.3087	61.5112
Frequencies --	63.0461	66.7397	70.8932
Frequencies --	81.6509	87.7808	95.8258
Frequencies --	110.2836	113.0717	120.7772
Frequencies --	122.3765	135.7177	147.0045
Frequencies --	156.0403	164.7000	184.9230
Frequencies --	193.4031	196.7009	209.6300
Frequencies --	210.9189	213.2763	228.1373
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Frequencies --	256.3574	264.6745	265.4486
Frequencies --	268.6856	288.6902	294.1304
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Frequencies --	401.1393	405.3616	406.1570
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Frequencies --	491.0262	512.3164	518.6403
Frequencies --	528.9037	543.2383	544.1484
Frequencies --	548.4016	563.4659	571.5760
Frequencies --	579.9949	598.3824	614.4486
Frequencies --	616.6684	617.8584	620.4380
Frequencies --	624.3743	634.6366	635.3335
Frequencies --	640.9034	656.0535	685.4977
Frequencies --	690.4137	692.0744	696.0154
Frequencies --	710.1990	710.5025	711.4969
Frequencies --	713.8182	729.4751	735.1018
Frequencies --	738.8439	746.2681	764.3738
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Frequencies --	797.7373	805.1385	809.3301
Frequencies --	817.5300	842.5572	844.5885
Frequencies --	858.7339	859.0456	859.9182
Frequencies --	864.1581	865.9595	879.0765
Frequencies --	887.9528	908.7955	909.3395
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Frequencies --	940.1742	963.5593	985.3149
Frequencies --	986.0254	990.7186	991.2193
Frequencies --	995.5027	997.4282	1002.9929
Frequencies --	1003.5075	1005.6111	1006.3261
Frequencies --	1013.2902	1019.9864	1026.7923
Frequencies --	1030.9638	1034.6693	1040.8363
Frequencies --	1042.5392	1046.4012	1050.4103
Frequencies --	1053.3783	1055.1678	1089.2061
Frequencies --	1090.3563	1090.7718	1091.0479
Frequencies --	1091.1776	1094.6057	1128.7440
Frequencies --	1129.8455	1133.7026	1182.0279
Frequencies --	1182.0624	1182.1459	1183.0602
Frequencies --	1183.4329	1192.6962	1203.7239
Frequencies --	1204.9765	1206.3804	1207.0840
Frequencies --	1230.5755	1268.0020	1280.3963
Frequencies --	1286.9902	1294.2104	1303.1940
Frequencies --	1323.4969	1327.6318	1331.3240
Frequencies --	1332.7800	1334.4873	1355.9918
Frequencies --	1365.9156	1367.7277	1369.7693
Frequencies --	1370.6184	1380.5701	1391.3303
Frequencies --	1400.0038	1402.7073	1428.4280
Frequencies --	1437.1658	1440.5851	1443.0277
Frequencies --	1445.0584	1447.7979	1448.4472
Frequencies --	1448.9830	1453.8677	1455.8613

Frequencies --	1496.7210	1497.3915	1502.4112
Frequencies --	1508.8222	1529.7886	1588.9804
Frequencies --	1590.9731	1594.1949	1596.0071
Frequencies --	1597.1782	1599.6631	1600.5601
Frequencies --	1622.5277	1623.2749	1624.0781
Frequencies --	1624.6757	2996.9217	3114.3164
Frequencies --	3150.0522	3150.9419	3151.5491
Frequencies --	3154.0092	3155.1742	3158.6257
Frequencies --	3159.4428	3161.4640	3162.3670
Frequencies --	3171.5173	3172.3438	3175.0750
Frequencies --	3177.2719	3184.0942	3184.2069
Frequencies --	3185.1281	3187.8895	3192.1330
Frequencies --	3195.8640	3196.0010	3197.3028
Frequencies --	3200.5890	3244.1472	3255.8743
Frequencies --	3268.2460	3276.5751	3300.0514

Catalyst 20:**distal conformation**

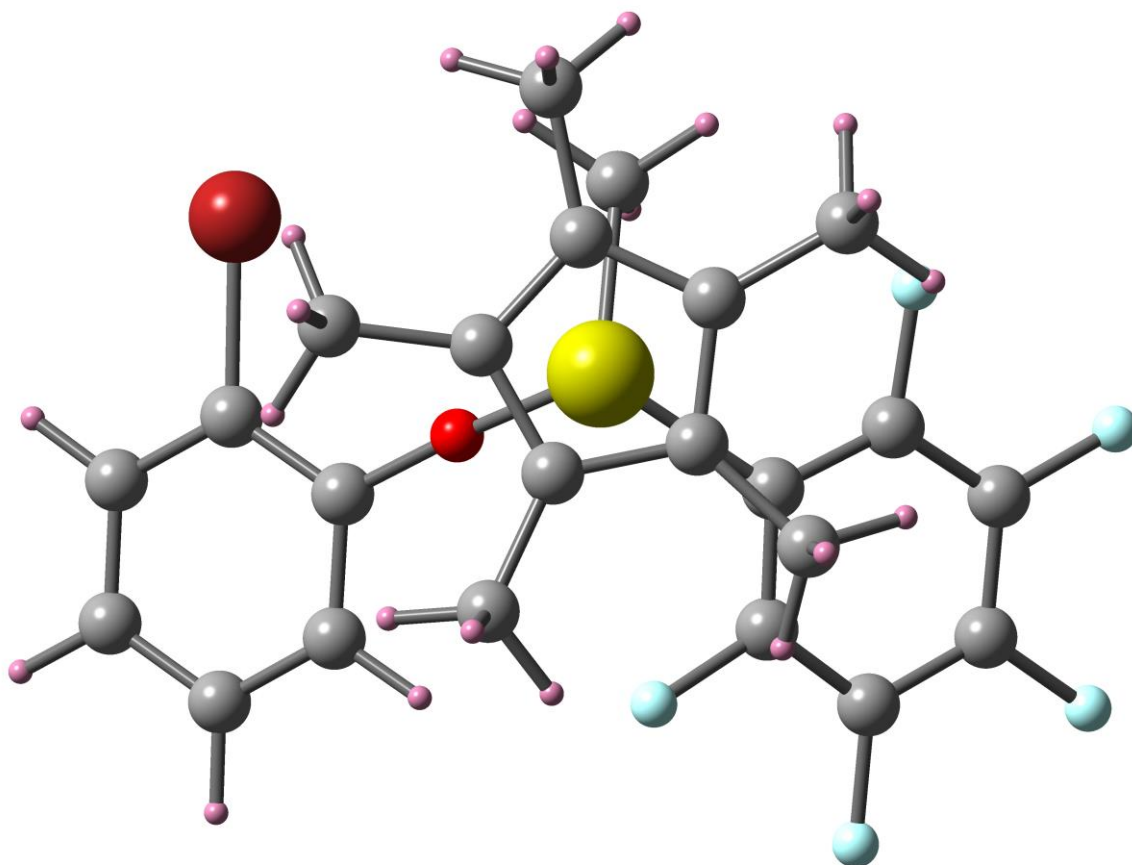
vacuum	toluene-like solvent	D3 dispersion
-1534.960218	-1534.9661905	-0.34871185

Ti	0.04837400	1.06312100	-0.30356300
C	0.08451600	1.91162100	-2.21473900
H	0.13199600	1.01996800	-2.86855800
H	-0.81065600	2.49638800	-2.47125400
H	0.97990100	2.52701100	-2.37581300
O	-1.41862800	0.04132000	-0.60736100
C	-2.65060600	-0.37717700	-1.04861100
C	-3.36942900	-1.44460000	-0.43887500
C	-3.23431100	0.26276600	-2.17805600
C	-4.62436600	-1.84796700	-0.94348600
C	-4.48458500	-0.13915000	-2.67952600
C	-5.18618600	-1.19738400	-2.06138300
H	-5.15635300	-2.66931500	-0.46275000
H	-4.90565500	0.36971800	-3.54917700
C	1.14528000	2.01584900	1.70174700
C	1.22967000	3.04154100	0.68934500
C	-0.25670000	1.76378900	1.96518400
C	-0.11216200	3.43100000	0.32689700
C	-1.03510200	2.63273200	1.10981900
C	1.76239600	-0.31154100	-0.31743100
C	2.86851300	-0.19294500	-1.17861100
C	1.77441300	-1.47537100	0.47138200

C	3.89189800	-1.15597800	-1.29309700
F	3.01372600	0.95177300	-1.98855800
C	2.76269300	-2.47600200	0.40476400
F	0.75312200	-1.67126300	1.42008500
C	3.83271800	-2.31416000	-0.49583700
F	4.95810700	-0.97872500	-2.17146300
F	2.70878200	-3.60728400	1.21483700
F	4.82611100	-3.27967300	-0.58608900
C	2.30786500	1.46353700	2.49424200
H	2.54336900	2.14383500	3.33177300
H	2.08633600	0.47971800	2.92594700
H	3.21834600	1.36726300	1.88787800
C	2.50215200	3.67730100	0.17881800
H	2.79039500	4.52360600	0.82772000
H	3.34489300	2.97388000	0.16819100
H	2.38922200	4.07340800	-0.83920500
C	-0.80985200	0.87923300	3.05862800
H	-1.78836700	0.45636600	2.79929700
H	-0.14449300	0.03979000	3.29242100
H	-0.93918300	1.46957800	3.98331700
C	-0.48511100	4.61196700	-0.53836700
H	-0.45257700	5.53723900	0.06336100
H	0.20266400	4.74962200	-1.38296400
H	-1.50159100	4.52575900	-0.94512500
C	-2.53691100	2.80910600	1.15396200
H	-3.05144700	1.90220900	1.49724500
H	-2.80102000	3.62042400	1.85513300
H	-2.95766200	3.07758700	0.17485200
H	-2.68331400	1.07168600	-2.65338200
H	-6.15710400	-1.51959800	-2.44133500
Br	-2.64720800	-2.40279500	1.10628000

Frequencies --	8.6152	15.7279	24.0391
Frequencies --	33.5744	42.8923	53.9052
Frequencies --	66.7608	88.0704	91.3623
Frequencies --	97.2476	102.4993	107.9330
Frequencies --	112.8711	115.9853	122.6260
Frequencies --	124.2036	127.1683	131.1956
Frequencies --	151.4492	157.5378	161.5835
Frequencies --	164.2381	173.8638	183.5746
Frequencies --	204.4693	212.4507	241.5295
Frequencies --	254.2409	264.3734	269.2547
Frequencies --	271.3982	284.6461	287.9890
Frequencies --	293.6478	296.1543	297.9984
Frequencies --	301.0487	310.7334	321.9697
Frequencies --	344.1434	356.4724	382.3570
Frequencies --	386.8662	391.1938	417.3068
Frequencies --	428.3119	447.6359	461.5721
Frequencies --	493.2572	502.4161	535.1663
Frequencies --	539.6315	542.5072	544.2904
Frequencies --	555.9273	573.2284	584.0215
Frequencies --	594.8723	603.8806	613.3200
Frequencies --	627.6362	634.5146	661.5998
Frequencies --	688.2380	693.9496	713.5339
Frequencies --	722.7237	730.5703	763.3746
Frequencies --	802.6692	804.6621	862.4490
Frequencies --	887.8109	912.7598	952.2851
Frequencies --	967.3028	970.7527	987.8264
Frequencies --	997.3049	1032.5966	1041.5406

Frequencies --	1043.3137	1044.4336	1047.7606
Frequencies --	1048.6739	1049.7101	1055.0354
Frequencies --	1087.1137	1088.4341	1124.3728
Frequencies --	1131.9029	1172.8229	1176.7458
Frequencies --	1177.9468	1182.4661	1191.3269
Frequencies --	1255.2119	1273.5632	1291.2765
Frequencies --	1353.1588	1354.0175	1396.9340
Frequencies --	1411.1623	1412.4382	1422.6033
Frequencies --	1424.7877	1427.7409	1430.0305
Frequencies --	1431.0727	1434.1806	1436.7282
Frequencies --	1448.1479	1450.5595	1455.1995
Frequencies --	1457.7184	1461.6370	1470.0280
Frequencies --	1478.5245	1490.4212	1491.3238
Frequencies --	1497.3136	1498.8742	1503.7920
Frequencies --	1505.8090	1510.6941	1512.2091
Frequencies --	1514.7572	1576.9045	1589.1681
Frequencies --	1597.9690	1600.2937	2982.1231
Frequencies --	3004.7027	3005.0791	3007.1684
Frequencies --	3008.2072	3009.3734	3095.6301
Frequencies --	3098.1711	3099.3573	3101.8329
Frequencies --	3105.9453	3110.8525	3136.3972
Frequencies --	3139.9648	3142.2770	3147.3435
Frequencies --	3149.2286	3157.4383	3168.1615
Frequencies --	3185.5256	3204.6864	3225.5487

proximal conformation

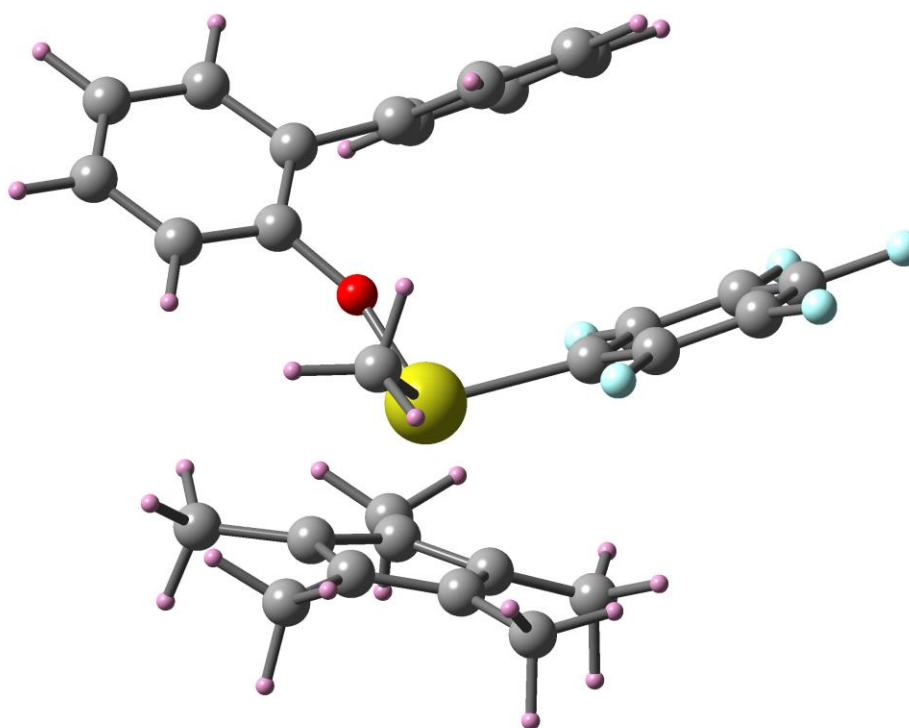
vacuum	toluene-like solvent	D3 dispersion
-1534.9642684	-1534.969783	-0.34901748

Ti	-0.01606600	0.79134800	-0.10165900
C	-0.38887300	1.46757200	-2.03154900
H	-0.22974000	0.54065400	-2.61609800
H	-1.42761600	1.79461900	-2.17492200
H	0.30854100	2.24430800	-2.37185100
O	-1.22922000	-0.54891600	-0.04701800
C	-2.16574300	-1.51623200	0.21895700
C	-1.86097600	-2.54777600	1.15004500
C	-3.43643100	-1.54911100	-0.42337300
C	-2.78840200	-3.56583000	1.43474400
C	-4.36778600	-2.56872500	-0.13650800
C	-4.04720800	-3.57878400	0.79481200
H	-2.52481200	-4.34719100	2.15049700
H	-5.33385400	-2.57415900	-0.64199000
C	1.13495800	2.05558600	1.68234000
C	0.90363900	3.01037800	0.62234500
C	-0.15344200	1.58920300	2.15179300
C	-0.52013500	3.13947700	0.43375200
C	-1.17685800	2.25530300	1.37799100
C	1.90350500	-0.27208700	-0.25881100

C	2.86792300	0.01332100	-1.24294300
C	2.22122800	-1.38115000	0.54243400
C	4.03841300	-0.74422900	-1.45225500
F	2.70127400	1.12924100	-2.08749000
C	3.36939400	-2.18096600	0.38796800
F	1.36218900	-1.73660000	1.60796900
C	4.28804800	-1.85833100	-0.62901700
F	4.95094400	-0.40752700	-2.44841200
F	3.61650300	-3.26923400	1.22149900
F	5.43249900	-2.62267900	-0.80903700
C	2.46825200	1.77119900	2.33562600
H	2.67442100	2.53575000	3.10555300
H	2.48866900	0.79420500	2.83462000
H	3.29998400	1.79952300	1.61943900
C	1.96345300	3.82368800	-0.08414900
H	2.13543700	4.77155600	0.45659000
H	2.92558600	3.29859200	-0.13715800
H	1.67263500	4.08435600	-1.11058400
C	-0.38991300	0.69887200	3.35110300
H	0.42324000	-0.02206300	3.50148200
H	-0.45928300	1.31367000	4.26592800
H	-1.32630500	0.13081600	3.27122500
C	-1.20806400	4.16580100	-0.43552600
H	-1.29677500	5.12019100	0.11280800
H	-0.65182000	4.37166000	-1.35931800
H	-2.22285600	3.85743900	-0.72005800
C	-2.66701200	2.18532000	1.62681800
H	-2.96854000	1.23412800	2.08443200
H	-2.96861500	2.99157900	2.31876000
H	-3.25280000	2.30897300	0.70645600
H	-0.88460100	-2.53490200	1.62814900
H	-4.77331900	-4.36506200	1.00806400
Br	-3.94053900	-0.19087900	-1.74799200

Frequencies --	13.0686	15.4785	22.9017
Frequencies --	35.0950	44.3132	54.1090
Frequencies --	69.3719	82.8366	93.4929
Frequencies --	97.1340	103.7939	111.6181
Frequencies --	113.6232	118.5130	125.1276
Frequencies --	127.2910	130.9725	144.8987
Frequencies --	154.0828	156.6320	165.7670
Frequencies --	172.5304	172.9917	191.9511
Frequencies --	206.9568	211.2812	224.9147
Frequencies --	230.4963	245.7761	264.7689
Frequencies --	267.4035	281.4419	287.4307
Frequencies --	292.1526	294.2459	295.5339
Frequencies --	298.4499	314.0579	319.4314
Frequencies --	343.7693	351.6275	384.1275
Frequencies --	385.7364	388.6579	414.1388
Frequencies --	428.0449	447.9023	460.7030
Frequencies --	487.5487	514.6075	535.3441
Frequencies --	539.3031	543.1481	544.5679
Frequencies --	554.0910	570.7302	583.5806
Frequencies --	595.8966	606.4269	611.1299
Frequencies --	628.0266	633.3240	657.2092
Frequencies --	684.5131	690.2280	713.2708
Frequencies --	721.4318	728.7204	766.4941
Frequencies --	801.6198	802.8323	869.8860
Frequencies --	884.2674	918.8471	958.1317

Frequencies --	965.4659	968.4729	991.9053
Frequencies --	994.8178	1030.5269	1037.1151
Frequencies --	1042.7223	1043.8261	1047.3947
Frequencies --	1049.0152	1049.9885	1054.7198
Frequencies --	1085.4640	1087.2281	1122.9250
Frequencies --	1133.0381	1172.6166	1174.1883
Frequencies --	1176.4836	1183.6196	1190.1319
Frequencies --	1258.5629	1277.9100	1289.7222
Frequencies --	1351.6740	1353.5318	1393.2821
Frequencies --	1409.7716	1411.2739	1421.0041
Frequencies --	1422.5234	1426.9057	1427.5793
Frequencies --	1430.0343	1431.0378	1435.1808
Frequencies --	1435.4202	1450.6788	1454.5652
Frequencies --	1456.7063	1462.5465	1471.0496
Frequencies --	1478.2150	1490.7574	1491.0183
Frequencies --	1496.8421	1498.6426	1503.6747
Frequencies --	1505.9158	1509.3229	1511.5023
Frequencies --	1515.1949	1575.7862	1586.9952
Frequencies --	1598.1790	1600.4840	2980.9712
Frequencies --	3004.6281	3005.3948	3007.2160
Frequencies --	3008.1237	3009.2361	3098.7631
Frequencies --	3099.6650	3100.5933	3101.6779
Frequencies --	3103.5387	3110.9799	3138.2678
Frequencies --	3142.2969	3143.1502	3146.6251
Frequencies --	3149.6180	3160.2955	3169.4560
Frequencies --	3185.6356	3203.6858	3237.6194

