

Is the reaction sequence in phosphine-catalyzed [8+2] cycloaddition controlled by the electrophilicity?

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S1. Computational Details

All theoretical calculations in this study were performed in the Gaussian16 program package.¹

All structures were optimized using M06-2X,² in conjunction with the 6-31G(d,p) basis set. The self-consistent reaction field (SCRF) polarizable continuum model (PCM)³ was applied to simulate the solvent effect and toluene was employed as solvent. All the optimized stationary points had been identified as minima (zero imaginary frequencies) and transition states (one imaginary frequency), *via* the vibrational analysis. The solution-translational entropy correction has been calculated with THERMO program.⁴ The entropy model has been successfully applied to typical cyclization reactions to predict activated entropy in solution. Furthermore, the single point energy at M06-2X/def2-TZVP⁵+PCM level has been also computed.

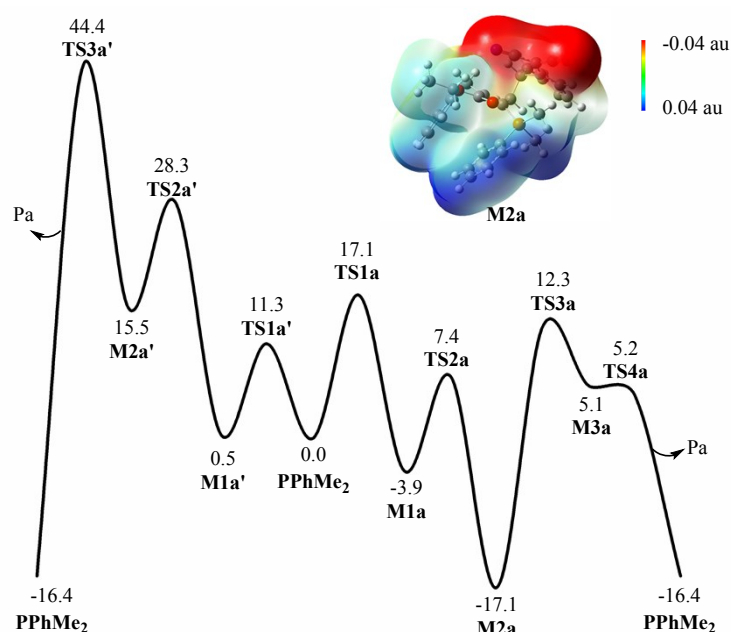
1. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. *Gaussian16*, Gaussian, Inc., Wallingford, CT, **2016**.
2. Zhao, Y.; and Truhlar, D.G. "The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals," *Theor. Chem. Acc.*, 120 (2008) 215-41. DOI: 10.1007/s00214-007-0310-x
3. Scalmani, G.; Frisch, M. J. Continuous Surface Charge Polarizable Continuum Models of Solvation. I. General formalism, *J. Chem. Phys.* **2010**, 132, 114110-24.
4. Fang, D.-C. THERMO; Beijing Normal University, Beijing, People's Republic of China, 2013.
5. Weigend F.; Ahlrichs, R. "Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy," *Phys. Chem. Chem.*

Phys., 2005, 7, 3297-305.

S2. The electrophilicity of some structures in the calculation at M062X/6-31G(d, p) level.

Species	R1	R2	R2a	R2c	R2b	R2d	M1
E ^H	-0.289	-0.268	-0.269	-0.235	-0.237	-0.275	-0.194
E ^L	0.003	-0.059	-0.066	-0.024	-0.041	-0.034	0.010
ω	0.947	1.739	1.886	1.085	1.341	1.349	0.562

S3. The calculation of phosphine catalyzed reaction of R2a and R1.



Scheme S1. The energy profile for the phosphine-catalyzed cycloaddition of R1 and R2a; the ESP map of M2a.

For the phosphine-catalyzed reaction between R1 and R2a, the rate-determined step would be the ring closure step, which the free energy barrier was calculated to be 30.4 kcal/mol. The ESP map clearly shows the cyano group could stabilize the intermediate M2a, leading to the free energy of stepwise cycloaddition increasing.

S4. The energy and free energy for the calculations of R1 and R2.

Species	E(au)	G(au)	E(au)	G(au)
	M062X/6-31G(d,p)	M062X/6-31G(d,p)	M062X/def2tzvp	
R1	-653.95415	-653.74687	-654.19176	-653.98448
R2	-837.46751	-837.26456	-837.77746	-837.57451
PPhMe₂	-652.65392	-652.51064	-652.79169	-652.64841
TS1	-1306.60006	-1306.23356	-1306.97215	-1306.60565
TS1-a	-1306.59367	-1306.22857	-1306.967274	-1306.602174
TS1-b	-1306.594	-1306.22776	-1306.968711	-1306.602471
M1	-1306.63048	-1306.26148	-1307.00811	-1306.63911