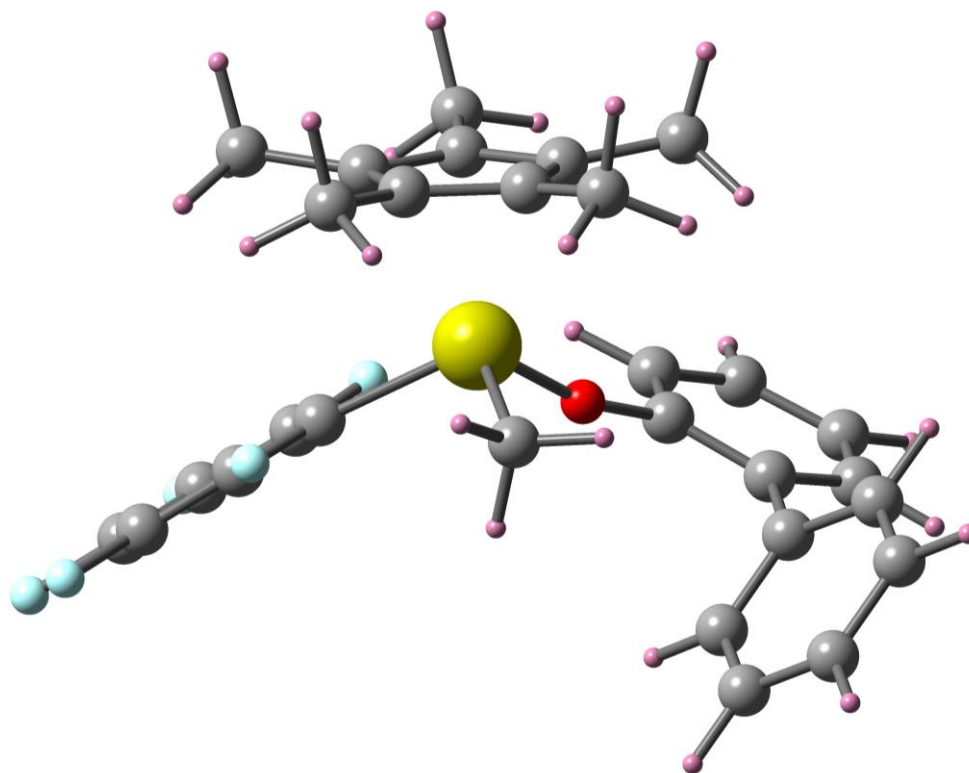
Catalyst 21:**distal conformation**

vacuum	toluene-like solvent	D3 dispersion
-1753.3483892	-1753.3551959	-0.41820584

Ti	0.18194800	-1.32410200	-0.30221400
C	0.32616300	-2.11490500	-2.23212600
H	0.23265200	-1.20644900	-2.85766800
H	1.29292500	-2.59344200	-2.45012800
H	-0.49108800	-2.80921500	-2.47253700
O	1.54529900	-0.16405500	-0.52658300
C	2.80623100	0.34296800	-0.79524700
C	3.13668400	1.70900100	-0.53440900
C	3.78091100	-0.53952700	-1.33274000
C	4.47798200	2.11284400	-0.77394500
C	5.09458700	-0.10273100	-1.57842700
C	5.45193500	1.23081200	-1.28238600
H	4.74333200	3.15380200	-0.58090700
H	5.82894200	-0.79649500	-1.99405800
C	-0.86119200	-2.33829700	1.71354100
C	-0.96578600	-3.33605000	0.67580100
C	0.54452400	-2.07825500	1.94399000
C	0.36817900	-3.71522000	0.27699100
C	1.30508400	-2.93495700	1.06127900
C	-1.62938000	-0.08354100	-0.30569700

C	-2.68511100	-0.23573500	-1.22187400
C	-1.77415200	1.01110700	0.56375400
C	-3.79325900	0.63181300	-1.30495500
F	-2.68160800	-1.31736500	-2.12666100
C	-2.85595400	1.91079400	0.53676900
F	-0.79599600	1.23789900	1.55058000
C	-3.87465300	1.72009300	-0.41629300
F	-4.80512400	0.42992600	-2.24105000
F	-2.94088300	2.97773300	1.42827300
F	-4.95337800	2.59355300	-0.47364400
C	-2.00195800	-1.82437000	2.56136700
H	-2.20356700	-2.53926800	3.37875300
H	-1.77180800	-0.85723000	3.02370800
H	-2.93366400	-1.71375600	1.99098500
C	-2.24753000	-3.95947600	0.17239200
H	-2.49422900	-4.85783900	0.76609400
H	-3.10093900	-3.27331300	0.24999400
H	-2.17216200	-4.27458200	-0.87717500
C	1.11489200	-1.18916200	3.02667500
H	0.53720900	-0.26497400	3.15316000
H	1.10755000	-1.72050700	3.99499900
H	2.15470400	-0.90342100	2.81938500
C	0.71893200	-4.88118000	-0.61758700
H	0.72274900	-5.81446900	-0.02722700
H	-0.00374800	-5.01617600	-1.43303800
H	1.71430500	-4.77889900	-1.06988100
C	2.80243200	-3.14401000	1.11012500
H	3.35015400	-2.22368100	1.34917700
H	3.04817900	-3.88305200	1.89323800
H	3.20182300	-3.53274000	0.16405000
H	3.49286100	-1.56637500	-1.54943500
H	6.46866000	1.58515400	-1.46244800
C	2.15428800	2.74235300	-0.06834600
C	2.37889400	3.45804900	1.13610700
C	1.04209600	3.10734600	-0.87041200
C	1.51638700	4.50204800	1.53246500
H	3.22617500	3.18741600	1.77009200
C	0.18735000	4.16000900	-0.48386800
H	0.86062100	2.58087300	-1.80939400
C	0.41848600	4.86005900	0.72071800
H	1.70079400	5.03131400	2.47039400
H	-0.65622700	4.43482700	-1.12181700
H	-0.25093700	5.66819000	1.02362800
Frequencies --	12.6330	21.3482	26.3924
Frequencies --	34.7604	41.2987	46.7760
Frequencies --	62.2782	65.5333	74.4073
Frequencies --	82.2527	89.1700	93.7951
Frequencies --	102.3653	114.4342	122.3992
Frequencies --	124.8485	126.8471	134.4586
Frequencies --	135.9188	142.2622	155.8310
Frequencies --	160.2747	162.5743	173.5844
Frequencies --	177.5073	188.6218	202.5298
Frequencies --	209.0304	227.3904	236.9763
Frequencies --	263.6802	265.1633	271.6781
Frequencies --	281.2905	286.6338	287.6127
Frequencies --	293.4992	297.1182	300.2993
Frequencies --	303.9075	324.2059	339.2766

Frequencies --	345.4511	355.1169	385.5691
Frequencies --	387.5343	389.0889	405.8608
Frequencies --	413.1293	428.3088	461.7600
Frequencies --	483.3276	498.7650	505.3067
Frequencies --	534.4113	539.9873	543.6005
Frequencies --	547.7343	554.6769	561.3369
Frequencies --	565.1939	584.4593	595.8305
Frequencies --	604.5203	615.9629	616.5628
Frequencies --	622.1948	634.7943	643.8111
Frequencies --	679.6310	690.9242	707.6544
Frequencies --	724.8368	730.0633	739.4499
Frequencies --	743.5870	765.2552	777.3657
Frequencies --	802.1353	805.1013	858.5774
Frequencies --	873.0493	886.6809	911.8304
Frequencies --	930.4199	955.2536	967.5731
Frequencies --	969.9799	983.7105	987.7823
Frequencies --	995.8746	1000.6830	1005.0417
Frequencies --	1038.2111	1040.4665	1043.1555
Frequencies --	1043.8201	1047.1210	1047.6138
Frequencies --	1049.7241	1052.7691	1062.5557
Frequencies --	1085.8100	1088.2915	1091.2055
Frequencies --	1124.1341	1124.8295	1173.0559
Frequencies --	1174.3930	1177.5738	1182.6155
Frequencies --	1183.2799	1189.7984	1204.5932
Frequencies --	1233.8694	1261.3847	1291.2855
Frequencies --	1300.6813	1330.6981	1355.5789
Frequencies --	1356.4043	1371.5567	1399.9343
Frequencies --	1410.5816	1412.7347	1422.1662
Frequencies --	1424.2270	1426.3252	1429.7356
Frequencies --	1430.3525	1431.8271	1434.4079
Frequencies --	1441.3641	1450.6622	1451.1773
Frequencies --	1454.2785	1458.6769	1462.5438
Frequencies --	1479.3295	1479.9743	1489.6118
Frequencies --	1492.1610	1497.4288	1499.8254
Frequencies --	1504.3272	1506.3363	1508.2420
Frequencies --	1510.6021	1511.8190	1517.2904
Frequencies --	1580.6419	1590.5444	1598.1003
Frequencies --	1601.6086	1611.2144	1626.1631
Frequencies --	2979.2921	3003.9773	3005.5645
Frequencies --	3006.5763	3008.0540	3009.1653
Frequencies --	3096.4005	3097.4502	3100.1933
Frequencies --	3101.9803	3102.3152	3104.4115
Frequencies --	3136.8514	3139.8104	3143.6437
Frequencies --	3145.7933	3148.7385	3152.8560
Frequencies --	3153.1737	3158.0305	3161.1526
Frequencies --	3172.2975	3173.9451	3180.1919
Frequencies --	3192.7831	3193.7287	3218.2306

proximal conformation

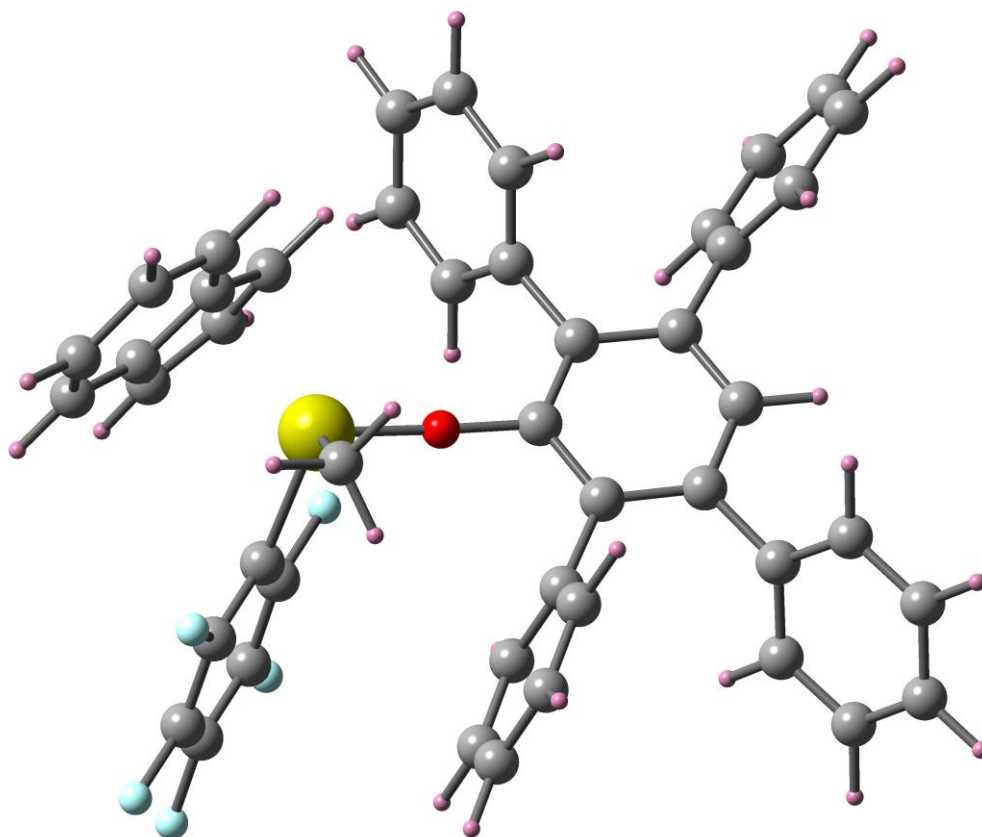
vacuum	toluene-like solvent	D3 dispersion
-1753.3512701	-1753.3582483	-0.41681392

Ti	-0.09218700	0.79380400	-0.05596000
C	0.52573000	1.31318900	1.86084500
H	0.33569700	0.36806100	2.40404200
H	1.60271200	1.52776100	1.91018900
H	-0.04824400	2.12455000	2.32549500
O	1.10281800	-0.51114000	-0.38698600
C	2.04762600	-1.36056800	-0.93778200
C	1.75372900	-1.99141400	-2.17451600
C	3.30480700	-1.58101200	-0.29362600
C	2.70838100	-2.80890100	-2.80635400
C	4.25408500	-2.39388000	-0.96762000
C	3.97374800	-2.99979700	-2.20885200
H	2.46369400	-3.29188600	-3.75506600
H	5.21806200	-2.57045700	-0.48674900
C	-1.51506200	2.30666400	-1.39109800
C	-0.93023800	3.14574200	-0.37153300
C	-0.43986200	1.78479500	-2.21080800
C	0.50123600	3.13021700	-0.54269500
C	0.80791100	2.28807900	-1.68317600
C	-1.96081300	-0.32621800	0.26584500
C	-2.82446400	-0.06426400	1.34419000
C	-2.33780900	-1.43612800	-0.50962300
C	-3.95526700	-0.84042100	1.66701500
F	-2.58381700	1.04887500	2.17690300

C	-3.45560400	-2.25181600	-0.24598700
F	-1.58057000	-1.78111300	-1.65051500
C	-4.27121600	-1.95063500	0.86151900
F	-4.76523000	-0.52736300	2.75614800
F	-3.77101400	-3.33912500	-1.05762100
F	-5.38010200	-2.73480900	1.15011100
C	-2.99092800	2.18587600	-1.69784400
H	-3.30847700	3.02188600	-2.34623600
H	-3.22951000	1.25477800	-2.22807300
H	-3.61090200	2.22365800	-0.79259600
C	-1.69592500	3.98648900	0.62355800
H	-1.93935100	4.96803800	0.17906300
H	-2.64220500	3.51832900	0.92269900
H	-1.11854100	4.18001400	1.53721100
C	-0.62433700	1.00237100	-3.49165300
H	-1.40007500	0.23031100	-3.40424900
H	-0.93020100	1.68463100	-4.30425000
H	0.30086300	0.50940800	-3.81425500
C	1.49962200	3.98598200	0.20170600
H	1.62014300	4.95560200	-0.31317800
H	1.18126200	4.19963700	1.22992600
H	2.49198000	3.51710300	0.25115500
C	2.17777800	2.12314400	-2.30369300
H	2.22686100	1.25682500	-2.97477900
H	2.43084300	3.01689000	-2.90057600
H	2.97184500	1.99746600	-1.55378600
H	0.77383600	-1.83851600	-2.61983200
H	4.72519900	-3.62749800	-2.69161800
C	3.65266400	-1.04198600	1.06371900
C	2.95624400	-1.48492200	2.21840800
C	4.74670000	-0.15500100	1.23826800
C	3.34414700	-1.06006400	3.50593100
H	2.12090200	-2.17865900	2.10708100
C	5.13063700	0.28098600	2.52517600
H	5.29556500	0.19841100	0.36240200
C	4.43229800	-0.17342000	3.66533800
H	2.79989200	-1.42192600	4.38148000
H	5.97354500	0.96765700	2.63563100
H	4.73186900	0.15665500	4.66269900

Frequencies --	6.7918	12.6369	23.3416
Frequencies --	30.2806	35.1283	38.6670
Frequencies --	57.2872	64.2079	82.4024
Frequencies --	84.9089	88.6938	97.8722
Frequencies --	100.4286	109.9333	114.8033
Frequencies --	121.6091	123.1846	130.9080
Frequencies --	137.1116	137.6188	143.8850
Frequencies --	151.0258	158.2479	164.8728
Frequencies --	181.3001	192.4514	203.2392
Frequencies --	213.2175	216.7175	234.6354
Frequencies --	260.6815	264.3145	267.4944
Frequencies --	284.2609	285.5482	288.8443
Frequencies --	293.3880	296.3911	300.1294
Frequencies --	304.7654	319.5935	339.4596
Frequencies --	346.2697	354.9308	383.7782
Frequencies --	384.7565	393.5197	406.3233
Frequencies --	410.2746	428.5526	460.6583
Frequencies --	472.3043	499.3769	512.5510

Frequencies --	535.6112	539.5323	543.4679
Frequencies --	551.0926	555.1801	562.9430
Frequencies --	572.6038	584.0018	595.2484
Frequencies --	603.0573	615.4278	615.7605
Frequencies --	620.8519	633.0889	643.6057
Frequencies --	683.6142	689.2415	710.4687
Frequencies --	721.2809	728.3428	739.9190
Frequencies --	743.5602	767.0842	778.3061
Frequencies --	801.2019	804.9527	862.0179
Frequencies --	875.7672	884.8950	915.5526
Frequencies --	932.9970	957.9618	969.1046
Frequencies --	970.9256	986.9213	989.2855
Frequencies --	994.2604	999.0593	1004.5849
Frequencies --	1035.9460	1037.5984	1042.4397
Frequencies --	1045.0575	1046.3390	1047.7479
Frequencies --	1048.8433	1050.8735	1061.7015
Frequencies --	1086.6399	1088.2547	1089.1023
Frequencies --	1123.6373	1125.0325	1173.2654
Frequencies --	1177.6285	1181.0442	1182.9151
Frequencies --	1184.1205	1189.2641	1204.3678
Frequencies --	1234.6655	1265.2995	1287.0769
Frequencies --	1300.6255	1330.0525	1353.9449
Frequencies --	1354.8395	1369.3923	1395.2690
Frequencies --	1409.9800	1412.5161	1421.7740
Frequencies --	1424.5385	1426.8938	1427.6930
Frequencies --	1432.3371	1433.3330	1436.2145
Frequencies --	1437.9318	1449.6314	1451.3616
Frequencies --	1454.2283	1457.8287	1463.3602
Frequencies --	1478.3803	1479.5511	1491.3911
Frequencies --	1492.7407	1498.4295	1499.2492
Frequencies --	1504.2008	1505.3867	1507.7850
Frequencies --	1509.9824	1514.6399	1520.5480
Frequencies --	1579.8772	1588.8946	1595.9124
Frequencies --	1599.6704	1611.8399	1625.0373
Frequencies --	2987.1627	3005.1737	3005.8636
Frequencies --	3006.5553	3007.8232	3009.7609
Frequencies --	3095.5190	3098.9108	3099.9606
Frequencies --	3101.0882	3103.9068	3112.9295
Frequencies --	3139.2671	3142.2846	3142.6886
Frequencies --	3147.5308	3150.1382	3151.8261
Frequencies --	3158.8265	3161.5789	3163.7191
Frequencies --	3171.7101	3173.4314	3180.6553
Frequencies --	3192.9076	3193.5764	3237.7451

Catalyst 22:

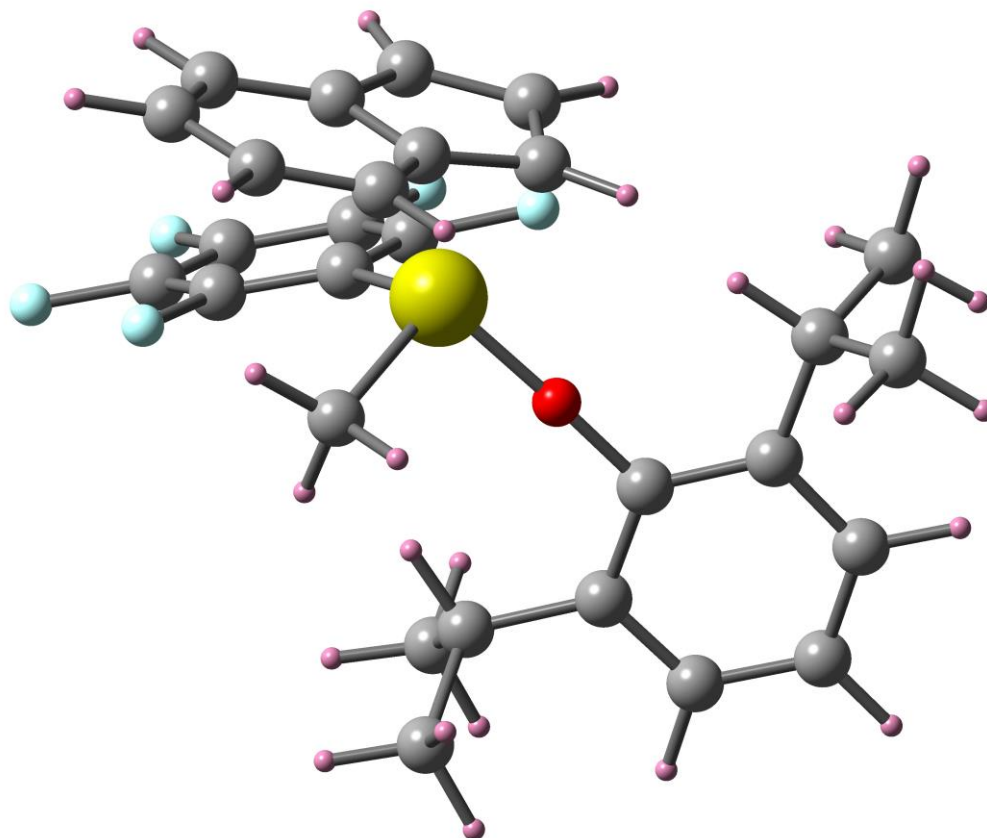
vacuum	toluene-like solvent	D3 dispersion
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Ti	-1.71471200	-0.89991300	-0.65300700
C	-1.91469900	0.03332000	-2.49078200
H	-1.84507100	1.10456600	-2.24307200
H	-1.07016800	-0.24357500	-3.14296600
H	-2.86645700	-0.17887100	-2.99353200
O	-0.04407700	-0.37318100	-0.27369900
C	1.27619600	0.04224200	-0.13924900
C	2.28299400	-0.92256100	0.18727300
C	1.58833400	1.41674300	-0.40085600
C	3.64779700	-0.50253000	0.17824600
C	2.96041500	1.80860300	-0.40109900
C	3.95368100	0.83882400	-0.14027900
C	-3.45006700	-2.59185300	0.02729100
C	-3.71195900	-2.60035600	-1.39731000
C	-2.10749500	-3.03158500	0.23364000
C	-2.47999000	-2.99238100	-2.06809500
C	-1.46524200	-3.18576800	-1.04657100
C	-2.88016200	0.18726800	0.83706000
C	-3.99072100	0.98897700	0.52470700
C	-2.53298400	0.17580000	2.19771600

C	-4.70600800	1.74715700	1.47220100
F	-4.44701400	1.05547200	-0.80619000
C	-3.20598200	0.90962300	3.19323800
F	-1.44592600	-0.61653100	2.62795900
C	-4.30604200	1.70693000	2.82180300
F	-5.79553500	2.53163700	1.10136300
F	-2.80912200	0.86035400	4.52799900
F	-4.99116300	2.44504400	3.77885100
H	4.99573300	1.15449500	-0.11640900
C	4.80383600	-1.40665900	0.52063000
C	4.94094800	-1.99272900	1.80556600
C	5.83576800	-1.62671900	-0.42918000
C	6.06637700	-2.77994300	2.12665300
H	4.17275400	-1.82316200	2.56060800
C	6.95988900	-2.41926600	-0.11343000
H	5.75238800	-1.18401800	-1.42429300
C	7.07987400	-3.00068800	1.16785500
H	6.15251300	-3.21588900	3.12489000
H	7.73694800	-2.58144200	-0.86445700
H	7.95019500	-3.61260600	1.41641800
C	3.42554600	3.22162500	-0.64141000
C	3.08068700	4.28165500	0.23622600
C	4.29743700	3.50600800	-1.72492300
C	3.58514300	5.58311700	0.03356500
H	2.42555700	4.08768800	1.08618200
C	4.79729000	4.80873500	-1.93542900
H	4.57620900	2.70565600	-2.41406700
C	4.44288100	5.85462600	-1.05541400
H	3.30978100	6.38189800	0.72640800
H	5.45932300	5.00471600	-2.78245500
H	4.83028900	6.86382100	-1.21373600
C	1.94507700	-2.35252200	0.51499000
C	1.32369800	-2.69019200	1.74426700
C	2.33030000	-3.40479800	-0.35489600
C	1.11204900	-4.03894100	2.10170100
H	1.02291600	-1.89792900	2.43111900
C	2.11021700	-4.75404200	-0.00596600
H	2.81905200	-3.16656000	-1.30144900
C	1.50427100	-5.07720200	1.22824700
H	0.64835800	-4.27612300	3.06232500
H	2.42262800	-5.54827600	-0.68816400
H	1.34425400	-6.12124800	1.50662700
C	0.51649900	2.43313100	-0.69163600
C	-0.35305100	2.88673300	0.33176000
C	0.40200800	3.01818300	-1.97826100
C	-1.30211500	3.90013000	0.08101600
H	-0.27220900	2.46068600	1.33331800
C	-0.55180200	4.02442700	-2.23599700
H	1.06252100	2.68523500	-2.78074700
C	-1.40669000	4.47284500	-1.20517600
H	-1.95356000	4.24456000	0.88761000
H	-0.62417500	4.45822400	-3.23601200
H	-2.14228100	5.25617200	-1.40076200
H	-4.17664800	-2.37884800	0.80375500
H	-1.62989500	-3.17506000	1.19565100
H	-0.46438000	-3.56685600	-1.20996900
C	-4.88670500	-2.32926700	-2.15932000

H	-5.80989500	-2.01990000	-1.66596300
C	-4.83719500	-2.48882900	-3.54753300
H	-5.73079800	-2.30366900	-4.14785600
C	-3.63031800	-2.90218900	-4.20626700
H	-3.63780400	-3.03113100	-5.29109600
C	-2.45670300	-3.14365300	-3.48596600
H	-1.54265300	-3.45496800	-3.99562400
Frequencies --	10.9084	14.5685	21.5423
Frequencies --	23.3954	27.3023	28.7931
Frequencies --	40.5537	41.4531	44.3169
Frequencies --	47.9927	53.6028	60.6359
Frequencies --	61.2328	64.9111	69.5331
Frequencies --	70.4244	77.1748	84.0115
Frequencies --	94.4961	110.2043	115.2728
Frequencies --	119.5098	120.5796	126.6192
Frequencies --	143.3355	147.0440	155.7780
Frequencies --	176.8977	193.6434	204.6288
Frequencies --	205.7972	210.1500	211.4919
Frequencies --	227.9255	236.4501	245.7242
Frequencies --	251.4403	255.4229	262.6743
Frequencies --	264.1813	266.9499	282.9848
Frequencies --	288.3387	294.7581	318.5353
Frequencies --	328.8076	330.5137	342.7013
Frequencies --	369.3767	384.9690	394.2514
Frequencies --	400.2698	403.8796	406.2780
Frequencies --	406.6931	408.1428	409.2694
Frequencies --	427.4125	437.7811	439.3511
Frequencies --	462.3127	490.7614	518.1807
Frequencies --	524.6950	528.5784	540.8935
Frequencies --	543.1853	543.6176	547.4189
Frequencies --	549.9643	566.7309	573.0907
Frequencies --	597.2879	601.6450	614.0095
Frequencies --	616.2534	617.5121	619.3745
Frequencies --	624.1324	633.6567	633.9805
Frequencies --	640.1643	656.0343	677.1155
Frequencies --	689.8992	690.5102	695.5228
Frequencies --	709.7505	709.8691	710.3503
Frequencies --	713.7558	727.7318	732.6502
Frequencies --	737.0647	741.8023	743.7004
Frequencies --	745.7934	764.6386	766.5268
Frequencies --	771.6884	783.1894	797.2832
Frequencies --	805.2387	810.9951	827.4168
Frequencies --	858.5782	858.9618	859.9316
Frequencies --	863.9772	866.5838	868.6500
Frequencies --	874.6970	885.5242	887.9548
Frequencies --	892.0354	909.2513	932.9087
Frequencies --	934.1104	936.6432	941.1761
Frequencies --	964.3081	969.6905	985.0864
Frequencies --	985.9969	989.2758	992.3252
Frequencies --	994.3880	995.9364	999.1471
Frequencies --	1003.5286	1004.4810	1006.2413
Frequencies --	1007.4331	1012.2426	1012.9687
Frequencies --	1019.9550	1027.3290	1039.0213
Frequencies --	1039.7760	1045.5505	1050.5044
Frequencies --	1053.3689	1054.4441	1062.7097
Frequencies --	1073.7548	1089.5957	1090.4072
Frequencies --	1091.0098	1091.4715	1128.7018
Frequencies --	1134.2476	1138.7807	1179.2581
Frequencies --	1182.1627	1182.4158	1182.5698
Frequencies --	1183.3096	1184.3468	1191.0723
Frequencies --	1204.2772	1205.5645	1207.0183

Frequencies --	1207.6643	1213.8899	1231.0844
Frequencies --	1242.5135	1268.3413	1270.8011
Frequencies --	1280.7155	1293.9388	1304.3437
Frequencies --	1324.2805	1328.8623	1332.1941
Frequencies --	1333.2329	1334.9834	1357.1673
Frequencies --	1362.7259	1366.6544	1368.0887
Frequencies --	1369.6798	1370.7324	1373.4764
Frequencies --	1380.7344	1402.9115	1421.4862
Frequencies --	1422.4779	1425.4416	1431.6719
Frequencies --	1440.8469	1443.3894	1445.6049
Frequencies --	1447.0579	1452.2953	1456.3755
Frequencies --	1467.9584	1497.0912	1497.8048
Frequencies --	1498.6338	1502.5655	1509.2998
Frequencies --	1529.8099	1562.4405	1589.4167
Frequencies --	1590.4836	1595.0575	1595.8808
Frequencies --	1597.4412	1599.9483	1600.3412
Frequencies --	1623.2245	1623.7422	1624.1803
Frequencies --	1624.5856	1629.3008	3002.8655
Frequencies --	3120.9643	3150.8607	3151.4843
Frequencies --	3153.4688	3155.3695	3158.0324
Frequencies --	3158.6390	3159.3257	3160.3914
Frequencies --	3160.6930	3161.8294	3167.4637
Frequencies --	3171.5679	3172.3077	3175.8872
Frequencies --	3176.4341	3180.6494	3183.1550
Frequencies --	3184.5311	3185.4043	3185.9506
Frequencies --	3193.4139	3193.9160	3195.8374
Frequencies --	3196.5301	3196.5661	3198.0539
Frequencies --	3255.9023	3271.4640	3290.9516

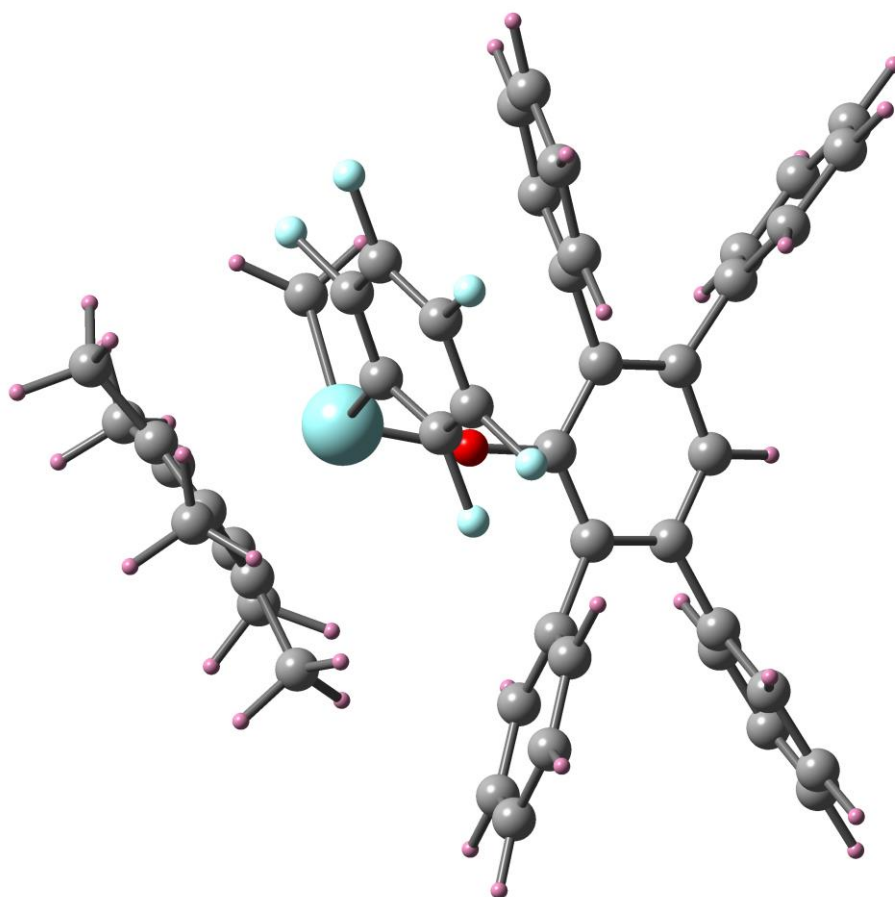
Catalyst 23:

vacuum	toluene-like solvent	D3 dispersion
-1715.2443804	-1715.2514622	-0.40771625

Ti	-0.31427900	1.03305300	0.17326100
C	-0.63228100	1.51505100	2.16931700
H	-0.55184900	0.55844100	2.71298800
H	0.16842100	2.19200500	2.51216500
H	-1.61463200	1.96612800	2.35997000
O	1.33732500	0.38888800	0.30645400
C	2.60620700	-0.18465600	0.42702000
C	3.67358200	0.29991200	-0.39226400
C	2.79557000	-1.23919100	1.37658300
C	4.94985100	-0.28545000	-0.22104200
C	4.09636600	-1.78210200	1.49845900
C	5.16679200	-1.31257500	0.71547300
H	5.78311100	0.06609000	-0.83084300
H	4.27216600	-2.58513300	2.21525600
C	-1.82791500	1.79079900	-1.65626400
C	-2.30869000	2.66986100	-0.60880300
C	-0.45842200	2.11077600	-1.90841700
C	-1.18975000	3.49640900	-0.17809000
C	-0.02291800	3.08484800	-0.94055500
C	-1.36152400	-0.81297100	-0.31929400

C	-2.44917800	-1.30750400	0.41991400
C	-0.94684200	-1.63981800	-1.37748300
C	-3.08494500	-2.53764500	0.15792300
F	-2.96466400	-0.54731900	1.48929700
C	-1.53881300	-2.87850300	-1.68965400
F	0.11642800	-1.22128100	-2.20485100
C	-2.62065400	-3.33112200	-0.90838600
F	-4.15784500	-2.97795600	0.92807200
F	-1.08259300	-3.65626700	-2.75034300
F	-3.22586600	-4.54833400	-1.19066100
C	3.47289300	1.40455400	-1.43886600
H	2.42595500	1.72028300	-1.39195400
C	1.65456800	-1.79355300	2.24304800
H	0.73223200	-1.27232200	1.96341000
H	6.16156800	-1.74777600	0.83083000
C	4.34203000	2.66014800	-1.13768800
H	4.13728800	3.05167500	-0.12840700
H	5.41840400	2.43814800	-1.19732500
H	4.12661800	3.45795900	-1.86747800
C	3.72083600	0.87638400	-2.88261900
H	3.07204400	0.01464900	-3.10319600
H	3.50630400	1.66679000	-3.62078400
H	4.76450800	0.55834400	-3.02823500
C	1.40991400	-3.30839000	1.98036500
H	0.52752900	-3.65215900	2.54416500
H	1.23020300	-3.50191500	0.91168500
H	2.26632100	-3.92473800	2.29362100
C	1.89408300	-1.51800600	3.75646800
H	2.02703200	-0.44202100	3.94794900
H	1.03191900	-1.86671700	4.34778600
H	2.78926000	-2.03963000	4.12898800
H	-2.42929700	1.08434600	-2.21733600
H	0.16219800	1.64873700	-2.67005500
H	0.95010300	3.56521300	-0.90749300
C	-3.59275400	2.83708300	-0.01032400
H	-4.43342600	2.21093300	-0.31481300
C	-3.75810800	3.83604100	0.95416900
H	-4.73799100	3.99302900	1.41041300
C	-2.66212800	4.67189700	1.35519100
H	-2.83747100	5.45190400	2.09962200
C	-1.38541500	4.50564500	0.81028300
H	-0.55625700	5.14235400	1.12526800
Frequencies --	14.6791	21.6142	25.5083
Frequencies --	27.6912	35.7868	47.0029
Frequencies --	49.6468	53.8242	67.1336
Frequencies --	80.6505	83.8116	91.0726
Frequencies --	113.5905	121.3183	125.1827
Frequencies --	125.9021	130.1430	151.2049
Frequencies --	155.9492	164.1660	181.4042
Frequencies --	205.2753	211.5373	221.0718
Frequencies --	223.9551	232.5441	238.3412
Frequencies --	239.4918	243.9257	254.9124
Frequencies --	264.6189	265.4535	272.3874
Frequencies --	283.4890	290.4398	295.4508
Frequencies --	305.6943	312.9761	321.6472
Frequencies --	336.8727	342.6551	377.0981
Frequencies --	385.9688	394.7267	420.3642

Frequencies --	426.9466	430.6504	434.4620
Frequencies --	438.9784	462.6644	524.0392
Frequencies --	538.3923	542.5777	543.1189
Frequencies --	544.2287	549.9568	562.5184
Frequencies --	571.5160	596.7078	601.3564
Frequencies --	602.0077	609.5156	628.4909
Frequencies --	635.5253	669.2862	691.7915
Frequencies --	725.6362	729.4469	737.2510
Frequencies --	739.4947	742.7634	762.3025
Frequencies --	767.1057	796.4676	798.4614
Frequencies --	815.1972	816.0674	867.4342
Frequencies --	873.3357	878.2138	878.9587
Frequencies --	887.2397	891.8551	920.1867
Frequencies --	930.9666	931.6583	938.4008
Frequencies --	941.2294	960.9607	963.4059
Frequencies --	970.9768	986.5819	995.8865
Frequencies --	1000.9118	1012.9842	1042.0252
Frequencies --	1055.1295	1059.7091	1070.8589
Frequencies --	1076.4805	1117.7255	1119.4649
Frequencies --	1120.3436	1139.2403	1166.0807
Frequencies --	1178.9009	1179.8505	1184.4412
Frequencies --	1193.3861	1198.9382	1203.8671
Frequencies --	1211.7068	1241.5254	1260.6947
Frequencies --	1268.8074	1277.9889	1294.0214
Frequencies --	1307.5706	1333.2959	1334.5201
Frequencies --	1338.2330	1356.4895	1362.0529
Frequencies --	1372.1978	1384.6223	1398.1727
Frequencies --	1398.7114	1404.3881	1416.3427
Frequencies --	1418.1868	1419.4375	1420.6598
Frequencies --	1424.8088	1430.8701	1441.9701
Frequencies --	1453.2660	1467.3510	1475.2295
Frequencies --	1487.5502	1487.9679	1489.4049
Frequencies --	1490.0460	1498.1481	1499.3992
Frequencies --	1500.9638	1506.8789	1507.8473
Frequencies --	1562.1895	1590.4991	1599.0184
Frequencies --	1600.8364	1607.9286	1629.4576
Frequencies --	2994.8235	3003.5915	3006.4242
Frequencies --	3007.8947	3011.3565	3098.1339
Frequencies --	3101.7392	3104.8204	3106.1759
Frequencies --	3108.2645	3110.6367	3115.2690
Frequencies --	3116.0146	3116.3309	3133.7732
Frequencies --	3143.6716	3154.3669	3159.8341
Frequencies --	3161.7671	3168.7580	3180.3833
Frequencies --	3181.6469	3195.4566	3195.5818
Frequencies --	3242.6363	3254.5154	3272.5971

Catalyst 24:

vacuum	toluene-like solvent	D3 dispersion
-2434.6573094	-2434.6678064	-0.65768109

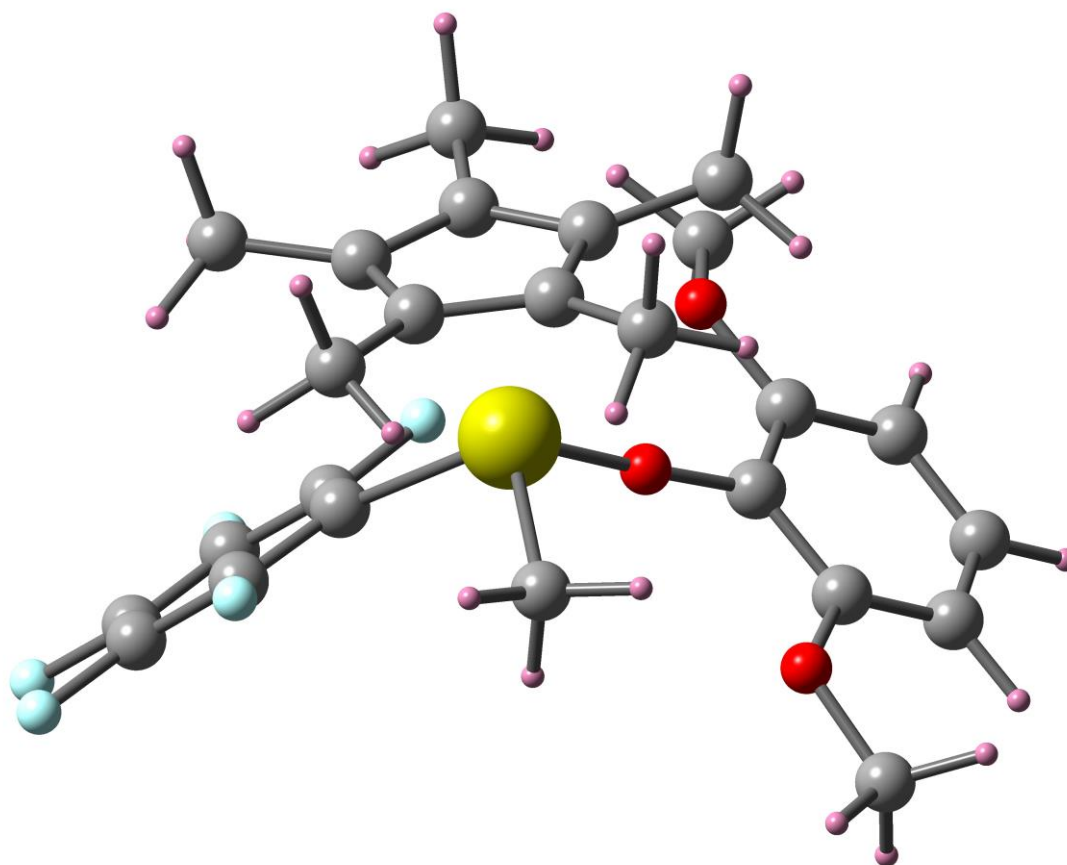
Zr	-1.71645000	-0.49995800	-1.02544600
C	-1.71579600	1.02641900	-2.65560200
H	-1.48814000	1.98175400	-2.15525600
H	-0.91244900	0.82893300	-3.38849600
H	-2.66671900	1.13342900	-3.19737600
O	0.15126800	-0.23528800	-0.39734800
C	1.48126200	0.09826200	-0.15801700
C	2.42789100	-0.92878400	0.17172200
C	1.88161600	1.47245200	-0.29197900
C	3.81607300	-0.58775100	0.20154600
C	3.27392700	1.78442200	-0.24718700
C	4.20814800	0.74338100	-0.05569700
H	5.26673400	0.99421900	-0.00572900
C	-2.40378800	-2.94328100	-0.99484900
C	-3.68128500	-2.26093900	-0.99653600
C	-1.76162200	-2.68872400	-2.27019000
C	-3.83285700	-1.59728500	-2.26929900
C	-2.65734100	-1.86472000	-3.06105700
C	-2.95382600	0.35885800	0.77555000
C	-3.91138400	1.37928100	0.65670200