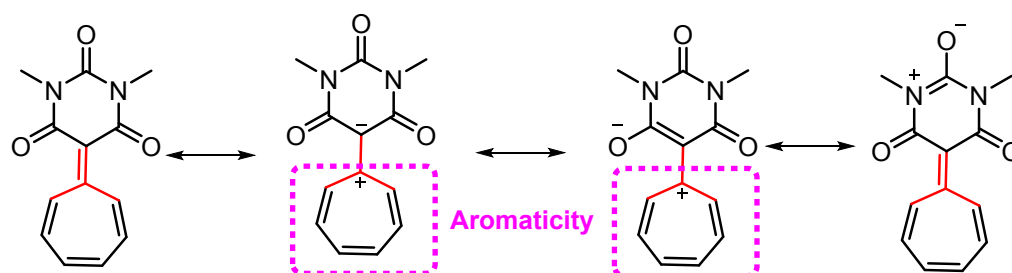
M1-a	-1306.62342	-1306.25366	-1307.001181	-1306.631421
M1-b	-1306.61226	-1306.24432	-1306.99226	-1306.62432
TS2	-2144.10765	-2143.51598	-2144.7855	-2144.19383
M2	-2144.13936	-2143.54249	-2144.81647	-2144.2196
TS3	-2144.12138	-2143.52293	-2144.79457	-2144.19612
M3	-2144.13115	-2143.53887	-2144.80102	-2144.20874
TS4	-2144.13115	-2143.53416	-2144.80097	-2144.20398
P	-1491.50578	-1491.07041	-1492.04289	-1491.60752
TS1'	-1490.11896	-1489.76045	-1490.56494	-1490.20643
TS1'-a	-1490.11996	-1489.75845	-1490.56581	-1490.20430
M1'	-1490.14639	-1489.78248	-1490.59725	-1490.23334
M1'-a	-1490.14243	-1489.77832	-1490.593712	-1490.229602
TS2'	-2144.08316	-2143.49204	-2144.76099	-2144.16987
M2'	-2144.09432	-2143.50028	-2144.77167	-2144.17763
TS3'	-2144.05693	-2143.46640	-2144.7316	-2144.14107
TS3''	-2144.02552	-2143.43431	-2144.704413	-2144.113203

S5. The energy and free energy for the calculations of different R2s.

Species	E(au) M062X/6-31G(d,p)	G(au) M062X/6-31G(d,p)	E(au) M062X/def2tzvp	G(au)
R2a	-493.9028	-493.79588	-494.0799	-493.97298
TS2a	-1800.53561	-1800.04408	-1801.085581	-1800.594051
M2a	-1800.58499	-1800.08689	-1801.13238	-1800.63428
TS3a	-1800.54385	-1800.04689	-1801.09733	-1800.58634
M3a	-1800.55128	-1800.05262	-1801.094422	-1800.59576
TS4a	-1800.55359	-1800.05619	-1801.09498	-1800.59758
M3a	-1800.54486	-1800.04473	-1801.087920	-1800.58779
Pa	-1147.91546	-1147.57902	-1148.320073	-1147.983633
TS1a'	-1146.55105	-1146.28827	-1146.86619	-1146.60341
M1a'	-1146.56748	-1146.30138	-1146.886727	-1146.620627
TS2a'	-1800.50179	-1800.01135	-1801.05126	-1800.56082
M2a'	-1800.5285	-1800.03319	-1801.07653	-1800.58122
TS3a'	-1800.4805	-1799.99060	-1801.02498	-1800.53508
R2b	-388.05789	-387.89290	-388.189257	-388.024267
TS2b	-1694.67095	-1694.11904	-1695.173974	-1694.622064
M2b	-1694.67812	-1694.12521	-1695.18135	-1694.62844
TS1b'	-1040.68758	-1040.36452	-1040.95829	-1040.63523
M1b'	-1040.69217	-1040.36797	-1040.96592	-1040.64172
TS2b'	-1694.63868	-1694.09074	-1695.17397	-1694.62603
M2b'	-1694.67843	-1694.1246	-1695.18135	-1694.62752
TS3b'	-1694.64748	-1694.09794	-1695.146019	-1694.596479
R2c	-309.46368	-309.3501	-309.57126	-309.45768
TS2c	-1616.0802	-1615.58176	-1616.56005	-1616.06161

M2c	-1616.11777	-1615.61454	-1616.59678	-1616.09355
TS1c'	-962.09233	-961.82295	-962.34007	-962.07069
M1c'	-962.09786	-961.82742	-962.34907	-962.07863
TS2c'	-1616.04297	-1615.55023	-1616.52705	-1616.03431
M2c'	-1616.11777	-1615.61454	-1616.59651	-1616.09328
TS3c'	-1616.08345	-1615.58292	-1616.55829	-1616.05776
R2d	-983.33141	-983.21512	-983.74521	-983.62892
TS2d	-2289.96106	-2289.45814	-2290.74308	-2290.24016
M2d	-2289.99738	-2289.49042	-2290.779	-2290.27204
TS1d'	-1635.97361	-1635.7008	-1636.523	-1636.25019
M1d'	-1635.98868	-1635.71373	-1636.54368	-1636.26873
TS2d'	-2289.93399	-2289.43345	-2290.71305	-2290.21251
M2d'	-2289.9567	-2289.45115	-2290.73158	-2290.22603
TS3d'	-2289.92235	-2289.42009	-2290.694789	-2290.192529

S6. The possible resonance structures of R2

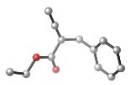
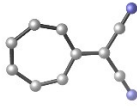
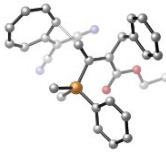
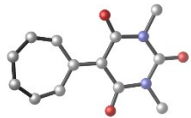


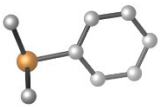
Scheme S6. The possible resonance structures of R2

S7. The energy and free energy for the calculations of R2 and methanol.

Species	E(au) M062X/6- 31G(d,p)	G(au) M062X/6- 31G(d,p)	E(au) M062X/def2tzvp	G(au)
MeOH	-115.66575	-115.62825	-115.71761	-115.68010
R1-sol	-953.14742	-952.8928	-953.50506	-953.25044
R1-sol-1	-953.14685	-952.89408	-953.50438	-953.25161
R1-2sol	-1068.82587	-1068.52488	-1069.231716	-1068.930726
R1-2sol-1	-1068.82803	-1068.52322	-1069.233707	-1068.928897
R1-3sol	-1184.50787	-1184.15216	-1184.961523	-1184.605813
M1'-sol	-1605.82755	-1605.41428	-1606.325877	-1605.91261
M1'-sol-1	-1605.83103	-1605.41791	-1606.329015	-1605.91589
M1'-sol-2	-1605.83081	-1605.41771	-1606.328772	-1605.91567
M1'-2sol	-1721.51728	-1721.05323	-1722.061912	-1721.59786
M1'-2sol-1	-1721.5152	-1721.05049	-1722.06054	-1721.59586
M1'-2sol-2	-1721.51922	-1721.05529	-1722.063982	-1721.600052
M1'-3sol	-1837.20177	-1836.68891	-1837.796671	-1837.283811

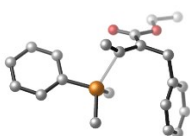
S8. The Coordination.