C	-2.72821000	-0.06739100	2.09357000
C	-4.59381000	1.95873800	1.74398200
F	-4.23101100	1.87815400	-0.62453500
C	-3.37166900	0.46503800	3.22682600
F	-1.79674100	-1.10624300	2.32616400
C	-4.31689200	1.49363900	3.04472000
F	-5.52907500	2.97455900	1.56142600
F	-3.09821900	-0.00223900	4.51063600
F	-4.97234500	2.04306100	4.13895400
C	-1.95693700	-3.95093400	0.04137800
H	-2.50593400	-4.89784300	-0.10932200
H	-0.88956800	-4.17485000	-0.03388400
H	-2.15564700	-3.62060100	1.06939700
C	-4.76451200	-2.43137700	0.04761500
H	-5.39308400	-3.30336800	-0.20646100
H	-4.35130500	-2.61045300	1.04857200
H	-5.42920700	-1.55967600	0.10886700
C	-0.49486500	-3.34928800	-2.77976400
H	0.30605600	-3.36200800	-2.03191100
H	-0.70064600	-4.39699100	-3.06105600
H	-0.10503100	-2.84425100	-3.67416000
C	-5.06992700	-0.86492600	-2.74236800
H	-5.75194000	-1.56504500	-3.25688300
H	-5.63094800	-0.41456200	-1.91325000
H	-4.83427800	-0.06206900	-3.45377600
C	-2.48804000	-1.54774800	-4.53074100
H	-1.43777200	-1.38516300	-4.80891500
H	-2.86090100	-2.39131500	-5.13824700
H	-3.05022800	-0.65528400	-4.83281200
C	4.92069900	-1.55577800	0.54706300
C	5.04021300	-2.12234000	1.84244300
C	5.93168400	-1.84596700	-0.40597500
C	6.12783700	-2.95851100	2.17051400
H	4.28633500	-1.90105200	2.59881900
C	7.01803200	-2.68754900	-0.08336500
H	5.86254000	-1.41615500	-1.40785200
C	7.12069200	-3.24867400	1.20842500
H	6.20090700	-3.37874500	3.17661200
H	7.78003100	-2.90194400	-0.83687400
H	7.96224200	-3.89751000	1.46273800
C	3.83108800	3.18224300	-0.34463900
C	3.55186900	4.16772200	0.63732800
C	4.73232700	3.51565200	-1.38950800
C	4.14633000	5.44519100	0.57203400
H	2.87488800	3.93260600	1.45941900
C	5.32315600	4.79542400	-1.46240000
H	4.96391500	2.77172700	-2.15516600
C	5.03228600	5.76731500	-0.48022100
H	3.91916900	6.18588500	1.34267500
H	6.00690400	5.03076000	-2.28179200
H	5.49008800	6.75807200	-0.53169200
C	2.01600800	-2.32486000	0.55855600
C	1.30735000	-2.54038900	1.77006600
C	2.45443900	-3.46130900	-0.16876900
C	1.08215300	-3.84439900	2.25768600
H	0.95581500	-1.68484500	2.34767100
C	2.21933400	-4.76806700	0.30891900

H	3.00601300	-3.32215600	-1.09997000
C	1.54385300	-4.96577800	1.53316200
H	0.55106500	-3.98183600	3.20250200
H	2.57975100	-5.62601900	-0.26390700
H	1.37964500	-5.97590500	1.91586300
C	0.87832300	2.58461500	-0.43569100
C	-0.02373400	2.87489200	0.62120500
C	0.87343100	3.43618100	-1.56983400
C	-0.89298800	3.98393700	0.55176600
H	-0.02588300	2.24484500	1.51264600
C	0.00296000	4.54280800	-1.64570800
H	1.55606400	3.23363300	-2.39631700
C	-0.88312300	4.82457100	-0.58288200
H	-1.56996700	4.19573900	1.38297600
H	0.01889300	5.18353600	-2.53044400
H	-1.55527400	5.68386500	-0.63741600

Frequencies --	11.1885	14.1039	15.7831
Frequencies --	21.4433	24.9325	26.9417
Frequencies --	41.2025	43.0627	44.6337
Frequencies --	46.4180	50.6254	56.0059
Frequencies --	59.8373	64.0161	69.4083
Frequencies --	78.2887	81.3500	84.5147
Frequencies --	86.9870	93.2122	98.6649
Frequencies --	108.4486	114.4799	116.1500
Frequencies --	116.8753	121.9829	132.4080
Frequencies --	137.0301	140.2747	152.6136
Frequencies --	154.5887	162.9585	164.4142
Frequencies --	172.9646	176.5214	180.7509
Frequencies --	192.6243	195.8928	205.3271
Frequencies --	212.8039	214.5163	216.0539
Frequencies --	228.2214	241.6363	249.8972
Frequencies --	255.9186	258.7232	263.7105
Frequencies --	264.9633	280.2797	288.4698
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Frequencies --	317.2673	321.6159	328.2690
Frequencies --	333.4267	346.3095	379.0180
Frequencies --	385.7737	387.7846	398.5542
Frequencies --	403.1372	406.4236	407.2902
Frequencies --	410.2565	410.7156	426.9315
Frequencies --	433.6569	460.5653	481.9924
Frequencies --	492.4759	519.4428	529.4036
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Frequencies --	553.3856	584.6892	585.1800
Frequencies --	592.7273	614.5305	615.6079
Frequencies --	616.5260	618.1892	619.9353
Frequencies --	624.1296	630.2647	633.0531
Frequencies --	640.5418	653.7473	656.9448
Frequencies --	686.4628	688.6448	693.4979
Frequencies --	701.1955	710.3821	710.9172
Frequencies --	711.2184	713.2841	715.6442
Frequencies --	724.2036	747.1080	764.2153
Frequencies --	770.7453	783.8848	795.8071
Frequencies --	799.8522	802.3586	804.9128
Frequencies --	858.1082	860.7306	861.5538
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Frequencies --	904.9288	931.3755	934.3220
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Frequencies --	965.7183	973.7910	986.6526
Frequencies --	987.3159	990.1400	990.8507

Frequencies --	992.4327	996.6323	1003.2432
Frequencies --	1004.0258	1005.6308	1005.9642
Frequencies --	1014.3050	1020.7838	1023.8528
Frequencies --	1036.4498	1043.6995	1044.2763
Frequencies --	1046.0732	1046.6733	1048.1723
Frequencies --	1048.8637	1050.8383	1051.3366
Frequencies --	1054.6094	1055.5657	1085.1917
Frequencies --	1086.7565	1088.4051	1089.6558
Frequencies --	1089.8622	1090.3613	1123.2845
Frequencies --	1128.8280	1129.6177	1172.2808
Frequencies --	1176.2464	1181.2812	1181.6059
Frequencies --	1181.7216	1182.2851	1189.3509
Frequencies --	1192.5534	1203.3822	1204.8236
Frequencies --	1206.1062	1207.3595	1227.4064
Frequencies --	1273.0671	1278.9531	1288.5607
Frequencies --	1301.4929	1322.5350	1326.8165
Frequencies --	1331.1832	1332.3760	1334.6354
Frequencies --	1357.6563	1365.2289	1367.6656
Frequencies --	1369.9073	1370.4587	1381.5785
Frequencies --	1398.5771	1413.1728	1415.0435
Frequencies --	1423.2658	1424.6049	1426.6209
Frequencies --	1429.9905	1432.4689	1438.6365
Frequencies --	1441.7088	1442.3508	1443.4526
Frequencies --	1444.6481	1446.5216	1447.5993
Frequencies --	1452.0796	1453.7098	1458.9654
Frequencies --	1463.5090	1486.7841	1492.7727
Frequencies --	1496.3022	1496.5881	1497.1822
Frequencies --	1501.3308	1501.3994	1502.0706
Frequencies --	1506.6080	1508.7619	1510.4761
Frequencies --	1514.3801	1515.8763	1518.3947
Frequencies --	1528.7519	1587.2876	1589.1994
Frequencies --	1593.1792	1595.1672	1596.8566
Frequencies --	1599.2836	1600.5148	1621.5518
Frequencies --	1623.0292	1623.3370	1623.9125
Frequencies --	2990.0998	3006.6981	3006.7594
Frequencies --	3007.2578	3008.0470	3009.5480
Frequencies --	3098.2809	3100.8107	3102.1772
Frequencies --	3102.9891	3104.7103	3110.4487
Frequencies --	3132.9445	3141.2272	3145.5642
Frequencies --	3148.1210	3149.8669	3149.9089
Frequencies --	3150.6568	3151.3889	3153.3030
Frequencies --	3157.9011	3158.1629	3160.9931
Frequencies --	3161.1944	3170.9510	3171.1234
Frequencies --	3175.7160	3175.8413	3182.8851
Frequencies --	3183.3880	3183.7126	3185.2768
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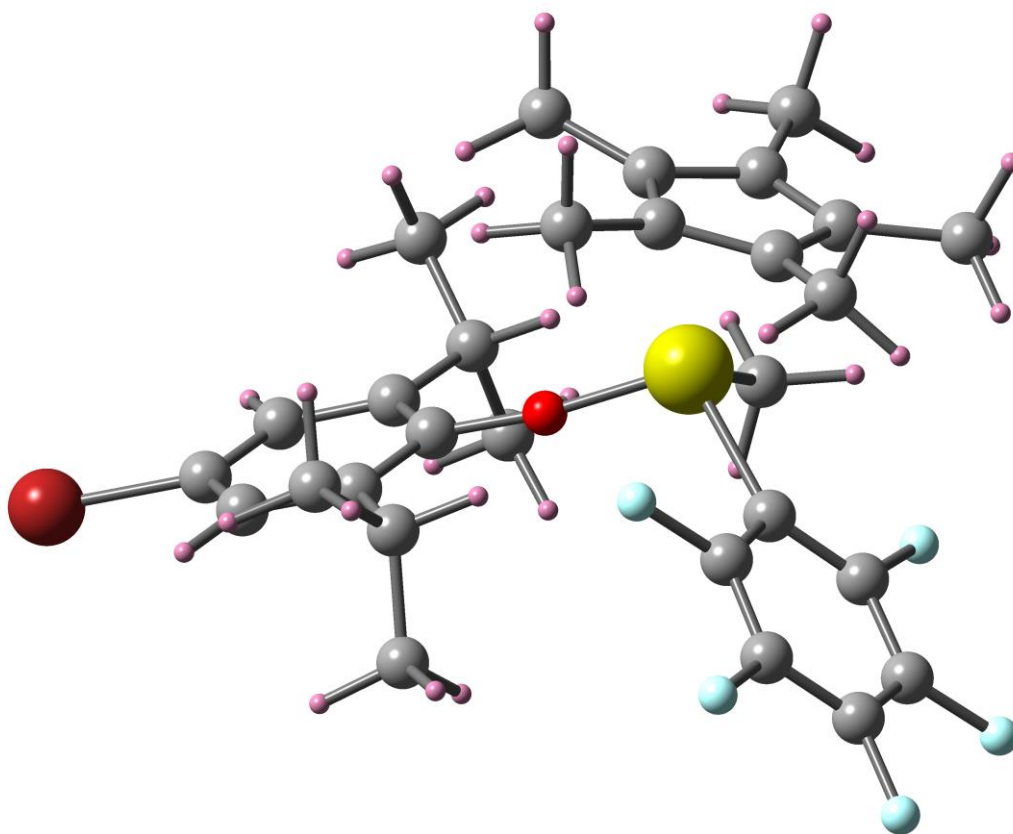
Catalyst 30:

vacuum	toluene-like solvent	D3 dispersion
-1751.3415946	-1751.3476426	-0.38032526

Ti	0.00069700	0.96066100	0.21464500
C	0.02776400	1.60271100	2.19790500
H	-0.08965300	0.64195900	2.73302300
H	1.00832800	2.02235700	2.46424900
H	-0.78017700	2.29112400	2.47564100
O	1.44452800	-0.10952100	0.28601800
C	2.60750600	-0.82806700	0.34337800
C	3.10534100	-1.53294500	-0.79629500
C	3.33389300	-0.91397000	1.57450200
C	4.27709100	-2.32137300	-0.69411200
C	4.50671000	-1.70026900	1.66274200
C	4.96469000	-2.40067200	0.53047700
H	4.65543800	-2.86284200	-1.55870700
H	5.05792300	-1.77300100	2.59785900
C	-1.37156600	2.29505900	-1.37513000
C	-1.00601800	3.22390400	-0.33272400
C	-0.15371600	1.83311800	-2.00859600
C	0.43237000	3.32698200	-0.30731300
C	0.96386200	2.47064500	-1.34868900
C	-1.69011000	-0.45488100	0.19974800

C	-2.85224700	-0.25439600	0.96589600
C	-1.65273000	-1.69466700	-0.46455600
C	-3.89123400	-1.19560100	1.10513800
F	-3.03574900	0.96531900	1.65270800
C	-2.65857100	-2.67748900	-0.37118100
F	-0.56191900	-2.00967300	-1.29540700
C	-3.78925500	-2.42497800	0.42764200
F	-5.01432100	-0.93178000	1.88778200
F	-2.55691900	-3.88851100	-1.05555200
F	-4.79731400	-3.37479500	0.53924500
C	-2.77764100	2.02609600	-1.86222100
H	-3.05146000	2.75852400	-2.64254500
H	-2.88171700	1.02625200	-2.30360900
H	-3.51916700	2.11567000	-1.05796900
C	-1.96985700	4.04383000	0.49309600
H	-2.28460700	4.93841200	-0.07330100
H	-2.87729800	3.48367600	0.75236200
H	-1.51741600	4.39656700	1.42903900
C	-0.07735200	0.96504800	-3.24342000
H	0.84199300	0.37004700	-3.26539700
H	-0.92439700	0.26958400	-3.31458500
H	-0.09406000	1.59782100	-4.14895500
C	1.24260000	4.28297900	0.53814200
H	1.33538400	5.25687400	0.02535600
H	0.77823200	4.47061700	1.51484400
H	2.26119300	3.91254400	0.71903800
C	2.41393900	2.39269600	-1.77138400
H	2.63463400	1.46052100	-2.30448900
H	2.65642500	3.23206000	-2.44706200
H	3.10171600	2.45407300	-0.91586000
H	5.86820100	-3.00920500	0.60284100
O	2.37849400	-1.36883000	-1.97922400
O	2.78909500	-0.18516300	2.63635900
C	2.59011700	-2.32981700	-3.06756800
H	1.79634200	-2.11381400	-3.79252900
H	3.57513000	-2.19079200	-3.54497300
H	2.48853500	-3.36641200	-2.70820000
C	3.43038400	-0.27150900	3.95100000
H	3.43449200	-1.30721600	4.33024900
H	4.46116800	0.12110300	3.92491200
H	2.81274600	0.35742100	4.60348500
Frequencies --	10.3387	18.9131	25.3631
Frequencies --	30.4136	36.5653	52.7652
Frequencies --	63.3782	67.2697	80.2362
Frequencies --	87.2935	90.4884	95.4813
Frequencies --	108.4357	112.6204	116.5357
Frequencies --	125.5787	128.5668	139.7270
Frequencies --	145.7260	146.4567	149.7587
Frequencies --	157.8866	165.9942	168.2729
Frequencies --	175.2152	184.6928	187.8051
Frequencies --	193.4064	201.9787	208.6750
Frequencies --	218.5238	231.3970	257.2241
Frequencies --	264.7521	265.7075	268.1422
Frequencies --	282.0456	285.5805	291.1293
Frequencies --	294.4384	299.0751	304.2297
Frequencies --	314.8823	331.8368	340.1931
Frequencies --	346.8634	355.7098	372.9963

Frequencies --	383.5742	385.0912	393.8383
Frequencies --	406.6256	428.3169	460.6683
Frequencies --	508.5798	522.0737	536.8613
Frequencies --	539.6056	542.9391	544.2228
Frequencies --	554.6817	567.4333	575.8987
Frequencies --	584.2805	592.1487	598.2000
Frequencies --	603.1057	608.1833	618.2771
Frequencies --	634.7421	676.7589	688.0515
Frequencies --	720.0522	721.8930	725.3231
Frequencies --	729.3761	753.6494	803.5537
Frequencies --	803.7221	836.5311	853.5840
Frequencies --	886.3534	909.5491	942.1681
Frequencies --	968.3448	974.8479	987.1783
Frequencies --	994.9926	1038.1656	1045.0865
Frequencies --	1045.7783	1050.8766	1052.0002
Frequencies --	1052.3594	1081.8474	1088.6619
Frequencies --	1089.8538	1102.4547	1125.0595
Frequencies --	1125.2129	1125.3716	1166.3608
Frequencies --	1170.5524	1174.4739	1176.6502
Frequencies --	1178.4380	1187.1893	1206.1041
Frequencies --	1232.8632	1252.7132	1287.5374
Frequencies --	1295.7104	1353.2820	1370.3759
Frequencies --	1394.7273	1410.2041	1411.5296
Frequencies --	1420.9717	1422.1285	1425.3881
Frequencies --	1427.1711	1429.5755	1431.1200
Frequencies --	1432.4995	1445.0675	1451.9201
Frequencies --	1453.3625	1455.9103	1459.0242
Frequencies --	1462.3629	1473.1312	1476.5331
Frequencies --	1479.0335	1483.3548	1485.3942
Frequencies --	1490.0889	1492.2253	1493.4582
Frequencies --	1495.3365	1498.1599	1502.3017
Frequencies --	1505.3630	1507.7374	1513.1636
Frequencies --	1516.6043	1518.0949	1589.2753
Frequencies --	1590.8003	1598.7609	1603.9885
Frequencies --	2988.6436	2993.3589	2996.9546
Frequencies --	3003.3900	3003.5141	3004.5802
Frequencies --	3005.5199	3007.2748	3090.8851
Frequencies --	3093.7070	3096.3314	3097.9807
Frequencies --	3098.3169	3101.9106	3104.0526
Frequencies --	3111.1032	3136.8801	3141.8044
Frequencies --	3147.9815	3150.7155	3156.7738
Frequencies --	3158.4501	3160.8084	3163.4419
Frequencies --	3172.9898	3211.4611	3220.0173

Catalyst 31:

vacuum	toluene-like solvent	D3 dispersion
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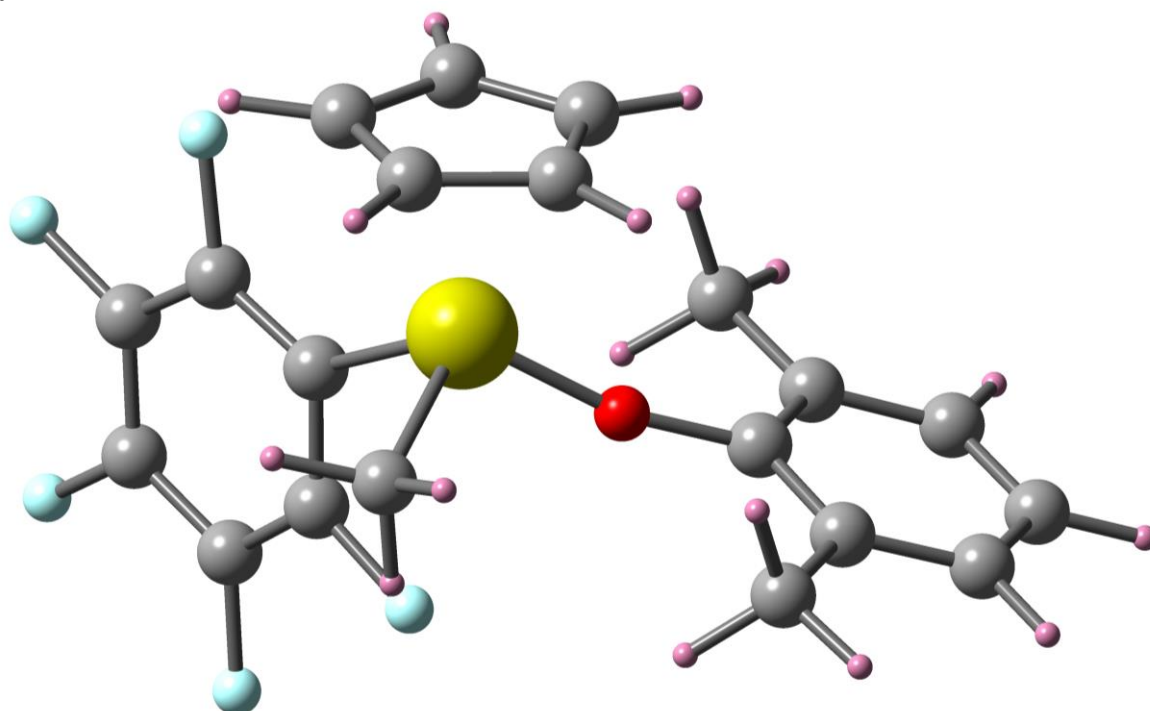
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C	1.11474500	2.06543400	-1.90769800
H	0.80761600	1.26630100	-2.60632800
H	0.42196200	2.91046200	-2.00365300
H	2.12826000	2.40012500	-2.16409700
O	-0.57172300	0.39630000	-0.14275400
C	-1.91900600	0.01717500	-0.14628800
C	-2.31360000	-1.19514200	0.51181700
C	-2.88743600	0.82289000	-0.83554700
C	-3.67686600	-1.57290900	0.47781600
C	-4.23792100	0.40083700	-0.84018200
C	-4.62086400	-0.77845100	-0.18638700
H	-3.98739500	-2.49226900	0.96992200
H	-4.98277100	0.99754000	-1.36216700
C	2.72125100	1.64114600	1.76750300
C	2.87367000	2.68503900	0.78328000
C	1.35758000	1.67945900	2.25244400
C	1.61970300	3.38870000	0.67201900
C	0.67484900	2.75923500	1.57325800
C	2.52185100	-0.60363200	-0.43304900

C	3.35975000	-0.70952500	-1.56293300
C	2.59175900	-1.72725000	0.40946500
C	4.16368000	-1.83048200	-1.86030300
F	3.45773000	0.35021200	-2.48384200
C	3.36578800	-2.87841500	0.17257400
F	1.85377600	-1.73522800	1.61456100
C	4.16189100	-2.93180100	-0.98577500
F	4.96196500	-1.86188400	-3.00065600
F	3.36414500	-3.95016300	1.06275600
F	4.94197800	-4.04757200	-1.25445200
C	-1.31510200	-2.12552900	1.20860600
H	-0.35598700	-1.60772000	1.25267500
C	-2.51998800	2.09197900	-1.61659000
H	-1.50154200	2.36744200	-1.33002600
C	3.85456600	0.82968100	2.35273600
H	4.40359100	1.44599800	3.08663300
H	3.50089500	-0.06492100	2.87726700
H	4.57990700	0.51192400	1.59184900
C	4.16248600	3.04933400	0.08215400
H	4.74718700	3.75401000	0.70016800
H	4.79941400	2.17269000	-0.09774900
H	3.98659600	3.53704700	-0.88569400
C	0.79936200	0.88419800	3.41088100
H	1.25548700	-0.10889900	3.49525700
H	0.99256700	1.41926500	4.35755900
H	-0.28731300	0.74712600	3.33407800
C	1.40231200	4.68750200	-0.06856300
H	1.72875300	5.53162900	0.56414200
H	1.97734800	4.74025900	-1.00202800
H	0.34598300	4.85825500	-0.31511800
C	-0.70894100	3.27233300	1.90298700
H	-1.38070200	2.47313000	2.24332600
H	-0.64919500	4.01743500	2.71613700
H	-1.18652100	3.76490500	1.04678700
C	-1.71610100	-2.46017400	2.67359600
H	-1.88003200	-1.54493400	3.26375000
H	-2.63384700	-3.06540500	2.73039400
H	-0.91032900	-3.03620900	3.15566200
C	-1.09545100	-3.42683300	0.38062200
H	-0.76546600	-3.19464200	-0.64409500
H	-0.32328900	-4.05248300	0.85546400
H	-2.01855400	-4.02317100	0.30881200
C	-2.51281600	1.81029700	-3.14946100
H	-2.17505700	2.70116900	-3.70328200
H	-1.83729100	0.97881200	-3.39875400
H	-3.51905200	1.54744800	-3.51147600
C	-3.43421300	3.30600600	-1.28567000
H	-3.48033200	3.49352800	-0.20205900
H	-3.04252800	4.21280500	-1.77506000
H	-4.46453000	3.16452200	-1.64471300
Br	-6.51500800	-1.32981300	-0.21049700

Frequencies --	9.9532	13.8683	24.5374
Frequencies --	28.0209	36.6275	51.7729
Frequencies --	58.6309	61.7461	69.5493
Frequencies --	75.3080	86.7091	91.2160
Frequencies --	102.6064	109.4849	111.6158

Frequencies --	117.2352	119.4558	122.5475
Frequencies --	126.6216	132.1253	133.4002
Frequencies --	135.2774	147.0331	155.6150
Frequencies --	162.9857	167.0889	174.2447
Frequencies --	181.6176	191.7582	206.8825
Frequencies --	210.0163	217.3146	220.4824
Frequencies --	224.9238	240.8859	247.2613
Frequencies --	248.5341	254.9152	259.0734
Frequencies --	264.3532	269.9207	289.6495
Frequencies --	290.5542	293.7902	300.8846
Frequencies --	302.0744	302.1994	306.7884
Frequencies --	310.5128	321.8932	327.3615
Frequencies --	328.4117	346.9154	361.1539
Frequencies --	382.2006	384.3099	389.5377
Frequencies --	417.3227	425.3246	430.9096
Frequencies --	434.7777	457.8822	461.2520
Frequencies --	500.4489	533.5503	540.0442
Frequencies --	542.4361	545.3902	556.9179
Frequencies --	563.4344	572.6463	585.3968
Frequencies --	593.3140	600.1639	606.1798
Frequencies --	613.6012	618.3427	624.1815
Frequencies --	634.1271	676.8930	686.8582
Frequencies --	716.6426	726.2692	770.0759
Frequencies --	774.9189	802.8238	806.9637
Frequencies --	807.9155	875.0265	887.0788
Frequencies --	893.3031	901.0626	914.3763
Frequencies --	930.9884	935.4051	947.4126
Frequencies --	962.5322	964.4858	971.2414
Frequencies --	972.3929	995.5154	1038.5820
Frequencies --	1041.8397	1044.3794	1047.3372
Frequencies --	1049.2591	1051.0207	1073.2540
Frequencies --	1087.7794	1088.4257	1089.2622
Frequencies --	1112.8610	1117.0711	1125.5857
Frequencies --	1126.6165	1169.7392	1173.6315
Frequencies --	1176.2907	1182.1476	1186.6355
Frequencies --	1189.9837	1192.1078	1264.1711
Frequencies --	1266.8288	1284.7336	1299.2912
Frequencies --	1325.6744	1337.5070	1341.9844
Frequencies --	1347.7526	1378.2157	1390.9611
Frequencies --	1398.7857	1399.8160	1411.8205
Frequencies --	1414.1603	1417.2236	1418.2736
Frequencies --	1423.2831	1424.6573	1425.7400
Frequencies --	1428.6170	1430.2167	1431.7490
Frequencies --	1435.3862	1439.2624	1450.5652
Frequencies --	1454.5199	1457.3668	1458.8715
Frequencies --	1463.1806	1479.9778	1487.3843
Frequencies --	1487.5272	1488.5030	1490.6595
Frequencies --	1493.6774	1494.8796	1500.1703
Frequencies --	1502.0293	1502.1152	1503.9110
Frequencies --	1505.6320	1506.4903	1508.2717
Frequencies --	1508.9670	1513.3797	1515.4861
Frequencies --	1519.3494	1577.3574	1587.4597
Frequencies --	1588.8938	1602.1126	2996.9521
Frequencies --	3005.2341	3006.2143	3006.5222
Frequencies --	3007.6780	3008.1044	3008.8241
Frequencies --	3009.8371	3011.6851	3012.6888
Frequencies --	3098.2820	3099.6947	3101.8342
Frequencies --	3104.0521	3105.0281	3106.1476
Frequencies --	3107.2438	3109.2396	3110.5696
Frequencies --	3113.6514	3116.6503	3119.0349
Frequencies --	3120.3902	3125.4400	3139.3372
Frequencies --	3143.2023	3147.3503	3150.6956
Frequencies --	3155.5262	3160.4313	3162.2102

Frequencies -- 3179.5850 3209.2603 3211.9395

Catalyst 33:

vacuum	toluene-like solvent	D3 dispersion
-1404.5192987	-1404.5261955	-0.28049707

Ti	0.39357500	1.24403700	0.46180800
C	0.39497600	1.45644800	2.54112800
H	0.32057000	0.41908000	2.90894400
H	1.29528800	1.92927400	2.96150800
H	-0.49409900	2.03032800	2.85399100
O	1.60341600	-0.03462600	0.19578900
C	2.65465400	-0.83251700	-0.23587900
C	2.56005800	-1.48071000	-1.50331300
C	3.78150900	-0.99744500	0.62320600
C	3.64539500	-2.29308400	-1.90687400
C	4.83860600	-1.81986800	0.16996400
C	4.77882400	-2.46049500	-1.08489200
H	3.59470600	-2.80217000	-2.87156300
H	5.71095100	-1.96195400	0.81115400
H	5.60506100	-3.09288700	-1.41584400
H	-0.51853900	2.46491400	-2.25499700
C	0.05203800	2.78415000	-1.39017800
C	-0.48402000	3.44237400	-0.22870200
C	1.46574700	2.63677300	-1.20412400
H	-1.52620400	3.69504300	-0.06958400
C	0.59743200	3.69459900	0.67437000
H	2.16069400	2.17582500	-1.89940400
C	1.80226300	3.18799800	0.07690300
H	0.52197700	4.17760800	1.64264000
H	2.79439800	3.21413200	0.51933200
F	-5.03630900	-2.26848600	0.03521400
C	-3.89834700	-1.47800600	0.08060400

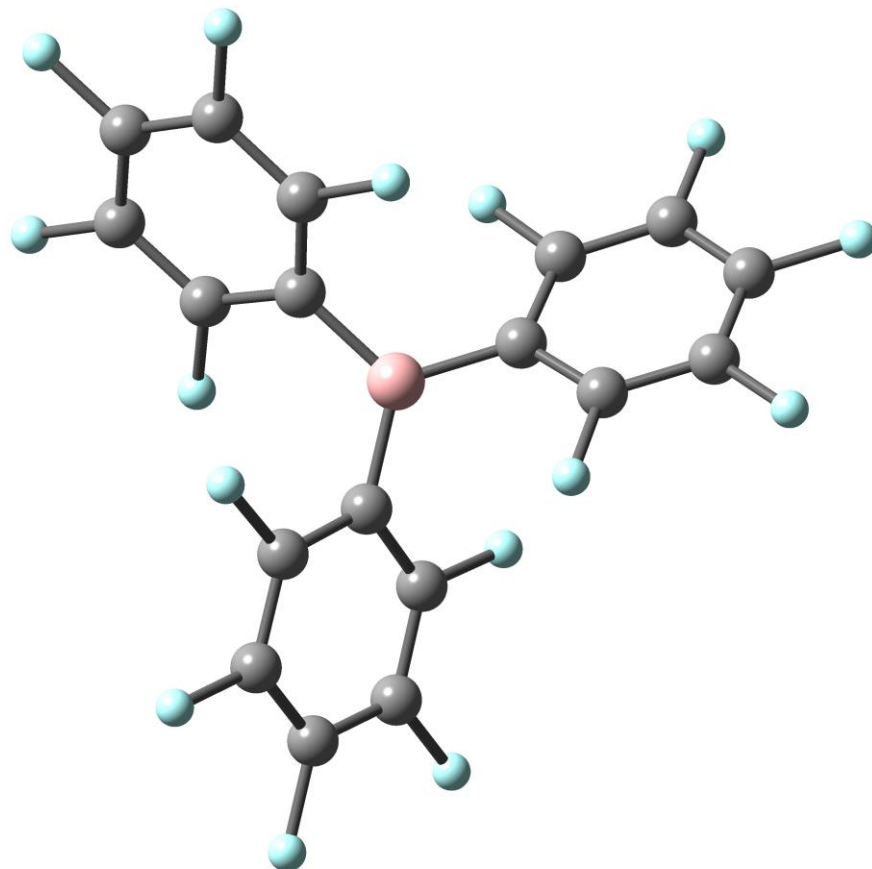
C	-3.86278100	-0.24275200	-0.59043700
C	-2.76409000	-1.90096000	0.79682300
C	-2.69350100	0.54382500	-0.52751800
F	-4.97996700	0.18275300	-1.30311000
C	-1.62681500	-1.07090800	0.81984100
F	-2.78567200	-3.12155200	1.46380700
C	-1.52225000	0.18089700	0.17111400
F	-2.76586700	1.75725400	-1.23690600
F	-0.53424200	-1.56891100	1.55678700
C	1.33346900	-1.33037800	-2.38666800
H	0.41954600	-1.64142000	-1.85840900
H	1.18136400	-0.28744400	-2.70581700
H	1.42761400	-1.94567600	-3.29187700
C	3.84218200	-0.32749300	1.98433500
H	3.84214100	0.77096000	1.89722700
H	2.97281200	-0.60012900	2.60089700
H	4.75217500	-0.62148900	2.52536800

Frequencies --	15.8513	22.2701	27.2674
Frequencies --	40.7063	64.9421	73.2596
Frequencies --	86.7657	94.2809	103.5289
Frequencies --	114.9973	123.5514	129.5209
Frequencies --	139.6047	149.7391	153.1216
Frequencies --	177.1959	200.1414	203.0760
Frequencies --	208.1629	216.8755	225.0620
Frequencies --	231.1200	245.0850	264.9759
Frequencies --	266.3359	272.0541	301.3084
Frequencies --	315.4119	327.5000	336.9248
Frequencies --	349.8662	356.4577	382.6154
Frequencies --	397.0621	428.3661	460.4016
Frequencies --	490.8863	509.3707	512.8574
Frequencies --	544.3782	550.8136	552.2682
Frequencies --	563.5405	570.2937	577.3789
Frequencies --	588.7106	597.9207	641.3464
Frequencies --	676.0555	688.4857	721.9672
Frequencies --	740.8551	742.7950	744.7916
Frequencies --	783.1623	794.0873	805.9185
Frequencies --	810.4895	842.1365	842.9947
Frequencies --	880.3296	890.8927	903.0253
Frequencies --	908.4191	922.2634	931.0247
Frequencies --	984.0632	1001.1864	1005.4033
Frequencies --	1028.2300	1035.6048	1043.3798
Frequencies --	1050.3008	1055.5091	1059.1120
Frequencies --	1090.4623	1093.8830	1110.0389
Frequencies --	1131.8930	1176.7575	1191.8257
Frequencies --	1192.4257	1219.1999	1278.5365
Frequencies --	1279.8357	1282.1028	1284.3580
Frequencies --	1341.0870	1362.1523	1389.2482
Frequencies --	1397.1206	1401.6984	1418.8951
Frequencies --	1419.8650	1429.3942	1431.5122
Frequencies --	1443.4395	1445.6389	1450.2160
Frequencies --	1457.1623	1472.0313	1485.3668
Frequencies --	1489.7915	1503.7177	1504.5082
Frequencies --	1587.2690	1598.6649	1604.6577
Frequencies --	1608.4277	2986.5625	3016.3077
Frequencies --	3018.8228	3102.8377	3103.6530
Frequencies --	3108.7720	3126.3476	3132.2419
Frequencies --	3132.8006	3160.2224	3171.6513
Frequencies --	3192.6207	3235.7727	3250.4563
Frequencies --	3261.9875	3269.1187	3287.6540

8. Additional Geometries

[\(return to table of contents\)](#)

B(C₆F₅)₃ Activator:

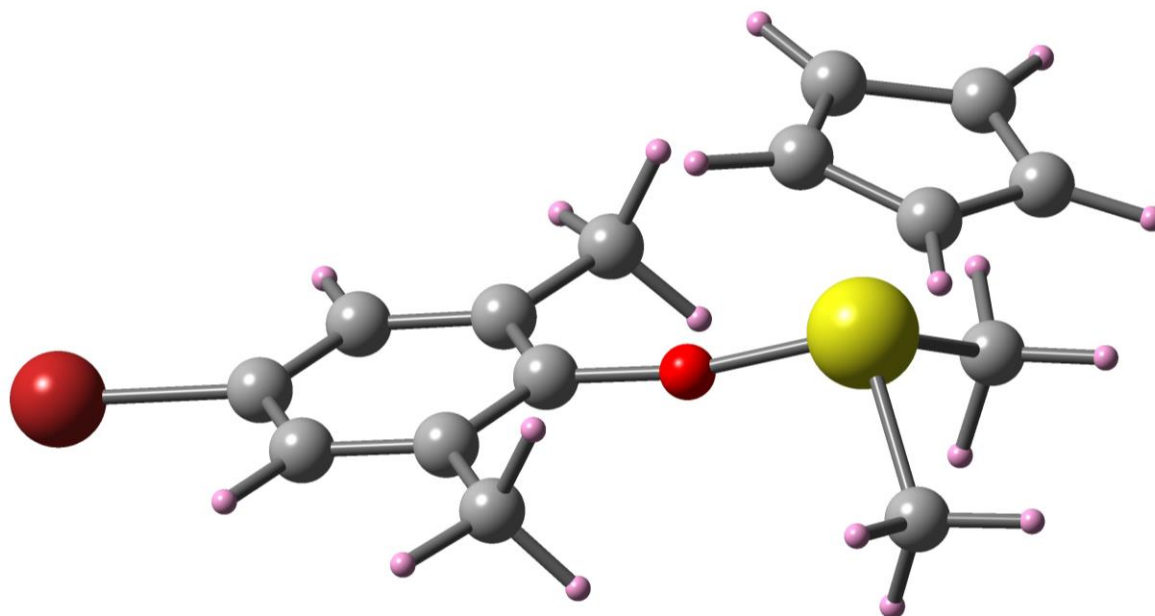


vacuum	toluene-like solvent	D3 dispersion
-2207.755517	-2207.7616892	-0.23126086

C	-0.40282700	1.52414500	0.00013200
C	0.23171500	2.47638300	0.83342900
C	-1.42557600	2.03716800	-0.83344500
C	-0.12059200	3.83720100	0.85827800
C	-1.79318100	3.39389400	-0.85856800
C	-1.13785200	4.29831800	-0.00012300
C	1.52314800	-0.41414500	-0.00053500
C	2.03031600	-1.44152400	0.83117300
C	2.47961100	0.21708100	-0.83173500
C	3.38493000	-1.81682000	0.85602100
C	3.83841100	-0.14269800	-0.85654800
C	4.29346700	-1.16459100	-0.00036900
C	-1.11875700	-1.11216200	0.00061800
C	-2.26130700	-1.03640100	0.83294800
C	-1.05310000	-2.25488800	-0.83220800
C	-3.26506400	-2.02048300	0.85800600

C	-2.04557500	-3.25030700	-0.85706300
C	-3.15686900	-3.13286900	0.00059200
F	-4.13702500	-4.10464000	0.00041700
F	-4.35020400	-1.90837200	1.70973900
F	-2.40024100	0.03660200	1.71321800
F	-1.94292000	-4.33624100	-1.70895700
F	0.01851800	-2.40254500	-1.71271800
F	1.17175500	-2.10008000	1.71126900
F	3.83168400	-2.81295600	1.70672000
F	5.62563900	-1.52544800	-0.00052500
F	4.72697900	0.49168300	-1.70712700
F	2.07100100	1.21965900	-1.71108100
F	1.22999300	2.06122700	1.71471400
F	0.51675500	4.72169300	1.71092200
F	-1.49113300	5.63258900	-0.00041600
F	-2.78460700	3.84668200	-1.71155700
F	-2.08722300	1.18242500	-1.71509200
B	0.00077100	-0.00086000	0.00012800

Frequencies --	17.6967	18.2354	30.5553
Frequencies --	30.6426	30.9701	34.3154
Frequencies --	95.6318	101.4191	102.1182
Frequencies --	118.9707	119.2363	120.6209
Frequencies --	136.7387	137.1893	149.9783
Frequencies --	152.8409	158.5688	158.6620
Frequencies --	212.8032	218.0167	218.6808
Frequencies --	265.8775	266.0820	266.2742
Frequencies --	268.2346	268.5558	269.3294
Frequencies --	295.1038	295.2159	295.3586
Frequencies --	320.1864	320.6874	331.0118
Frequencies --	343.4051	374.9435	375.2295
Frequencies --	380.3889	381.5169	382.4401
Frequencies --	426.2781	426.7134	426.8216
Frequencies --	456.1621	456.3382	473.8504
Frequencies --	536.1207	541.2468	541.4305
Frequencies --	548.9237	606.5069	606.7613
Frequencies --	641.4006	641.5789	644.9591
Frequencies --	651.9160	652.4695	655.6512
Frequencies --	731.8270	732.2109	737.3612
Frequencies --	762.9672	763.4875	779.3398
Frequencies --	817.8536	913.6078	913.7342
Frequencies --	917.1406	966.0895	966.1578
Frequencies --	1048.3298	1072.3427	1072.9749
Frequencies --	1073.1434	1127.4978	1127.7130
Frequencies --	1238.1661	1260.2953	1260.7076
Frequencies --	1348.5144	1349.0855	1349.4669
Frequencies --	1354.3171	1354.4040	1355.4056
Frequencies --	1436.6848	1438.1604	1438.3211
Frequencies --	1470.4093	1472.2138	1472.5017
Frequencies --	1591.7911	1592.8677	1593.2196
Frequencies --	1622.1443	1622.5544	1624.3538