R1		R2a
		
C -1.50945 3.17196 0.46145		C -3.02142 0.67880 0.00015
C -1.05444 2.08070 -0.08383		C -3.02142 -0.67885 -0.00005
H -1.27023 3.42389 1.49040		C -1.88464 -1.55081 -0.00012
H -2.14897 3.85070 -0.09513		C -1.88463 1.55075 0.00016
C -0.57682 0.99739 -0.65171		C -0.55487 -1.27193 -0.00006
C 0.75510 0.95580 -1.37614		C -0.55487 1.27184 0.00002
H 0.61624 0.41657 -2.31748		C 0.13217 -0.00004 -0.00017
H 1.06021 1.97906 -1.60803		H -3.98793 -1.17420 -0.00019
C 1.82061 0.27152 -0.54437		H -2.12790 -2.61006 -0.00017
C 2.48816 0.98112 0.45732		H 0.10108 -2.13811 -0.00004
C 2.13264 -1.07420 -0.74207		H -2.12786 2.61001 0.00025
C 3.45642 0.36144 1.24065		H -3.98793 1.17416 0.00020
H 2.24410 2.02856 0.62024		H 0.10113 2.13800 0.00003
C 3.10103 -1.69725 0.04153		C 1.52327 -0.00002 -0.00020
H 1.60123 -1.63183 -1.50705		C 2.27839 -1.21077 -0.00001
C 3.76627 -0.98150 1.03330		N 2.87789 -2.20366 0.00031
H 3.97154 0.92576 2.01185		C 2.27828 1.21081 -0.00008
H 3.33594 -2.74405 -0.12434		N 2.87751 2.20386 -0.00003
H 4.52317 -1.46609 1.64189		TS2a
C -1.33124 -0.28795 -0.60273		
O -0.99367 -1.27363 -1.22106		C 0.97516 1.42899 -0.48422
O -2.41458 -0.23884 0.17914		C 0.23090 0.30204 -0.14244
C -3.17835 -1.45391 0.24954		H 0.73137 2.37552 -0.01762
C -4.32995 -1.20419 1.19697		H 1.51692 1.50087 -1.41606
H -2.52511 -2.25963 0.59684		C -0.66900 0.22849 0.92825
H -3.52095 -1.71371 -0.75657		C -0.98868 1.47578 1.70905
H -4.94397 -2.10399 1.27799		H -1.48092 1.18976 2.64131
H -3.96022 -0.94422 2.19120		H -0.06181 1.98798 1.99863
H -4.95680 -0.38669 0.83403		C -1.87852 2.43458 0.93738
R2		C -1.54899 3.78139 0.78450
		C -3.06471 1.96785 0.35911
C -4.42002 0.67975 0.40115		C -2.37661 4.64548 0.06772
C -4.41991 -0.68037 0.40033		

C	-3.39754	-1.51454	-0.14367	H	-0.63287	4.15792	1.23473
C	-3.39782	1.51478	-0.14183	C	-3.89465	2.82579	-0.35493
C	-2.09711	-1.23670	-0.43757	H	-3.32777	0.91901	0.47588
C	-2.09732	1.23765	-0.43612	C	-3.55135	4.16977	-0.50584
C	-1.35881	0.00044	-0.24874	H	-2.10044	5.68961	-0.04314
H	-5.30899	-1.18693	0.76533	H	-4.81543	2.44818	-0.79011
H	-3.69198	-2.54747	-0.31381	H	-4.19735	4.83959	-1.06437
H	-1.51342	-2.06771	-0.80920	C	-1.26207	-1.02796	1.27246
H	-3.69248	2.54788	-0.31058	O	-0.99198	-2.10748	0.73211
H	-5.30919	1.18571	0.76679	O	-2.19322	-0.96052	2.24888
H	-1.51379	2.06927	-0.80661	C	-2.76209	-2.21020	2.64964
C	0.02891	0.00032	-0.09085	C	-3.75386	-1.91449	3.75360
C	0.77860	-1.25842	0.04146	H	-1.96147	-2.87513	2.98757
C	0.77911	1.25877	0.04114	H	-3.23973	-2.68026	1.78450
C	2.91048	-0.00033	-0.00470	H	-4.21917	-2.84149	4.09668
O	4.12662	-0.00058	-0.01861	H	-3.25261	-1.44179	4.60097
O	0.28182	-2.36967	0.16858	H	-4.53791	-1.24310	3.39578
O	0.28292	2.37036	0.16763	P	0.33499	-1.08628	-1.31974
N	2.17305	1.17358	0.01338	C	1.26391	-2.58471	-0.90442
N	2.17254	-1.17398	0.01347	H	2.32641	-2.33320	-0.93385
C	2.90015	2.44060	0.08783	H	0.97924	-2.96145	0.07340
H	3.95514	2.22960	-0.05685	H	1.06920	-3.33365	-1.67693
H	2.52913	3.11196	-0.68626	C	1.23696	-0.49751	-2.79130
H	2.73453	2.90794	1.06027	H	2.26812	-0.24396	-2.53047
C	2.89899	-2.44133	0.08860	H	1.24066	-1.31454	-3.51720
H	2.52756	-3.11294	-0.68509	H	0.73936	0.36795	-3.23032
H	3.95410	-2.23104	-0.05626	C	-1.33288	-1.40629	-1.94290
H	2.73311	-2.90803	1.06131	C	-1.79356	-2.69390	-2.21731
PPhMe ₂				C	-2.15217	-0.29734	-2.17297
				C	-3.07241	-2.86980	-2.73677
P	-1.65781	-0.22505	-0.57578	H	-1.17473	-3.55919	-2.00333
C	-2.12262	-1.24756	0.90417	C	-3.43308	-0.48268	-2.68525
H	-3.20894	-1.36822	0.92673	H	-1.80421	0.70456	-1.93148
H	-1.67487	-2.24037	0.81996	C	-3.89098	-1.76657	-2.97065
H	-1.78961	-0.78518	1.83744	H	-3.43423	-3.87085	-2.94561
C	-2.31533	1.40709	-0.00075	H	-4.07152	0.37847	-2.85351
H	-2.04376	2.19796	-0.70383	H	-4.89034	-1.90976	-3.36831
H	-3.40602	1.34040	0.02103	C	4.47802	2.67217	-0.93325
H	-1.95769	1.67149	0.99899	C	5.02858	1.65685	-1.69964
				C	4.96387	0.27906	-1.44029
				C	3.62505	2.55558	0.16656
				C	4.34173	-0.41663	-0.41949
				C	3.01968	1.42403	0.71373
				C	3.46239	0.04211	0.59768