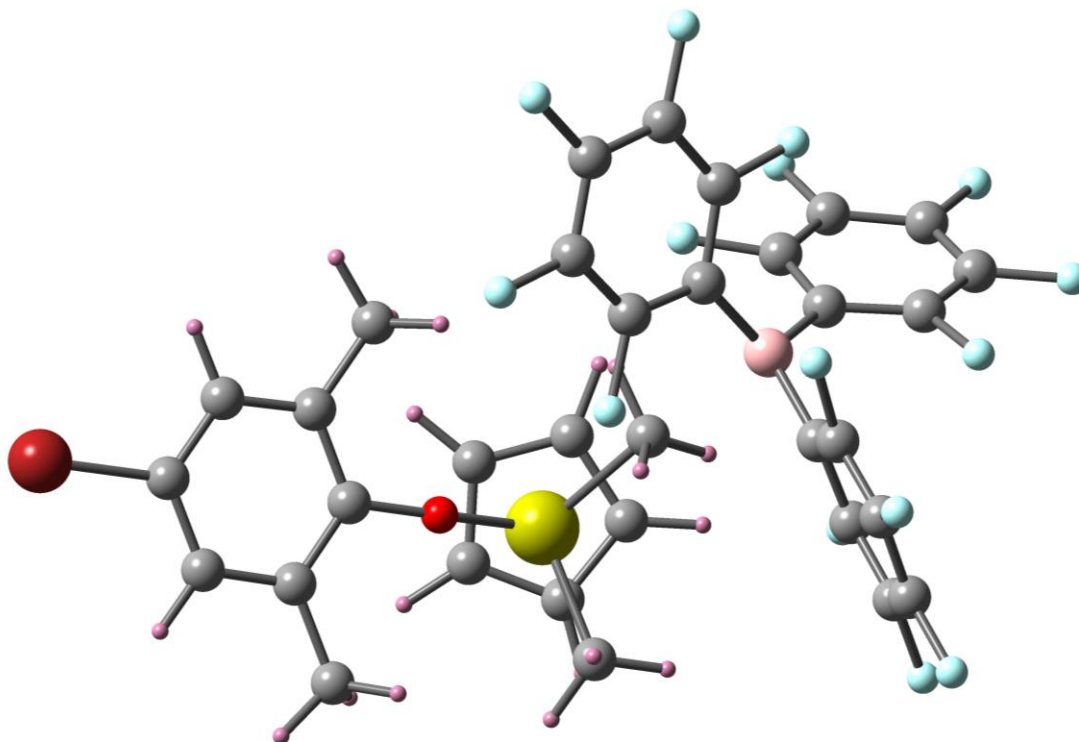
Precatalyst 1:

vacuum	toluene-like solvent	D3 dispersion
-729.32764055	-729.33229740	-0.2237939

C	3.26319200	1.61791800	-1.65227400
H	2.68508100	1.46610300	-2.58360600
H	3.01253300	2.60579400	-1.23273100
H	4.34143300	1.59058100	-1.88270900
O	0.91444600	0.00011100	-0.53019500
C	-0.45435100	0.00007700	-0.34057300
C	-1.14579600	-1.24547600	-0.25784900
C	-1.14584400	1.24558300	-0.25760500
C	-2.54870300	-1.22646100	-0.07760000
C	-2.54875400	1.22646900	-0.07736700
C	-3.23185600	-0.00001800	0.01308800
H	-3.09309100	-2.16828600	-0.01341400
H	-3.09318100	2.16825900	-0.01301500
H	4.45670200	-2.19298300	1.03779000
C	4.16338800	-1.16150000	1.20376900
C	4.90251100	-0.00047100	0.80354800
C	2.96153200	-0.71884500	1.85485400
H	5.84497500	-0.00047000	0.26260400
C	4.16370000	1.16057100	1.20427200
H	2.19238800	-1.35561500	2.28262300
C	2.96170300	0.71793700	1.85513500
H	4.45724500	2.19205100	1.03870100
H	2.19270500	1.35471300	2.28315300
C	3.26323500	-1.61664100	-1.65356400
H	3.01252300	-2.60485600	-1.23487000
H	4.34152800	-1.58905700	-1.88371500
H	2.68528100	-1.46400600	-2.58484900
Ti	2.71592400	0.00014300	-0.42692100

C	-0.40638400	2.56730900	-0.36614600
H	0.29878500	2.70367300	0.46943400
H	0.18331600	2.61785700	-1.29313200
H	-1.10703000	3.41361000	-0.35707200
C	-0.40627900	-2.56714500	-0.36672100
H	0.18340600	-2.61741600	-1.29373500
H	0.29890800	-2.70370100	0.46880900
H	-1.10689200	-3.41347700	-0.35786200
Br	-5.18857900	-0.00007500	0.26318900

Frequencies --	18.3892	20.9685	23.0538
Frequencies --	62.8283	73.8451	108.9473
Frequencies --	111.5527	141.1170	141.3924
Frequencies --	147.4809	164.1667	176.4402
Frequencies --	184.5121	194.5945	198.9665
Frequencies --	207.7273	220.5359	226.0567
Frequencies --	238.1836	241.1881	257.2772
Frequencies --	317.8002	349.7343	375.5476
Frequencies --	420.0166	485.1746	500.8086
Frequencies --	507.9968	509.8653	556.6565
Frequencies --	561.8447	564.1243	572.5740
Frequencies --	575.7282	582.5641	591.9964
Frequencies --	638.8290	665.8422	737.8811
Frequencies --	771.6250	788.2859	795.3323
Frequencies --	799.9422	841.0318	841.1528
Frequencies --	868.3430	884.0277	885.9703
Frequencies --	894.9929	924.5234	950.4377
Frequencies --	1011.2187	1024.2010	1029.7853
Frequencies --	1049.2128	1054.8312	1057.4435
Frequencies --	1086.3561	1086.8591	1123.6882
Frequencies --	1128.4638	1162.9712	1177.6118
Frequencies --	1236.9216	1262.6439	1278.2251
Frequencies --	1293.5676	1353.9067	1393.6093
Frequencies --	1397.9065	1413.1858	1419.3412
Frequencies --	1424.3285	1429.9843	1434.2199
Frequencies --	1436.5183	1438.7820	1443.0553
Frequencies --	1444.1868	1447.5336	1482.3108
Frequencies --	1482.7432	1500.1938	1502.4685
Frequencies --	1589.5157	1592.1378	2970.1066
Frequencies --	2973.7607	3016.7667	3017.1944
Frequencies --	3088.1057	3093.0227	3104.4127
Frequencies --	3104.5233	3112.0504	3113.2502
Frequencies --	3134.4508	3134.6199	3195.2481
Frequencies --	3197.1903	3233.3135	3234.4484
Frequencies --	3249.5058	3259.9357	3275.2879

Catalyst 1 Activation Transition State:

vacuum	toluene-like solvent	D3 dispersion
-2937.0651556	-2937.0751054	-0.49173103

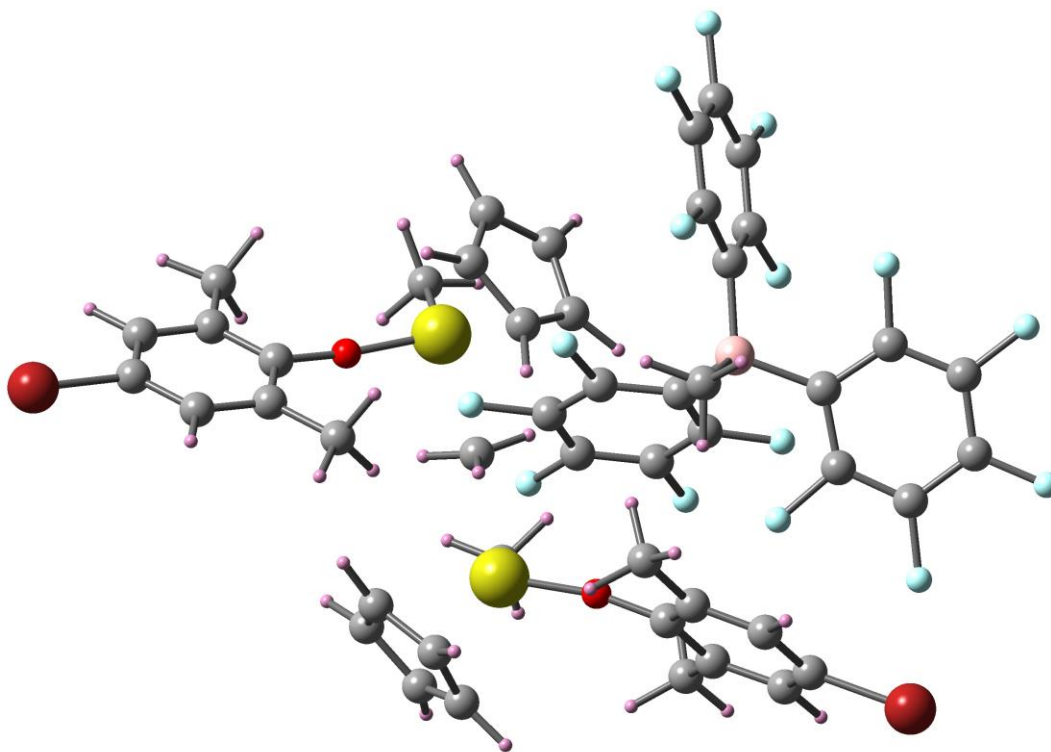
Imaginary frequency corresponding to vibration along the reaction coordinate: -184 cm^{-1} .

Ti	-1.23094100	-2.48656800	-0.08136900
C	-0.90428300	-3.27973600	1.82456100
H	-1.00859600	-2.41186300	2.50282800
H	-1.63320800	-4.04996100	2.12057600
H	0.11300300	-3.69604000	1.90718600
O	-2.71388400	-1.51408900	0.14844700
C	-3.98127300	-0.94775600	0.08646700
C	-4.23717900	0.08650100	-0.86147800
C	-4.98333900	-1.40369700	0.99324400
C	-5.53193500	0.65384200	-0.89946100
C	-6.26602900	-0.81261100	0.92377300
C	-6.52925700	0.20015400	-0.01686400
H	-5.74674200	1.44802100	-1.61359500
H	-7.04510800	-1.14523200	1.60880000
H	0.17611200	-2.55895700	-2.91552400
C	-0.38962500	-3.22791800	-2.27468000
C	0.15652000	-4.14824700	-1.31776500
C	-1.81983700	-3.34876400	-2.24021600
H	1.21081100	-4.29139900	-1.09664000
C	-0.93202400	-4.83535700	-0.68785100
H	-2.52427800	-2.79897500	-2.85685600

C	-2.15742000	-4.33735000	-1.25398200
H	-0.84690000	-5.59956500	0.07719500
H	-3.16107400	-4.66613100	-0.99910100
F	-0.69360600	5.58324900	-1.13286300
C	-0.01807500	4.41159200	-0.84074500
C	1.17837700	4.09200800	-1.50319400
C	-0.51428300	3.52688500	0.13312800
C	1.84405500	2.88874900	-1.19550700
F	1.69826500	4.96485400	-2.44705900
C	0.19089600	2.34414500	0.41267200
F	-1.68665000	3.83055900	0.81073400
C	1.38016600	1.94320100	-0.24651000
F	3.05113900	2.68648700	-1.86914500
F	-0.34879000	1.54775300	1.43098600
B	2.17405900	0.57588500	0.09502500
C	3.18964500	0.00738400	-1.03115600
C	2.56836200	0.30811100	1.64175600
C	0.39105800	-0.98701000	-0.11573100
C	4.56878600	-0.20560400	-0.78266600
C	2.81053600	-0.26704700	-2.36788600
C	2.70503100	1.34683900	2.59645500
C	2.86886700	-0.97596300	2.16060900
H	0.14033900	-0.42335800	-1.01221800
H	1.23658300	-1.66814500	-0.15983200
H	0.10991200	-0.56107500	0.84719400
C	5.47924100	-0.69187500	-1.74187200
F	5.12220100	0.10890900	0.46053700
C	3.67666500	-0.76534900	-3.35596700
F	1.49407100	-0.02517200	-2.78834000
C	3.05015000	1.13846900	3.94650100
F	2.53701700	2.68188000	2.22171400
C	3.20688900	-1.23609900	3.49921300
F	2.85785900	-2.09375000	1.31357600
C	5.02886900	-0.98607700	-3.03939400
F	6.81503800	-0.87442800	-1.41813000
F	3.21196600	-1.02899500	-4.63771300
C	3.29320300	-0.16606400	4.40741200
F	3.16035200	2.20957500	4.82013600
F	3.46555800	-2.53100400	3.92664300
F	5.90294100	-1.47156100	-3.99548200
F	3.62602200	-0.39442800	5.73064900
C	-3.16000100	0.59316100	-1.80401000
H	-2.28005800	0.94365000	-1.24588500
H	-2.81758600	-0.19311500	-2.49445800
H	-3.53138500	1.43015500	-2.41026900
C	-4.69878800	-2.48470400	2.02065900
H	-4.41016200	-3.43361300	1.54174800
H	-3.87193400	-2.19475400	2.68602500
H	-5.58355300	-2.67772200	2.64215100
Br	-8.32311200	1.00393200	-0.09300500

Frequencies --	-183.8661	4.5614	8.5315
Frequencies --	16.8737	20.0249	27.4211
Frequencies --	28.6398	30.3710	32.8762
Frequencies --	36.6830	37.3286	43.4041
Frequencies --	48.5035	48.8595	72.9966
Frequencies --	77.1507	96.7297	100.6667

Frequencies --	102.9649	109.1374	114.0004
Frequencies --	121.8193	123.3887	133.1781
Frequencies --	135.1972	147.5569	149.0618
Frequencies --	151.8367	152.5186	155.5909
Frequencies --	157.6088	161.0066	162.9741
Frequencies --	167.0030	180.7594	197.3821
Frequencies --	210.0547	216.7000	219.1624
Frequencies --	221.2567	222.7961	225.4808
Frequencies --	231.2921	241.1089	248.8848
Frequencies --	258.1735	262.0123	264.7461
Frequencies --	265.4727	265.7275	271.7371
Frequencies --	274.4960	277.3224	281.3837
Frequencies --	295.9716	305.8494	307.5048
Frequencies --	316.6161	329.2604	329.4745
Frequencies --	333.2902	339.1174	352.2322
Frequencies --	365.7820	378.9334	379.7496
Frequencies --	380.6457	383.0718	384.2485
Frequencies --	390.9587	430.1714	430.7226
Frequencies --	431.1013	431.3722	455.1898
Frequencies --	455.2862	469.0332	498.6573
Frequencies --	503.0345	509.3144	513.7843
Frequencies --	541.9011	542.1153	550.1872
Frequencies --	561.3282	564.4850	567.6301
Frequencies --	572.4262	579.0362	584.7154
Frequencies --	604.1211	604.5974	640.4267
Frequencies --	640.6359	642.6640	645.8358
Frequencies --	653.7044	654.5606	663.5747
Frequencies --	723.4794	730.2579	731.7273
Frequencies --	734.5964	748.0293	755.6706
Frequencies --	755.9259	768.3730	779.3298
Frequencies --	793.2533	799.0797	800.6444
Frequencies --	807.2210	840.4125	841.2340
Frequencies --	842.0027	853.9356	868.1064
Frequencies --	884.3231	888.8547	895.3551
Frequencies --	907.5698	908.3591	910.4071
Frequencies --	929.2380	947.8881	948.9272
Frequencies --	950.5240	1012.6207	1027.6893
Frequencies --	1033.1229	1037.4453	1051.1879
Frequencies --	1056.5025	1058.6673	1060.9815
Frequencies --	1061.8836	1063.1311	1088.8347
Frequencies --	1089.4058	1090.6975	1091.7731
Frequencies --	1125.6993	1127.5780	1180.7988
Frequencies --	1218.5310	1225.9723	1235.6938
Frequencies --	1236.5413	1266.7271	1283.3021
Frequencies --	1289.9174	1333.9770	1334.8949
Frequencies --	1336.8678	1341.1510	1344.5367
Frequencies --	1344.8963	1354.1795	1391.0921
Frequencies --	1396.8651	1402.5263	1412.3910
Frequencies --	1414.6044	1419.6360	1422.9928
Frequencies --	1425.3421	1429.2357	1430.8282
Frequencies --	1432.2100	1434.5813	1441.5592
Frequencies --	1444.5564	1447.2099	1473.3143
Frequencies --	1473.5787	1474.0129	1486.7269
Frequencies --	1487.4856	1500.6216	1503.1941
Frequencies --	1589.7774	1592.4116	1592.9962
Frequencies --	1594.8810	1595.2294	1621.4318
Frequencies --	1621.7110	1623.6572	2976.2951
Frequencies --	3019.4332	3025.4469	3084.8459
Frequencies --	3096.7056	3106.2457	3113.2145
Frequencies --	3123.9600	3136.4115	3139.1762
Frequencies --	3200.5782	3202.5539	3238.0514
Frequencies --	3238.7625	3254.1412	3264.1604
Frequencies --	3271.5156	3278.4699	3290.7776

Catalyst 1 Dimerization Geometries:**conformation 1**

vacuum	toluene-like solvent	D3 dispersion
-3666.4012455	-3666.4243198	-0.73396683

Ti	-1.62496500	2.20608700	1.60371000
C	-0.60370600	1.01795500	2.95723200
H	0.12304700	0.48843000	2.31662800
H	-0.05145000	1.57875800	3.72527100
H	-1.26940200	0.29575500	3.45540500
O	-0.29945600	3.01221800	0.74285000
C	0.61704000	3.88637100	0.16081600
C	0.35823800	4.37982600	-1.15125200
C	1.79270600	4.23509800	0.88891100
C	1.30523800	5.25189500	-1.73244800
C	2.71822100	5.10596700	0.26886500
C	2.46825200	5.60772100	-1.02217200
C	-3.36521200	3.83295200	1.56467300
C	-4.03322900	2.63360700	1.99649200
C	-2.42534400	4.20666300	2.58520600
C	-3.50217900	2.26450100	3.27440100
C	-2.50894500	3.23204300	3.63910200
B	3.27027600	-1.54141400	-0.07498800
C	3.02846900	-1.77696100	1.57590600
C	3.26184500	-3.09636400	-0.70880400
C	1.77037600	-2.19019000	2.07326700

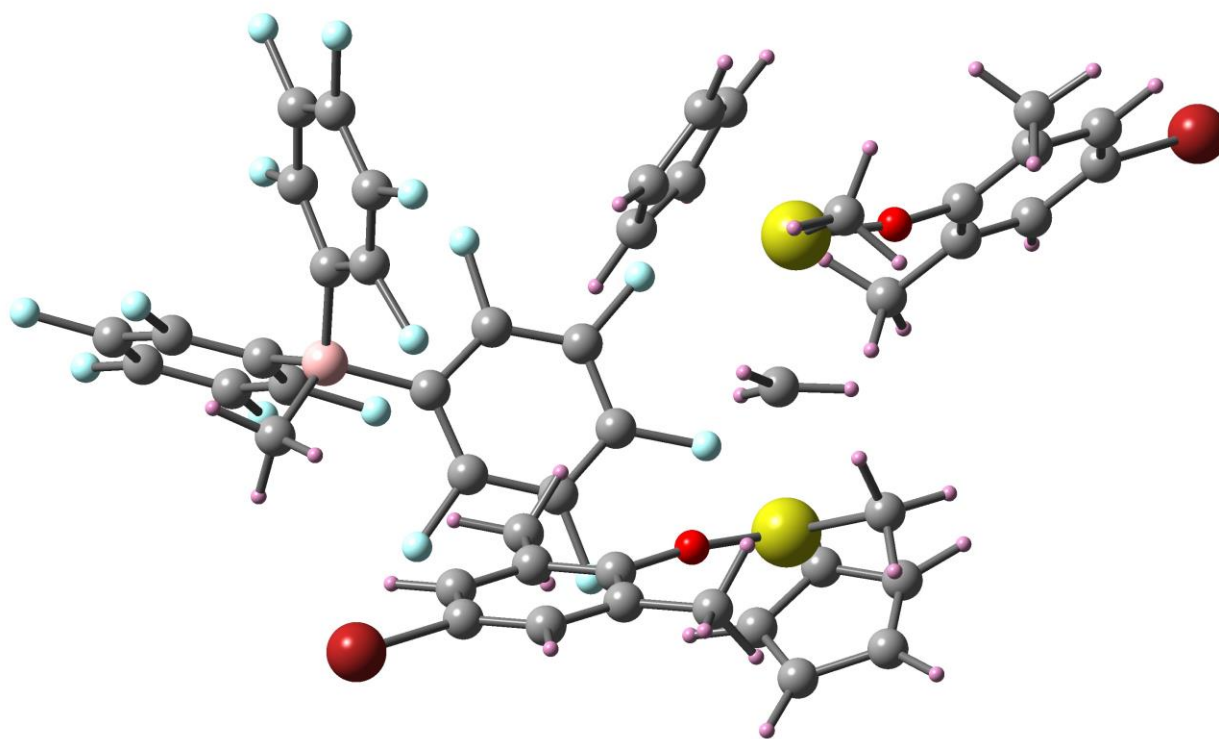
C	3.99709300	-1.64129600	2.60241300
C	2.38230000	-3.58988900	-1.69566200
C	4.14633100	-4.09293800	-0.22433000
C	1.46310400	-2.40844500	3.42982700
F	0.69381600	-2.43543800	1.19084000
C	3.74262900	-1.84366200	3.97546200
F	5.31691300	-1.29709800	2.30338600
C	2.34809900	-4.92513300	-2.14860800
F	1.44164700	-2.75187900	-2.33078600
C	4.16469400	-5.43480300	-0.64652400
F	5.11146500	-3.75079900	0.72975100
C	2.45965800	-2.22534700	4.39969300
F	0.17314100	-2.78303400	3.81976900
F	4.75134800	-1.67195800	4.92007300
C	3.24703600	-5.86272900	-1.62089600
F	1.42017000	-5.32137700	-3.11566600
F	5.07773600	-6.34180500	-0.11537900
F	2.18036800	-2.41550500	5.74954700
F	3.23055900	-7.18426700	-2.05219800
C	4.66307300	-0.69263600	-0.43512300
C	5.59430000	-1.01928000	-1.44702200
C	4.91609700	0.57340100	0.14624700
C	6.68266700	-0.20473900	-1.82798300
C	5.98012900	1.42542300	-0.19415800
C	6.88441500	1.03068700	-1.19413700
F	4.06007800	1.06775400	1.15250300
F	6.14122600	2.65870600	0.44143500
F	7.94549600	1.85346700	-1.55717500
F	7.55496300	-0.61033000	-2.83569300
F	5.47483900	-2.21144300	-2.17822200
H	3.63277200	5.37263300	0.79656300
C	2.07372900	3.68802500	2.27538300
H	1.25374600	3.91490400	2.97444500
H	2.20112200	2.59731900	2.24905200
H	2.99759300	4.11621700	2.68478900
C	-0.88205300	3.97760200	-1.93031900
H	-0.92767400	2.88558800	-2.06436300
H	-1.80510400	4.29099800	-1.41686100
H	-0.88281100	4.43786300	-2.92735700
H	1.13262000	5.63919800	-2.73591100
Ti	-3.31027700	-1.05327200	-1.17877900
C	-2.36968000	0.57376500	0.14361600
H	-2.83715700	1.35007900	-0.47111700
H	-1.34051900	0.26495200	-0.05678200
H	-2.92757200	0.13350300	0.97547800
C	-2.69462900	-2.75244900	-0.16355100
H	-1.59641300	-2.81673600	-0.13610000
H	-3.08346800	-2.61823200	0.86263000
H	-3.09225500	-3.69050200	-0.57940200
O	-5.02336100	-0.89731100	-0.68295600
C	-6.40302100	-0.78201300	-0.54930000
C	-7.06459000	0.39114300	-1.02049600
C	-7.11449500	-1.84385700	0.08663500
C	-8.46380600	0.48803200	-0.83893700
C	-8.51308000	-1.71036800	0.24372500
C	-9.17302100	-0.55467100	-0.21461900
H	-8.98746300	1.37700500	-1.18887600