C	0.14613	-0.03705	-0.23732
C	0.95182	-1.17944	-0.34159
C	0.75822	1.18085	0.07186
C	2.32256	-1.11176	-0.11986
H	0.50016	-2.13437	-0.60262
C	2.13472	1.25312	0.28223
H	0.16695	2.08781	0.15029
C	2.91975	0.10845	0.19236
H	2.92691	-2.01036	-0.19664
H	2.59207	2.20895	0.51911
H	3.99053	0.16542	0.35957

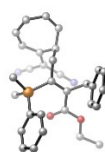
TS1



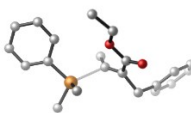
C	-1.12304	0.17179	2.72736
C	-0.23359	0.23078	1.75169
H	-0.94195	0.75155	3.62955
H	-2.03983	-0.40489	2.66924
C	1.00315	0.71527	1.40743
C	2.25544	-0.06189	1.77140
H	3.09832	0.63000	1.84657
H	2.11508	-0.52768	2.75191
C	2.55554	-1.13115	0.74267
C	1.96782	-2.39547	0.84623
C	3.35060	-0.85261	-0.37373
C	2.16238	-3.35676	-0.14481
H	1.35459	-2.62581	1.71542
C	3.54249	-1.80937	-1.36743
H	3.80409	0.13056	-0.46261
C	2.94492	-3.06413	-1.25930
H	1.70768	-4.33838	-0.04266
H	4.16110	-1.57550	-2.22860
H	3.09603	-3.81097	-2.03199
C	1.04886	1.81397	0.47570
O	0.08388	2.39789	-0.01231
O	2.31913	2.18267	0.15559
C	2.42916	3.28029	-0.75240
C	3.90441	3.51936	-0.99220
H	1.93953	4.15774	-0.31842
H	1.89981	3.03668	-1.67908
H	4.04238	4.36373	-1.67178

H	5.62830	1.95514	-2.55395
H	5.53750	-0.34409	-2.12276
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H	3.30041	3.49536	0.60635
H	4.72989	3.68796	-1.22700
H	2.41517	1.61261	1.59469
C	2.95314	-0.87985	1.53098
C	3.36920	-2.24038	1.52700
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M2a

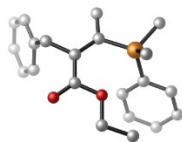


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C	0.31677	-1.12141	-1.48974	C	4.46358	0.52560	-1.62314
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H	2.12093	-1.40461	1.60638	H	4.41301	-1.34930	-0.60367
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C	5.39418	0.50002	-0.93225	N	4.03512	-3.31066	1.44055
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				N	1.05326	-0.56155	3.26873
				TS3a			

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H	2.13356	-3.48189	-1.84218
H	2.94243	-3.25159	-0.27531
C	1.74013	-0.78176	0.82977
C	0.52319	-0.96196	1.49077
C	2.85651	-0.30108	1.51375
C	0.42900	-0.65754	2.84652
H	-0.35191	-1.31632	0.95015
C	2.75554	-0.00911	2.86982
H	3.79292	-0.13226	0.99032
C	1.54288	-0.18594	3.53518
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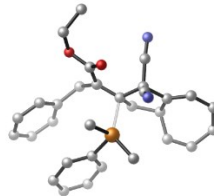
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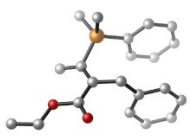
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H	-2.64020	0.51699	2.34617
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C	-3.28581	0.12786	0.35228
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H	-5.91946	0.49428	-1.77964
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C	-0.29449	-0.19234	1.92050
O	-0.82017	-0.93128	2.75570
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H	-4.55198	-2.39097	-1.53933
H	-3.56334	-0.27069	-1.84805
H	-3.89865	-0.56303	3.32388
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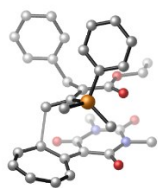
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C	-0.61829	0.19814	1.23991
C	-1.22504	1.41885	1.91085
H	-2.00511	1.04600	2.57958
H	-0.49612	1.92299	2.55698
C	-1.84714	2.45998	1.00232
C	-1.25266	3.70718	0.79815
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C	-1.79984	4.62568	-0.09892
H	-0.34898	3.96159	1.34815
C	-3.58663	3.08250	-0.57312
H	-3.51052	1.20749	0.50245
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H	-1.31888	5.58749	-0.24939
H	-4.50673	2.83958	-1.09671
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O	-0.79187	-2.14218	0.99067
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C	3.15687	-1.43915	1.95124	C	-3.28388	-2.23130	1.73507
H	1.18274	-2.32175	2.09631	C	-4.74369	-1.92733	1.99778
H	1.59549	-1.27594	3.45159	H	-2.85506	-2.86742	2.51698
H	3.67858	-2.21734	2.51446	H	-3.14255	-2.74417	0.77866
H	3.25526	-1.66054	0.88551	H	-5.31995	-2.85435	2.05189
H	3.64985	-0.48346	2.15521	H	-4.86383	-1.38818	2.94064
P	1.38382	1.60185	-0.30610	H	-5.15452	-1.31079	1.19301
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H	2.16020	3.30513	1.17323	H	2.19064	-1.47430	-2.25799
C	1.73934	2.80057	-1.62895	H	1.39371	-0.54616	-3.56026
H	1.28659	2.47877	-2.56712	C	-0.01718	1.68949	-1.94843
H	1.37153	3.79028	-1.35431	H	0.84875	2.35046	-2.01456
H	2.82384	2.84387	-1.75466	H	-0.47980	1.60159	-2.93400
C	2.03445	0.04467	-0.95862	H	-0.73837	2.11299	-1.24452
C	1.18685	-1.05655	-1.09980	C	-0.93125	-1.02652	-1.77828
C	3.37131	-0.03689	-1.35343	C	-0.75629	-2.35625	-2.17692
C	1.68816	-2.24283	-1.62485	C	-2.22016	-0.50426	-1.64566
H	0.15083	-0.98415	-0.77759	C	-1.86564	-3.15621	-2.41670
C	3.86726	-1.22899	-1.87424	H	0.23697	-2.78153	-2.27101
H	4.03883	0.81463	-1.24548	C	-3.32850	-1.31588	-1.87482
C	3.02603	-2.33114	-2.00686	H	-2.36647	0.53291	-1.36822
H	1.03350	-3.10153	-1.72901	C	-3.15226	-2.64203	-2.25616
H	4.90820	-1.29614	-2.17201	H	-1.72510	-4.18859	-2.71839
H	3.41372	-3.26131	-2.40940	H	-4.32662	-0.90451	-1.75953
M1-b				H	-4.01507	-3.27587	-2.43534
				C	4.80273	1.52306	-1.04378
C	-1.89428	1.43143	-1.47070	C	5.79824	0.66748	-0.42118
C	-1.19591	1.01487	-0.37451	C	5.55457	-0.46611	0.27680
H	-2.76175	0.88000	-1.80360	C	3.54716	1.71489	-0.60788
H	-1.64261	2.33275	-2.01282	C	4.25134	-1.04154	0.55732
C	-1.40020	-0.05348	0.56224	C	3.02174	1.17105	0.69665
C	-0.27413	-0.66196	1.36389	C	3.12042	-0.33693	0.70671
H	0.37469	0.08164	1.85026	H	6.83699	0.90966	-0.63142
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C	0.26813	-2.21859	-0.58192	H	2.88223	2.34997	-1.19152
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				C	1.74495	-0.96273	1.00700
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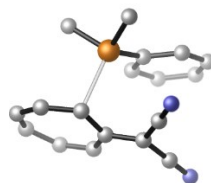
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H	2.22655	-1.44503	2.06879	C	0.01235	-0.52930	0.94055
C	2.38766	-3.37199	-0.72430	H	1.15887	-0.27214	2.71080
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H	3.75667	-2.99147	0.89569	C	-1.26223	-0.14193	0.82329
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H	-5.96253	0.83116	-0.70073	H	-1.43891	1.49404	-1.32737
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P	0.16910	2.13499	0.03566	H	0.32291	5.39145	1.17510
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H	-1.05022	3.31988	1.68625	H	0.45579	5.35032	-1.30373
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C	3.28914	-0.02107	-1.39248	C	4.72951	-0.13596	-0.83325
H	1.24427	0.37111	-1.94091	C	4.45858	-1.45477	-0.63456
C	4.28794	0.18726	-0.44327	C	2.63273	0.99112	-0.13650
H	4.81706	1.12659	1.42048	C	3.13708	-2.00562	-0.42555
H	3.47568	-0.65661	-2.25124	C	2.37766	-0.03302	0.93694
H	5.26030	-0.27700	-0.57308	C	2.16453	-1.33288	0.20888
TS2				H	5.74486	0.11754	-1.12930
				H	5.26672	-2.16497	-0.78759
				H	2.92605	-2.98432	-0.85390
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				H	3.97427	1.75840	-1.55614
				H	3.25841	-0.10805	1.58613



C	-0.39748	-1.91198	1.04582
C	0.10439	-0.96078	0.14644
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H	-0.58018	-2.92905	0.73405
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H	0.02040	0.33725	2.57373
C	2.09852	-0.22065	2.50105
C	2.00889	-1.00553	3.65060
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C	3.11377	-1.71613	4.11948
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C	4.42959	-0.86037	2.29427
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H	3.02453	-2.32420	5.01458
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H	2.56852	3.01115	-1.66113
H	2.58048	5.40490	-0.88948
H	1.50152	4.96740	0.45111
H	3.17367	4.34982	0.40815
P	0.18945	-1.51981	-1.59271
C	-0.96169	-0.89348	-2.83614
H	-0.80927	-1.47314	-3.75089
H	-1.97733	-1.05601	-2.46684
H	-0.81572	0.16887	-3.00319
C	-0.17665	-3.30585	-1.61475
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H	0.50886	-3.85473	-0.96844