H	-9.07351800	-2.51067500	0.72553400
C	-6.32204600	1.52107600	-1.71420100
H	-5.42173500	1.82253100	-1.15930900
H	-6.00014500	1.22809100	-2.72582900
H	-6.96612400	2.40467600	-1.81751300
C	-6.40896000	-3.08983200	0.58921600
H	-5.89120800	-3.61661700	-0.22684100
H	-5.64845400	-2.84444200	1.34580900
H	-7.12311100	-3.78971800	1.04260200
C	-1.74047000	-1.92030300	-2.89524000
C	-3.07683900	-2.29942000	-3.25200500
C	-1.67034800	-0.48888900	-2.90719400
C	-3.83495000	-1.10397000	-3.50069800
C	-2.96487700	0.01824700	-3.28208400
C	2.08405100	-0.55563100	-0.68876200
H	2.28052300	-0.34095800	-1.75157100
H	1.08192500	-0.99433900	-0.61601800
H	2.08412900	0.40476500	-0.15087100
H	-0.78194000	0.09759100	-2.69525300
H	-0.92441800	-2.59112900	-2.65582900
H	-3.44794700	-3.31749200	-3.32959500
H	-4.87514400	-1.06239700	-3.80919900
H	-3.23019700	1.06416100	-3.40886400
H	-3.56513500	4.38647800	0.65173700
H	-1.77850700	5.07894700	2.56819300
H	-1.92670900	3.23024300	4.55482700
H	-3.79005600	1.39794700	3.86278800
H	-4.81594600	2.10846300	1.45769900
Br	3.76692400	6.81794200	-1.85679300
Br	-11.11461500	-0.38965600	0.02531500

Frequencies --	5.0539	6.0002	7.6452
Frequencies --	9.2315	10.3956	11.6453
Frequencies --	15.7165	18.0156	21.1115
Frequencies --	26.3450	28.8641	30.1494
Frequencies --	33.3678	35.5978	37.3306
Frequencies --	42.2810	44.4345	46.5576
Frequencies --	48.2339	51.4268	56.2102
Frequencies --	58.6042	62.7925	67.7905
Frequencies --	81.6951	87.9650	93.7218
Frequencies --	100.0958	107.8485	108.9126
Frequencies --	111.5098	119.3265	123.5230
Frequencies --	128.0828	133.0232	134.0055
Frequencies --	140.3620	141.2496	146.1376
Frequencies --	146.7045	151.0807	153.2795
Frequencies --	153.7994	154.8824	156.8873
Frequencies --	158.6304	160.0807	165.7789
Frequencies --	166.7589	174.4060	182.1191
Frequencies --	183.6936	189.1167	202.3132
Frequencies --	202.6027	208.4891	213.1333
Frequencies --	219.5420	220.4605	220.9867
Frequencies --	222.1484	222.9626	224.2331
Frequencies --	231.6475	233.4703	235.1497
Frequencies --	243.8106	249.3334	253.4599
Frequencies --	254.5113	258.2342	262.7025
Frequencies --	263.9244	264.0286	264.9025
Frequencies --	270.9190	274.3420	275.1055
Frequencies --	275.6695	279.6605	292.0341
Frequencies --	300.8134	306.1437	317.0562

Frequencies --	322.4362	328.3217	334.4954
Frequencies --	335.0848	337.9587	345.4095
Frequencies --	353.3808	358.1726	365.2040
Frequencies --	367.0902	377.9877	378.9322
Frequencies --	379.7140	394.0705	394.3899
Frequencies --	399.4234	428.2369	430.0719
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Frequencies --	435.1756	454.8838	455.3028
Frequencies --	469.2991	502.5934	502.7450
Frequencies --	509.2476	510.3866	511.0788
Frequencies --	520.4833	538.7444	541.1032
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Frequencies --	567.2261	568.4071	570.1488
Frequencies --	573.9864	575.8766	577.2069
Frequencies --	577.8173	583.1167	589.5147
Frequencies --	593.9654	630.5342	634.8640
Frequencies --	636.2553	637.4363	643.2877
Frequencies --	661.0294	663.8185	673.0978
Frequencies --	711.4759	712.3595	726.1686
Frequencies --	731.1249	734.2667	741.0475
Frequencies --	746.9667	763.5997	768.6049
Frequencies --	786.3354	787.7123	799.4674
Frequencies --	803.7026	804.6500	807.8287
Frequencies --	811.6338	812.1501	823.8936
Frequencies --	831.5950	833.7766	841.1629
Frequencies --	841.7227	841.9552	844.5847
Frequencies --	874.1715	876.2221	880.6199
Frequencies --	883.4264	886.9389	892.8813
Frequencies --	894.8585	896.2211	896.9917
Frequencies --	905.1570	905.8485	919.8130
Frequencies --	927.7034	938.4269	948.3426
Frequencies --	949.6432	951.0537	981.1501
Frequencies --	989.7447	1010.5757	1012.6295
Frequencies --	1021.2675	1027.2368	1029.3123
Frequencies --	1032.3140	1033.1594	1033.6694
Frequencies --	1042.2758	1046.9729	1048.2678
Frequencies --	1050.1392	1053.1887	1055.7760
Frequencies --	1058.6595	1059.1470	1062.7213
Frequencies --	1066.7154	1088.4579	1090.0787
Frequencies --	1091.3422	1096.1136	1123.3981
Frequencies --	1125.3779	1128.3880	1128.6515
Frequencies --	1192.1443	1193.3500	1202.2095
Frequencies --	1205.7527	1207.7818	1208.5568
Frequencies --	1213.5795	1266.2741	1267.1856
Frequencies --	1282.1261	1285.9006	1287.4011
Frequencies --	1288.2471	1311.1584	1314.7100
Frequencies --	1318.6117	1329.9629	1337.3871
Frequencies --	1344.2287	1348.0533	1349.3097
Frequencies --	1353.0908	1355.6690	1367.0653
Frequencies --	1390.3263	1392.7755	1398.0262
Frequencies --	1398.5759	1407.6472	1412.7582
Frequencies --	1413.5408	1416.2636	1416.8124
Frequencies --	1418.6033	1418.9253	1421.2822
Frequencies --	1422.8573	1426.8136	1427.4419
Frequencies --	1429.4279	1431.1146	1436.5851
Frequencies --	1437.6453	1443.9666	1446.3590
Frequencies --	1446.9993	1449.2885	1462.7343
Frequencies --	1465.5588	1467.2517	1485.5003
Frequencies --	1489.6863	1491.3140	1491.5946
Frequencies --	1498.8974	1499.0674	1499.7569
Frequencies --	1502.4753	1503.7074	1510.4277
Frequencies --	1586.9114	1587.7301	1590.6832

Frequencies --	1591.5166	1594.2213	1596.3854
Frequencies --	1597.5298	1613.1248	1617.3986
Frequencies --	1619.3834	2987.1673	2991.6385
Frequencies --	3012.6988	3014.2862	3022.2072
Frequencies --	3023.8637	3025.5405	3027.4156
Frequencies --	3098.2585	3104.8470	3107.1305
Frequencies --	3107.9449	3112.7490	3116.0179
Frequencies --	3120.0721	3131.0268	3134.4486
Frequencies --	3135.6800	3136.5956	3140.6237
Frequencies --	3142.6446	3149.3831	3199.5907
Frequencies --	3200.9183	3203.1922	3208.4348
Frequencies --	3218.4875	3231.3175	3236.8469
Frequencies --	3238.8412	3241.3844	3245.2823
Frequencies --	3254.9373	3259.5502	3261.5081
Frequencies --	3267.3470	3277.9420	3296.6154

conformation 2

vacuum	toluene-like solvent	D3 dispersion
-3666.4031326	-3666.425317	-0.73244489

Ti	-2.68579700	3.38256600	-1.34827900
C	-4.35557000	4.38064700	-0.57027100
H	-4.15596900	4.44178300	0.51583200
H	-4.43967800	5.40430700	-0.96720000
H	-5.30435800	3.85245700	-0.75137100
O	-1.35829000	4.36930200	-0.70016200
C	-0.24244600	5.15626400	-0.41198600
C	1.05628300	4.56878100	-0.46421300
C	-0.44638400	6.52200100	-0.05313200
C	2.16590700	5.38506000	-0.14395900

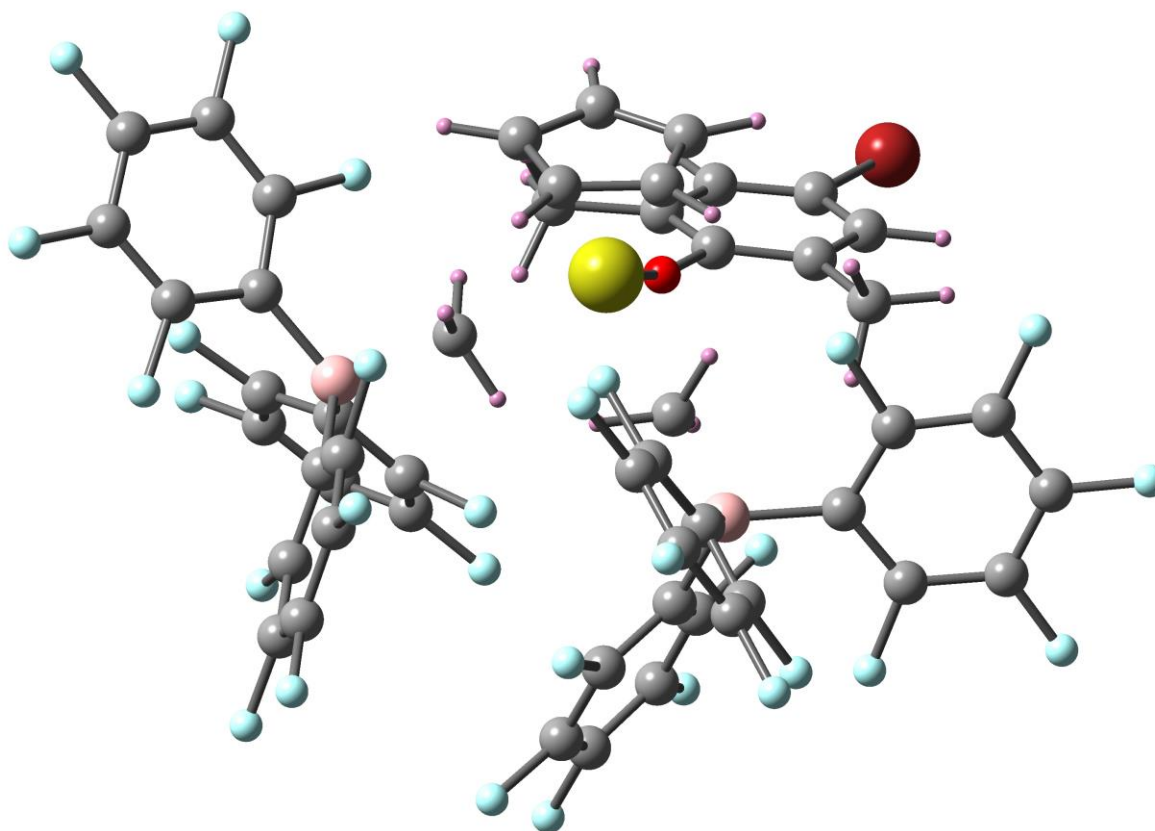
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C	-1.83970500	2.69288200	-3.46244000
C	-2.87641000	1.73797600	-3.18068200
C	-2.45498400	3.98228200	-3.61166500
C	-4.12942500	2.43439500	-3.15922500
C	-3.87322700	3.81990000	-3.42560400
B	4.27427400	-1.40728900	-0.30717400
C	2.80385300	-1.47351000	-1.12378100
C	5.34030000	-2.57376300	-0.84793000
C	2.40369900	-0.59135400	-2.15439100
C	1.79797400	-2.41069300	-0.78024600
C	6.63357200	-2.69990100	-0.27895100
C	5.15680900	-3.41209800	-1.97001900
C	1.12633200	-0.59396700	-2.75266400
F	3.27231800	0.37522300	-2.67416100
C	0.51017900	-2.45220500	-1.34592300
F	2.05508100	-3.39973600	0.17579100
C	7.63877300	-3.56469100	-0.74677100
F	6.97669800	-1.94432300	0.85259900
C	6.13141400	-4.29359100	-2.48449200
F	3.94101400	-3.41779600	-2.67947200
C	0.16378400	-1.52331100	-2.33807800
F	0.78973400	0.34678300	-3.73555700
F	-0.44570700	-3.38309300	-0.91546800
C	7.38780100	-4.37454300	-1.86755400
F	8.87844100	-3.63021700	-0.11380200
F	5.85781300	-5.08356800	-3.60042900
F	-1.12641200	-1.50807200	-2.88533600
F	8.36603100	-5.23480400	-2.35546900
C	3.89241400	-1.52929600	1.32695200
C	4.24424100	-2.57790300	2.21112200
C	3.16476700	-0.50139100	1.97032900
C	3.98563700	-2.57625100	3.59815800
C	2.87050900	-0.45346700	3.34525700
C	3.29830400	-1.49814000	4.17852900
F	2.61263200	0.56297800	1.21752800
F	2.13670000	0.61035700	3.88524000
F	3.02268000	-1.47587600	5.54262800
F	4.38409800	-3.64331600	4.39930700
F	4.85690200	-3.73979600	1.73450000
H	0.55936900	8.34958200	0.52984200
C	-1.83091500	7.14204300	0.00601200
H	-2.32036500	7.13124500	-0.98105800
H	-2.48705100	6.59756400	0.70089300
H	-1.77679800	8.18666000	0.34017900
C	1.27695200	3.12067500	-0.85544300
H	0.60772200	2.44400200	-0.30473500
H	1.10043600	2.96670900	-1.93093200
H	2.30520100	2.80607800	-0.64461200
H	3.16615700	4.95464100	-0.17023000
Ti	-3.38162900	0.12947800	1.80329300
C	-2.81713200	1.59756300	0.09901100
H	-2.13461000	0.91832300	-0.41665600
H	-2.43019800	2.24861000	0.88888100
H	-3.88336800	1.57662700	-0.14619800
C	-4.35008800	1.54771300	2.99937800

H	-3.66866400	2.30615300	3.41446800
H	-5.08214400	2.02414800	2.32010700
H	-4.89951800	1.07718100	3.82923800
O	-4.76795700	-0.76772200	1.13306100
C	-5.73056400	-1.68410300	0.71304000
C	-5.48579700	-2.46683700	-0.45405200
C	-6.94225300	-1.79138700	1.45866100
C	-6.48951200	-3.37342400	-0.86738300
C	-7.91727600	-2.71310700	1.01417700
C	-7.68583300	-3.49123600	-0.13604900
H	-6.32449500	-3.98143800	-1.75591400
H	-8.84912700	-2.81348800	1.56941600
C	-4.19583300	-2.35874600	-1.24484800
H	-3.93165100	-1.31242800	-1.45364400
H	-3.34905100	-2.80853700	-0.70527000
H	-4.27749600	-2.88091500	-2.20697400
C	-7.20244300	-0.95017200	2.69541300
H	-6.45069800	-1.13881500	3.47801500
H	-7.16786100	0.12502900	2.46427500
H	-8.19032300	-1.17372800	3.11943000
C	-1.38165800	0.38169300	3.27820500
C	-2.35402000	-0.44980600	3.92400800
C	-0.97095400	-0.27013900	2.07073000
C	-2.54314500	-1.62579000	3.11542300
C	-1.68771200	-1.51294200	1.96695300
C	5.06811800	0.03175700	-0.52253000
H	5.89270500	0.11423000	0.19996700
H	5.50515700	0.09808400	-1.53018200
H	4.42009500	0.90768400	-0.38499300
H	-0.21773300	0.09475700	1.37997000
H	-1.01164200	1.33460400	3.64495000
H	-2.84573400	-0.23806400	4.86793700
H	-3.19042900	-2.46720900	3.34621800
H	-1.56513200	-2.25854100	1.18897900
H	-0.78604300	2.46526500	-3.57992700
H	-1.94123700	4.90908400	-3.85132900
H	-4.61874200	4.60625200	-3.48432500
H	-5.10467600	1.99416200	-2.96876300
H	-2.72669000	0.67233600	-3.04099500
Br	3.53439800	7.84569600	0.64278600
Br	-9.05996000	-4.76013600	-0.73272300

Frequencies --	2.7132	5.5796	7.4307
Frequencies --	11.3684	12.3285	17.5517
Frequencies --	19.2684	20.7969	22.2446
Frequencies --	24.9496	27.5316	30.5521
Frequencies --	32.6635	36.8304	38.3036
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Frequencies --	154.4375	155.3803	158.7292
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Frequencies --	169.6690	180.8848	183.3919
Frequencies --	190.1848	194.1092	206.3958
Frequencies --	208.6002	212.9436	216.4033
Frequencies --	216.7757	217.5043	221.1238
Frequencies --	222.1495	229.5811	233.3536
Frequencies --	234.8258	237.0792	239.4043
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Frequencies --	256.1599	261.1569	261.4188
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Frequencies --	577.9082	583.4787	586.0189
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Frequencies --	730.0376	731.6169	742.8319
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Frequencies --	784.2445	788.8485	789.8727
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Frequencies --	1208.4956	1265.3790	1267.5121
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Frequencies --	1353.8870	1354.7962	1372.8003
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Frequencies --	1399.2013	1409.0163	1412.4479
Frequencies --	1413.7620	1414.8268	1417.3699
Frequencies --	1420.9220	1424.1483	1424.5479
Frequencies --	1424.6704	1428.8009	1429.4583
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Frequencies --	1590.9650	1594.2622	1597.3272
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Frequencies --	1618.2338	2979.0013	2981.2886
Frequencies --	3018.0568	3019.0481	3025.5743
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Frequencies --	3100.8447	3101.7100	3106.2321
Frequencies --	3106.4189	3115.1282	3122.1348
Frequencies --	3125.2089	3127.1276	3129.8595
Frequencies --	3137.0179	3137.5537	3137.7669
Frequencies --	3143.6757	3162.9933	3198.9780
Frequencies --	3201.5733	3205.1759	3205.7392
Frequencies --	3222.2752	3233.7431	3237.6569
Frequencies --	3241.9343	3243.7492	3246.9571
Frequencies --	3262.3448	3264.6536	3267.8862
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Catalyst 1 Double Activation Product:

vacuum	toluene-like solvent	D3 dispersion
-5144.7990126	-5144.8102725	-0.78388588

C	-2.45882300	-1.03443800	1.59000600
C	-2.05647100	-2.25898100	2.17393800
C	-2.21341300	0.08131500	2.42763900
C	-1.53214900	-2.38015400	3.47782500
C	-1.70013500	0.01967800	3.73185000
C	-1.36205400	-1.23395800	4.27147100
C	-3.48853300	-2.26892300	-0.68936800
C	-4.59955100	-3.00657900	-0.20866000
C	-2.89304400	-2.85702500	-1.82291700
C	-5.08146800	-4.19637700	-0.78209000
C	-3.33438100	-4.04194800	-2.44423100
C	-4.44382100	-4.72250700	-1.91953600
C	-4.40500500	0.13823400	-0.05914800
C	-5.28628700	0.47057500	1.00137400
C	-4.83525000	0.65065500	-1.30504800
C	-6.45115500	1.25190700	0.84957500
C	-5.98041500	1.43984300	-1.51223900
C	-6.80265700	1.74878900	-0.41656600
C	-1.70543900	-0.04083600	-0.73167300
H	-2.11047700	0.16103000	-1.73065700
H	-1.55774000	0.81970400	-0.07371100