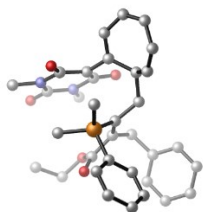
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C	0.20870	-1.94634	-1.14202
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C	0.50779	-2.96931	1.04178
N	0.44156	-3.91405	1.70310

TS1a'

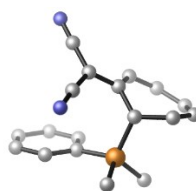


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C	-2.12976	-2.15031	-0.96867
C	-3.03201	0.32268	0.64837
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C	-1.69853	0.16226	1.09712
C	-0.85381	-1.02486	0.92011
H	-3.94797	-1.71422	-1.95704
H	-2.01979	-3.00024	-1.63918
H	-0.35385	-2.81462	-0.07565
H	-3.57523	1.12317	1.14407
H	-4.69772	0.07113	-0.59897
H	-1.49026	0.68904	2.02473
C	0.32661	-1.06695	1.68792
P	-0.31498	1.69412	-0.11638
C	0.32351	3.24687	0.61743
H	-0.53117	3.86809	0.89527
H	0.88432	3.00702	1.52354
H	0.95543	3.79151	-0.08884
C	-1.41049	2.21981	-1.48151
H	-1.77523	1.34154	-2.01907
H	-2.27891	2.72551	-1.04997
H	-0.89660	2.89289	-2.17092
C	1.09376	0.85071	-0.86944
C	2.38568	1.02882	-0.35261
C	0.87636	-0.12017	-1.85575
C	3.44014	0.26328	-0.83283
H	2.56510	1.75503	0.43449
C	1.93991	-0.88241	-2.33351
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C	2.27753	-0.98088	-3.38659	H	4.04529	-1.29571	-2.18899
C	4.23787	-1.75865	-1.55565	C	1.26610	-2.12496	1.54641
H	2.61596	-2.10944	-0.18572	N	2.02369	-2.99498	1.41139
C	3.62129	-0.94963	-3.74663	C	0.72394	0.02719	2.50023
H	1.52006	-0.64511	-4.08799	N	1.04149	0.95161	3.13288
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H	4.99741	-2.04879	-0.83677				
H	3.90520	-0.60909	-4.73665				
H	5.64660	-1.30363	-3.11585				
C	-3.56191	-3.87121	1.18127				
C	-4.04275	-3.81945	-0.13562				
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C	-2.98262	-2.85035	1.90158				
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C	-2.58650	-1.54726	1.50122				
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H	-4.42064	-4.74469	-0.56049				
H	-4.68812	-2.82236	-1.85572				
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H	-3.66640	-4.82376	1.69575				
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C	-2.73967	0.64302	0.34444				
C	-2.69397	1.34959	-0.92204				
C	-2.31385	1.35010	1.54250				
C	-1.49733	3.22756	0.15560				
O	-0.93427	4.31116	0.08253				
O	-3.14070	0.95623	-2.00280				
O	-2.48303	0.96449	2.70141				
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C	-1.15756	3.29897	2.53200				
H	-1.14827	2.60653	3.36866				
H	-0.15332	3.66017	2.30806				
H	-1.79508	4.15546	2.76527				
C	-1.85842	3.22051	-2.24808				
H	-2.79707	3.16470	-2.79597				
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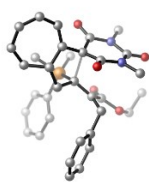


M1a'



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H	-0.06793	-1.16633	-2.25829
H	-0.72756	-2.29276	-1.10008
C	-0.87160	0.71902	-0.80005
C	-1.33504	0.89798	-2.23980
H	-1.36528	1.96421	-2.47028
H	-0.64488	0.43808	-2.94432
C	-2.72843	0.29930	-2.31657
C	-2.94301	-0.97297	-2.85238
C	-3.80851	0.97638	-1.73915
C	-4.20470	-1.56236	-2.79754
H	-2.11922	-1.50380	-3.32114
C	-5.06784	0.38849	-1.67957
H	-3.65926	1.97515	-1.33448
C	-5.26802	-0.88784	-2.20311
H	-4.35533	-2.54956	-3.22286
H	-5.89376	0.92706	-1.22583
H	-6.24976	-1.34822	-2.15750
C	-1.34739	1.80947	0.11528
O	-1.78757	1.63446	1.23293
O	-1.24884	3.01124	-0.45158
C	-1.64420	4.14668	0.34974
C	-0.57310	4.49419	1.36496
H	-2.60136	3.91817	0.82505
H	-1.78057	4.94525	-0.38001
H	-0.81166	5.45168	1.83497
H	-0.52459	3.73349	2.14760
H	0.40351	4.57298	0.87811
P	-0.07358	-0.61105	1.48513
C	0.57399	0.84066	2.38135
H	1.54434	0.55746	2.79657
H	0.71170	1.68132	1.70137
H	-0.13484	1.12316	3.16083
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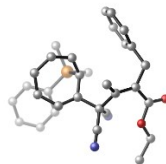
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C	2.84533	0.11579	0.92220
C	1.03174	1.68108	-1.04566
C	1.34612	0.16123	0.94980
C	0.68193	1.32369	0.23716
H	3.92698	0.26000	-2.31085
H	1.99325	1.42798	-2.91302
H	0.38394	2.41120	-1.52404
H	3.31958	-0.01412	1.89053
H	4.69524	0.02706	-0.02327
H	1.04710	0.20205	2.00120
C	-0.41789	1.90757	0.93721
P	0.55038	-1.44904	0.43225
C	0.31787	-2.40333	1.95141
H	1.30102	-2.56703	2.40040
H	-0.29807	-1.82275	2.64400
H	-0.15237	-3.36477	1.73647
C	1.61237	-2.41834	-0.66671
H	1.78883	-1.87087	-1.59327
H	2.57167	-2.58085	-0.17261
H	1.12268	-3.37299	-0.86944
C	-1.03980	-1.19534	-0.36733
C	-2.22782	-1.33026	0.35928
C	-1.07228	-0.80661	-1.71253
C	-3.44490	-1.08149	-0.26520
H	-2.21064	-1.59850	1.41008
C	-2.29473	-0.55853	-2.32547
H	-0.15118	-0.67864	-2.27371
C	-3.47795	-0.69657	-1.60294
H	-4.36621	-1.17888	0.29829
H	-2.32234	-0.25138	-3.36515
H	-4.43002	-0.49731	-2.08370
C	-0.97660	1.24834	2.05381
N	-1.37923	0.62131	2.95325
C	-1.08034	3.04952	0.42534



C	-0.39713	-1.54293	0.92534
C	-0.23819	-0.25805	0.07089
H	0.08888	-1.34764	1.87929
H	0.18986	-2.34788	0.46587
C	0.75406	0.67481	0.51287
C	1.14802	0.80606	1.97845
H	1.40904	1.85138	2.16775
H	0.30788	0.57752	2.63765
C	2.32690	-0.06433	2.39136
C	2.20833	-0.97367	3.44482
C	3.55650	0.02224	1.72642
C	3.27772	-1.78638	3.81993
H	1.26321	-1.04586	3.97940
C	4.62687	-0.78512	2.09853
H	3.66841	0.73362	0.91297
C	4.49082	-1.69686	3.14552
H	3.15941	-2.48955	4.63857
H	5.57418	-0.69817	1.57406
H	5.32619	-2.32672	3.43427
C	1.38908	1.52623	-0.43222
O	1.30024	1.41715	-1.66616
O	2.17734	2.49003	0.11040
C	2.82780	3.37234	-0.81080
C	1.86870	4.42240	-1.34082
H	3.26042	2.78602	-1.62544
H	3.63171	3.82847	-0.22887
H	1.35729	4.92292	-0.51592
H	2.41351	5.16640	-1.92867
H	1.11819	3.95232	-1.97903
P	-0.14214	-0.70097	-1.75257
C	-0.59252	0.43168	-3.11623
H	-1.50225	0.07501	-3.59662
H	-0.71748	1.44049	-2.73791
H	0.25811	0.44467	-3.79911
C	-1.30204	-2.07283	-2.06344
H	-2.32557	-1.74116	-1.87291
H	-1.19752	-2.32839	-3.12173
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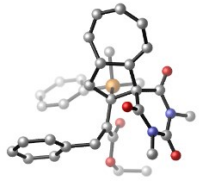
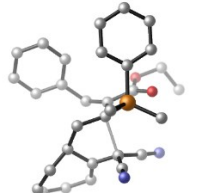
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C	-1.79356	-2.69390	-2.21731
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C	-3.07241	-2.86980	-2.73677
H	-1.17473	-3.55919	-2.00333
C	-3.43308	-0.48268	-2.68525
H	-1.80421	0.70456	-1.93148
C	-3.89098	-1.76657	-2.97065
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H	-4.07152	0.37847	-2.85351
H	-4.89034	-1.90976	-3.36831
C	4.47802	2.67217	-0.93325
C	5.02858	1.65685	-1.69964
C	4.96387	0.27906	-1.44029
C	3.62505	2.55558	0.16656
C	4.34173	-0.41663	-0.41949
C	3.01968	1.42403	0.71373
C	3.46239	0.04211	0.59768
H	5.62830	1.95514	-2.55395
H	5.53750	-0.34409	-2.12276
H	4.55170	-1.48335	-0.39684
H	3.30041	3.49536	0.60635
H	4.72989	3.68796	-1.22700
H	2.41517	1.61261	1.59469
C	2.95314	-0.87985	1.53098
C	3.36920	-2.24038	1.52700
N	3.71511	-3.34862	1.48025
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N	1.31109	-0.17412	3.39686

M2a'

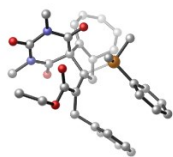


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C	-0.63427	1.97761	1.24232
C	-1.49583	-0.86564	1.95987
C	-0.56879	0.78799	0.31532
C	-0.50897	-0.48376	1.13086