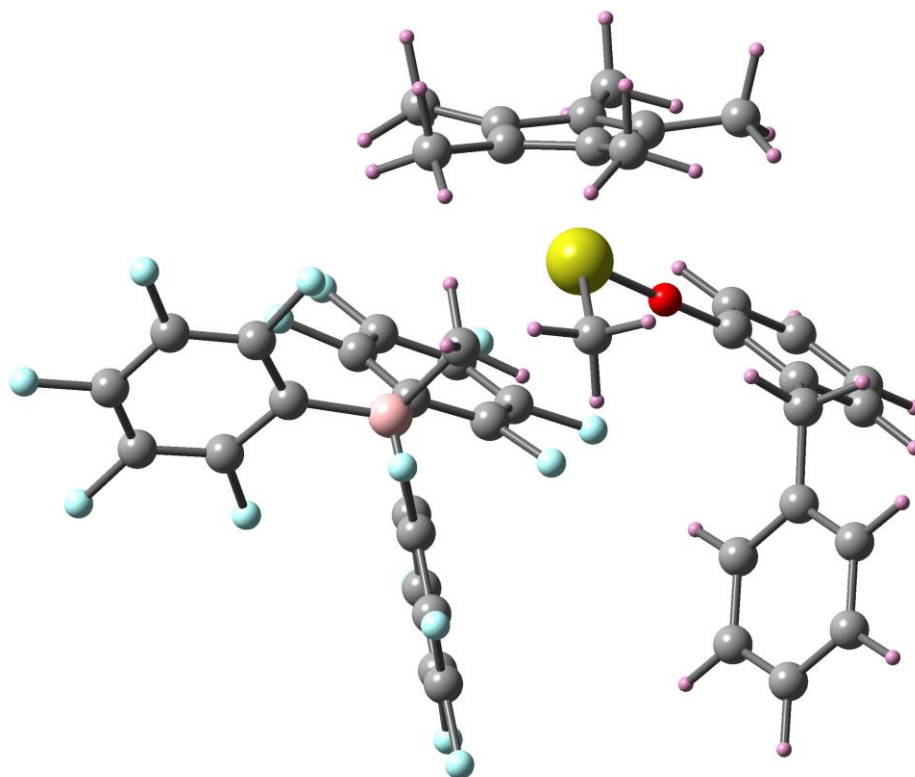
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F	-7.93716700	2.52557800	-0.58379600
F	-7.25763600	1.53275800	1.94244300
F	-5.05385900	0.01317500	2.29617900
F	-6.29777000	1.91448700	-2.78077200
F	-4.09182300	0.37180900	-2.47718900
F	-5.26961700	-2.56498300	0.93585300
F	-6.17382900	-4.85499400	-0.23658900
F	-4.90150800	-5.88834400	-2.50978500
F	-2.68407100	-4.53306800	-3.56968200
F	-1.76187400	-2.26552200	-2.42863700
F	-2.13403900	-3.45750100	1.45311600
F	-1.16331200	-3.62283200	3.97386300
F	-0.84395000	-1.33190600	5.55000300
F	-1.51248000	1.17198800	4.47978500
F	-2.48375600	1.37701500	1.94125000
B	-3.06377500	-0.84797300	0.05999700
F	6.75385400	-3.73690800	-2.37964500
C	6.09906500	-2.52000700	-2.27065800
C	5.09731000	-2.33056700	-1.29614600
C	6.44391300	-1.46543000	-3.13188100
C	4.37459800	-1.12499300	-1.11417900
F	4.87808300	-3.42678100	-0.45966700
C	5.78493200	-0.23400100	-2.98362000
F	7.41976900	-1.62999400	-4.09934700
B	3.19679300	-0.91624700	0.03661100
C	4.79716300	-0.10102200	-1.99249300
F	6.11488100	0.83839600	-3.80537000
C	3.68365000	0.04374600	1.29768300
C	2.53006400	-2.35567400	0.51536400
C	1.84099600	-0.02363000	-0.74237200
F	4.24482700	1.19886200	-1.88468600
C	5.02755500	0.39498300	1.57485800
C	2.77332900	0.58042200	2.24039100
C	2.65699200	-2.92046900	1.80802000
C	1.80019000	-3.18149100	-0.37304800
H	2.33808000	0.91060600	-1.02655800
H	1.62729000	-0.73725400	-1.54232700
H	1.13090900	0.04298400	0.08718200
C	5.42941600	1.21594400	2.64943100
F	6.07524200	-0.09413000	0.78904100
C	3.11670600	1.40202100	3.32713400
F	1.40110000	0.25904200	2.15109300
C	2.08995700	-4.15195400	2.19546300
F	3.41470200	-2.28236700	2.79403400
C	1.20914800	-4.41169700	-0.04086900
F	1.66305600	-2.79914000	-1.72900400
C	4.46759700	1.73081400	3.53346700
F	6.77051200	1.51346900	2.84388800
F	2.14332300	1.87909200	4.19332400
C	1.35167100	-4.90495200	1.26705100
F	2.26527900	-4.63091100	3.48334800
F	0.49793800	-5.13657900	-0.98690700
F	4.84175900	2.54175100	4.59062400
F	0.78516800	-6.11209500	1.62838000
Ti	0.09023500	1.06080000	-1.81209100
O	0.05350100	2.63731100	-1.02269200

C	0.00715600	4.01597100	-0.78313100
C	1.23277200	4.71639100	-0.56837900
C	-1.26689600	4.65861600	-0.73253300
C	1.15923000	6.10661800	-0.33013800
C	2.58123500	4.02166700	-0.56311000
C	-1.28843400	6.05028700	-0.49183700
C	-2.57362800	3.90256400	-0.88102500
C	-0.08770300	6.76148600	-0.30031600
H	2.07859100	6.66575800	-0.16188900
H	2.61987100	3.23629600	0.20525000
H	2.81541300	3.55145900	-1.52907800
H	3.38557600	4.73604800	-0.34612400
H	-2.24655500	6.56622600	-0.44536300
H	-2.59770100	3.27659200	-1.78396400
H	-2.74353300	3.24652500	-0.01483600
H	-3.41973300	4.59909500	-0.94008800
Br	-0.15295300	8.68841800	0.02470700
C	-0.55692200	1.92791700	-3.89240700
C	0.87828200	1.95687900	-3.83458300
C	-0.97022900	0.54840600	-3.94376700
H	-1.20942700	2.79466200	-3.93297600
C	1.34595500	0.59590600	-3.84611700
H	1.49868700	2.84772900	-3.82044600
C	0.20457400	-0.27277800	-3.90298000
H	-1.99217000	0.19093100	-4.00513200
H	2.38414700	0.28532700	-3.82131000
H	0.22022700	-1.35789400	-3.90725700

Frequencies --	1.1185	8.3234	9.5474
Frequencies --	12.2604	14.5966	18.9193
Frequencies --	21.1826	23.5112	25.8969
Frequencies --	27.8519	29.6668	30.0374
Frequencies --	31.2941	32.5670	35.9047
Frequencies --	38.6313	40.5588	43.4686
Frequencies --	45.5167	46.8899	47.8336
Frequencies --	52.9211	54.6937	66.4841
Frequencies --	79.0523	88.6461	94.4767
Frequencies --	99.8745	103.9273	106.3049
Frequencies --	108.5610	111.3157	113.8594
Frequencies --	117.5593	119.1476	120.8391
Frequencies --	123.2964	125.5105	128.6637
Frequencies --	129.6659	137.2732	142.1951
Frequencies --	146.8475	149.2684	150.2057
Frequencies --	153.4382	154.3828	155.0901
Frequencies --	156.4898	158.1476	159.5002
Frequencies --	161.1236	162.5431	162.9441
Frequencies --	166.2859	171.2292	186.7240
Frequencies --	201.2451	216.3969	216.8480
Frequencies --	217.9946	219.6848	220.0925
Frequencies --	221.6526	224.6952	241.7511
Frequencies --	249.8743	259.0065	261.4577
Frequencies --	263.9878	264.6053	264.9107
Frequencies --	264.9851	265.1397	265.4468
Frequencies --	266.8177	270.0536	273.0191
Frequencies --	273.9775	274.4992	275.4595
Frequencies --	276.6508	280.9669	289.4328
Frequencies --	292.1210	296.1951	299.4852
Frequencies --	301.6740	307.1097	309.8954
Frequencies --	319.6123	320.3640	322.5144
Frequencies --	327.9375	330.6187	334.7667

Frequencies --	341.3537	344.0766	348.0039
Frequencies --	356.6650	360.4635	364.8571
Frequencies --	366.0194	373.8916	378.2639
Frequencies --	379.3964	379.5866	380.2888
Frequencies --	381.6670	382.9039	389.2276
Frequencies --	392.6131	403.6272	415.1293
Frequencies --	430.8956	431.2017	432.0419
Frequencies --	432.6581	432.8226	433.5878
Frequencies --	445.3729	452.6389	457.0514
Frequencies --	457.2311	457.8687	458.2748
Frequencies --	459.3730	469.7979	479.8834
Frequencies --	502.9676	510.2412	530.9461
Frequencies --	541.0921	541.5534	542.3775
Frequencies --	543.5527	548.1885	549.7112
Frequencies --	553.5091	561.0126	565.9849
Frequencies --	573.4353	574.7391	591.3374
Frequencies --	597.3804	598.5959	601.8054
Frequencies --	606.6455	635.4884	636.3643
Frequencies --	639.2811	639.7971	640.8289
Frequencies --	642.2997	648.8072	652.7168
Frequencies --	654.2933	660.8983	664.1755
Frequencies --	679.6596	718.8192	724.1137
Frequencies --	727.5158	730.2496	731.9704
Frequencies --	732.5308	734.9109	751.0973
Frequencies --	757.3463	759.0972	759.7388
Frequencies --	763.5707	766.9459	795.7201
Frequencies --	803.3938	808.5467	813.1455
Frequencies --	823.0324	837.1199	841.0675
Frequencies --	846.2857	861.4728	874.5004
Frequencies --	879.7359	884.1867	890.2181
Frequencies --	890.9972	894.4877	902.6778
Frequencies --	903.4721	908.9475	913.2883
Frequencies --	915.9613	916.8021	924.2116
Frequencies --	929.6124	951.1795	953.5660
Frequencies --	988.8689	1011.5492	1013.4457
Frequencies --	1022.6909	1028.4409	1030.1176
Frequencies --	1032.2310	1033.0543	1034.8815
Frequencies --	1038.9459	1049.1955	1049.7744
Frequencies --	1051.4806	1052.8173	1053.9561
Frequencies --	1056.4952	1058.5438	1058.7286
Frequencies --	1061.5239	1072.2699	1079.5436
Frequencies --	1092.9883	1094.2819	1096.0098
Frequencies --	1104.6107	1119.2570	1127.2363
Frequencies --	1178.2171	1217.4429	1219.7200
Frequencies --	1220.4045	1221.8113	1222.3808
Frequencies --	1223.0998	1269.9279	1283.8372
Frequencies --	1287.8742	1318.2932	1318.6707
Frequencies --	1320.3782	1320.6228	1325.1027
Frequencies --	1326.0051	1336.7064	1337.9142
Frequencies --	1340.3925	1342.1937	1345.1122
Frequencies --	1350.5022	1355.2295	1384.9625
Frequencies --	1396.5806	1407.4945	1410.4763
Frequencies --	1413.8789	1414.4634	1417.0293
Frequencies --	1418.8428	1419.5042	1422.8931
Frequencies --	1423.7555	1425.5469	1427.6403
Frequencies --	1430.8611	1431.9956	1435.9929
Frequencies --	1442.9190	1448.4430	1470.3027
Frequencies --	1471.0246	1471.8078	1472.6022
Frequencies --	1473.3532	1474.3815	1493.3556
Frequencies --	1494.8930	1504.3305	1505.4354
Frequencies --	1579.4390	1588.6270	1590.6510
Frequencies --	1591.2719	1593.0316	1593.5175
Frequencies --	1594.0861	1596.5798	1620.0278

Frequencies --	1620.5286	1621.2529	1621.9409
Frequencies --	1622.9272	1625.3611	2999.9813
Frequencies --	3012.9334	3034.0113	3034.8722
Frequencies --	3124.0412	3126.8309	3145.3489
Frequencies --	3145.6259	3157.3724	3187.0171
Frequencies --	3195.9037	3203.1941	3204.6075
Frequencies --	3207.2919	3251.1677	3262.2904
Frequencies --	3268.0331	3281.5488	3293.5735

Catalyst 15 proximal to distal conformation transition state:

vacuum	toluene-like solvent	D3 dispersion
-3312.6374347	-3312.6503766	-0.63983084

Ti	1.67070000	-2.00460000	-0.80180000
C	2.10900000	-0.95830000	-2.54820000
H	2.03460000	0.10060000	-2.24350000
H	3.10350000	-1.13740000	-2.97840000
H	1.34670000	-1.16810000	-3.31570000
O	2.74990000	-1.22520000	0.38140000
C	3.60790000	-0.62400000	1.30250000
C	4.67470000	0.22680000	0.89380000
C	3.35870000	-0.88310000	2.67570000
C	5.47490000	0.79090000	1.92010000
C	4.16570000	-0.30110000	3.66650000
C	5.23690000	0.53840000	3.28450000
H	6.29190000	1.45540000	1.63170000
H	3.95430000	-0.48980000	4.72050000
C	1.80790000	-4.19920000	0.04790000
C	0.57180000	-4.20840000	-0.71010000
C	2.90030000	-3.99800000	-0.88030000
C	0.89900000	-4.01340000	-2.10340000
C	2.33490000	-3.88860000	-2.21330000
F	-0.64040000	5.65560000	-2.17960000
C	-0.90320000	4.41360000	-1.61800000

C	-1.23690000	4.29810000	-0.25900000
C	-0.84630000	3.24870000	-2.39970000
C	-1.49100000	3.02700000	0.29690000
F	-1.31570000	5.44290000	0.52640000
C	-1.10540000	2.00470000	-1.79490000
F	-0.53840000	3.33410000	-3.75390000
C	-1.41620000	1.81210000	-0.42730000
F	-1.84520000	3.03930000	1.64690000
F	-1.06360000	0.89960000	-2.66870000
B	-1.73450000	0.27850000	0.16490000
C	-1.70930000	0.14670000	1.82600000
C	-3.20690000	-0.11940000	-0.50870000
C	-0.44070000	-0.75310000	-0.28440000
C	-2.64230000	-0.57760000	2.60350000
C	-0.62680000	0.64520000	2.59100000
C	-4.35410000	0.66630000	-0.23260000
C	-3.46670000	-1.15840000	-1.42330000
H	0.42900000	-0.20450000	0.10370000
H	-0.62010000	-1.70850000	0.23340000
H	-0.44770000	-0.86300000	-1.37580000
C	-2.55680000	-0.74360000	4.00260000
F	-3.73360000	-1.22290000	2.00390000
C	-0.49150000	0.50970000	3.98330000
F	0.42460000	1.32160000	1.94610000
C	-5.62550000	0.45810000	-0.79620000
F	-4.25960000	1.71870000	0.68340000
C	-4.71650000	-1.41280000	-2.02280000
F	-2.44410000	-2.05000000	-1.80820000
C	-1.47590000	-0.18760000	4.70420000
F	-3.52490000	-1.46750000	4.69040000
F	0.60770000	1.04120000	4.65200000
C	-5.81210000	-0.59550000	-1.70810000
F	-6.69760000	1.27520000	-0.45820000
F	-4.86940000	-2.46690000	-2.92060000
F	-1.36570000	-0.34500000	6.07920000
F	-7.05430000	-0.82390000	-2.28240000
C	3.11440000	-3.88770000	-3.50600000
H	4.12630000	-3.47920000	-3.38630000
H	3.22350000	-4.92480000	-3.86800000
H	2.61320000	-3.31780000	-4.29870000
C	4.37350000	-4.06430000	-0.54750000
H	4.72350000	-5.10970000	-0.60400000
H	4.98610000	-3.47980000	-1.24760000
H	4.58980000	-3.70090000	0.46520000
C	-0.06430000	-4.06260000	-3.26630000
H	0.24290000	-3.40360000	-4.09010000
H	-0.10200000	-5.08860000	-3.67340000
H	-1.08500000	-3.78780000	-2.98100000
C	-0.78850000	-4.56320000	-0.15230000
H	-1.61020000	-4.12820000	-0.73020000
H	-0.91370000	-5.65990000	-0.17690000
H	-0.91020000	-4.25360000	0.89510000
C	1.93410000	-4.51130000	1.52220000
H	1.92470000	-5.60500000	1.67220000
H	2.87050000	-4.13340000	1.95040000
H	1.10300000	-4.10240000	2.11500000
H	2.52030000	-1.52220000	2.95060000

H	5.87130000	0.99960000	4.04340000
C	4.99000000	0.54320000	-0.56580000
H	6.01760000	0.20710000	-0.78300000
H	4.33130000	-0.04280000	-1.21550000
C	4.87400000	2.02440000	-0.95910000
C	5.86540000	2.61980000	-1.77810000
C	3.76110000	2.81330000	-0.57030000
C	5.74920000	3.96140000	-2.20410000
H	6.73490000	2.03350000	-2.08770000
C	3.64170000	4.15400000	-0.99260000
H	2.98990000	2.38900000	0.07620000
C	4.63420000	4.73400000	-1.81390000
H	6.52620000	4.40000000	-2.83480000
H	2.77840000	4.74570000	-0.67900000
H	4.54010000	5.77180000	-2.14090000

Frequencies --	-7.3308	5.5728	9.2807
Frequencies --	15.8037	22.1215	26.4840
Frequencies --	26.7825	29.0558	33.5310
Frequencies --	33.9328	38.1066	41.7259
Frequencies --	44.3653	47.8740	61.5354
Frequencies --	62.6858	72.1915	73.8890
Frequencies --	97.4238	102.1890	107.1549
Frequencies --	111.3338	112.3797	114.7735
Frequencies --	118.6618	121.3572	122.2724
Frequencies --	125.3354	126.8212	136.0167
Frequencies --	136.5646	137.4250	142.9637
Frequencies --	147.5597	148.7003	155.4796
Frequencies --	158.6471	162.1451	168.0272
Frequencies --	170.0743	174.2988	182.0008
Frequencies --	195.4236	201.2983	213.5020
Frequencies --	213.8513	217.9888	222.1925
Frequencies --	233.7593	235.8834	257.0101
Frequencies --	263.9608	264.8297	265.0901
Frequencies --	269.0542	272.0445	273.4815
Frequencies --	274.4603	284.5187	286.4523
Frequencies --	289.2958	292.3791	299.0500
Frequencies --	300.4506	301.1756	301.4780
Frequencies --	308.5645	318.6171	325.5936
Frequencies --	330.6799	335.0584	338.4020
Frequencies --	346.1388	351.9101	367.8682
Frequencies --	378.7394	379.0770	379.7791
Frequencies --	380.4550	393.6696	401.6660
Frequencies --	407.3705	416.3244	430.8570
Frequencies --	431.9091	433.7388	446.9334
Frequencies --	453.7860	457.3333	457.7818
Frequencies --	467.4754	474.4573	478.7880
Frequencies --	510.8277	527.9000	530.7769
Frequencies --	535.7376	540.2062	543.4872
Frequencies --	548.7137	553.7420	567.2008
Frequencies --	575.4970	582.4083	586.7953
Frequencies --	600.8537	603.1256	610.3487
Frequencies --	615.1290	623.0115	632.9920
Frequencies --	636.1074	636.7510	640.7280
Frequencies --	648.1502	649.6952	665.4190
Frequencies --	682.2808	701.4404	709.0972
Frequencies --	716.3339	726.8655	731.0254
Frequencies --	741.1299	743.5618	750.1233
Frequencies --	763.9005	769.0692	770.3859
Frequencies --	799.3292	804.3182	813.2996
Frequencies --	820.2470	840.2266	850.3905

Frequencies --	861.8326	876.6624	880.1797
Frequencies --	900.5932	912.2649	912.4558
Frequencies --	915.0991	940.5815	956.3660
Frequencies --	967.7187	967.9143	970.0424
Frequencies --	988.8685	999.5117	1002.6400
Frequencies --	1008.0623	1018.8055	1020.4021
Frequencies --	1028.2827	1041.2762	1042.5793
Frequencies --	1044.8082	1046.5239	1047.0501
Frequencies --	1048.2935	1048.8440	1051.9542
Frequencies --	1052.8676	1054.7808	1066.4172
Frequencies --	1087.5143	1088.2634	1089.0769
Frequencies --	1091.4310	1113.1976	1125.8417
Frequencies --	1157.0131	1170.3385	1175.4217
Frequencies --	1182.8995	1184.2396	1193.0433
Frequencies --	1196.6395	1203.8989	1212.2741
Frequencies --	1212.9641	1214.1729	1214.8528
Frequencies --	1217.6577	1231.4303	1298.0816
Frequencies --	1313.0038	1320.5114	1320.9004
Frequencies --	1325.2143	1338.8883	1344.8550
Frequencies --	1352.0806	1358.9492	1375.2778
Frequencies --	1379.6292	1408.5938	1412.4555
Frequencies --	1414.7836	1419.8024	1423.3129
Frequencies --	1424.3265	1425.8190	1428.6144
Frequencies --	1430.0213	1432.4304	1435.1035
Frequencies --	1443.2678	1445.5896	1447.2891
Frequencies --	1454.0104	1456.5870	1458.3587
Frequencies --	1460.8308	1467.2103	1467.7725
Frequencies --	1471.2284	1479.0456	1480.3810
Frequencies --	1487.7123	1490.5553	1493.3705
Frequencies --	1494.4862	1497.5740	1499.6275
Frequencies --	1504.2187	1505.4844	1506.7140
Frequencies --	1511.1511	1514.1033	1517.0330
Frequencies --	1586.1185	1594.4768	1596.6864
Frequencies --	1599.0448	1604.1749	1615.6027
Frequencies --	1617.9779	1619.7224	1623.1509
Frequencies --	1626.1585	2988.2830	2993.8695
Frequencies --	3009.6345	3011.3417	3011.8861
Frequencies --	3013.6965	3014.4159	3036.6343
Frequencies --	3095.0879	3101.8274	3103.3803
Frequencies --	3104.8823	3106.3652	3110.9857
Frequencies --	3123.8106	3135.6373	3139.6380
Frequencies --	3142.4285	3145.3159	3146.5078
Frequencies --	3147.6353	3151.4547	3157.6791
Frequencies --	3167.2320	3167.5336	3168.1251
Frequencies --	3173.1115	3177.8784	3178.5532
Frequencies --	3193.8840	3194.6076	3210.1250