C	1.47753	-1.46072	-2.09271	H	-3.67224	1.70223	2.71356
C	2.44221	-1.64925	-1.10115	H	-3.55150	-0.65071	2.58562
C	1.71873	-1.92264	-3.39102	H	-1.40747	-1.82899	2.45693
C	3.64268	-2.28160	-1.41299	H	0.20485	2.66507	1.18595
H	2.27335	-1.29151	-0.09171	H	-1.64169	3.10340	2.68359
C	2.92079	-2.55193	-3.69657	H	0.35598	0.86742	-0.27121
H	0.97599	-1.79265	-4.17418	C	0.79894	-1.27230	0.93751
C	3.88525	-2.73165	-2.70716	P	-1.88367	0.85589	-1.00878
H	4.38602	-2.41482	-0.63326	C	-1.08326	0.57422	-2.60707
H	3.10221	-2.90159	-4.70743	H	-0.27128	1.29641	-2.71934
H	4.82239	-3.22362	-2.94653	H	-0.67178	-0.43531	-2.65520
C	-3.22342	-4.11041	0.62260	H	-1.82470	0.71702	-3.39612
C	-4.56240	-3.59192	0.84963	C	-2.54730	2.53685	-1.07702
C	-4.94606	-2.30450	0.73738	H	-3.10087	2.77328	-0.16850
C	-2.06608	-3.44115	0.71109	H	-1.70034	3.22457	-1.15828
C	-4.12415	-1.15042	0.40812	H	-3.18948	2.62740	-1.95576
C	-1.85189	-2.01951	1.18524	C	-3.23583	-0.32692	-0.86065
C	-2.79799	-0.99998	0.56947	C	-2.97167	-1.68674	-1.05502
H	-5.33321	-4.33110	1.05323	C	-4.52762	0.10682	-0.54653
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H	-4.67120	-0.29037	0.02976	H	-1.97045	-2.02879	-1.30342
H	-1.15917	-3.99722	0.47441	C	-5.55397	-0.82220	-0.42456
H	-3.16657	-5.16185	0.34771	H	-4.73536	1.16002	-0.38460
H	-2.01664	-1.98718	2.27060	C	-5.29057	-2.17912	-0.60437
C	-2.12253	0.31106	0.33751	H	-3.80066	-3.66512	-1.06248
C	-2.52910	1.11825	-0.81649	H	-6.55728	-0.48760	-0.18436
C	-1.95179	1.04402	1.61181	H	-6.09191	-2.90313	-0.50046
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O	-1.15012	4.22484	0.24962	C	2.01147	-0.30873	1.20266
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H	-0.22233	3.60802	2.51914	H	4.43190	1.11019	-0.73106
H	-1.93099	3.89630	2.90493	C	2.79962	2.38098	-0.19706
H	-1.12591	2.42652	3.52278	C	2.03354	2.40599	-1.36995
C	-2.26973	3.28768	-1.98202	C	2.69996	3.46593	0.67666
H	-2.74656	2.68234	-2.74875	C	1.19323	3.47922	-1.65613
H	-2.90518	4.13428	-1.71740	H	2.11885	1.56321	-2.05500
H	-1.30962	3.67175	-2.33187	C	1.85824	4.54473	0.39793
M3				H	3.29658	3.46593	1.58558
				C	1.09618	4.55320	-0.76673
				H	0.63420	3.50141	-2.58958

	H	1.79760	5.37642	1.09341			
	H	0.44879	5.39498	-0.99327			
	C	3.51526	-1.18860	-0.59620			
	O	4.29437	-1.13281	-1.54737			
	O	3.08259	-2.42849	-0.13792			
	C	3.30920	-3.51575	-1.02738			
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	H	4.38527	-3.63567	-1.18423			
	H	2.85613	-3.29086	-2.00084			
	H	2.88840	-5.62863	-1.01364			
	H	3.09959	-4.91353	0.59933			
	H	1.60511	-4.62829	-0.30571			
	C	0.70334	-1.75969	-0.45922			
	N	0.42094	-2.10931	-1.52663			
	C	0.86247	-2.44647	1.82345			
	N	0.88041	-3.36058	2.52990			
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C	-0.32117	-1.62169	0.80755	C	1.64325	-3.72344	0.58345
C	-0.36926	-0.24671	0.06645	C	2.51338	-3.14272	1.58874
H	0.12406	-1.44357	1.78692	C	2.43326	-1.91449	2.15154
H	0.34914	-2.32205	0.30021	C	0.86444	-3.05572	-0.29333
C	0.61390	0.74976	0.61330	C	1.43443	-0.88695	1.91400
C	0.99373	0.87139	2.07672	C	0.69843	-1.61212	-0.37399
H	1.25022	1.92182	2.25867	C	0.68413	-0.74420	0.80798
H	0.15040	0.64167	2.73430	H	3.29225	-3.80212	1.96572
C	2.17135	0.01580	2.52425	H	3.15464	-1.67983	2.93019
C	2.02760	-0.92176	3.54919	H	1.31479	-0.15175	2.70532
C	3.42883	0.15624	1.92394	H	0.31431	-3.62605	-1.03673
C	3.10071	-1.71317	3.95796	H	1.67829	-4.80561	0.49397
H	1.05862	-1.03529	4.03159	H	0.26478	-1.21477	-1.28372
C	4.50303	-0.62902	2.33096	C	-0.33334	0.40077	0.63909
H	3.55409	0.88963	1.13202	P	2.97845	-1.02091	-1.26971
C	4.34246	-1.57098	3.34759	C	2.74346	-0.28829	-2.93724
H	2.96326	-2.44065	4.75199	H	2.20445	-1.01267	-3.55372
H	5.47239	-0.50186	1.85736	H	2.14100	0.61937	-2.86471
H	5.18110	-2.18393	3.66231	H	3.70470	-0.06127	-3.40577
C	1.22914	1.52120	-0.33045	C	3.96668	-2.52484	-1.64309
O	1.03093	1.34021	-1.58904				
O	2.11234	2.47540	0.06047				
C	2.66046	3.30595	-0.96701				
C	1.64058	4.30666	-1.48064				
H	3.04049	2.67965	-1.77842				
H	3.49963	3.81187	-0.48470				
H	2.11850	5.02397	-2.15356				
H	0.85546	3.78140	-2.02837				
H	1.18666	4.84939	-0.64809				
P	0.03717	-0.48452	-1.81213				
C	-0.54673	0.46055	-3.28194				
H	-1.39748	-0.03166	-3.74800				
H	-0.78724	1.48182	-3.00247				
H	0.30880	0.50527	-3.96100				
C	-0.93056	-2.02294	-2.20348				
H	-2.00089	-1.85163	-2.05954				
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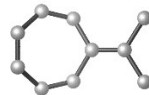
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C	2.06720	-1.60442	-3.34513	H	4.86285	-2.27062	-2.21473
C	3.84213	-1.96992	-1.23713	C	4.14667	0.10083	-0.43357
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C	3.31480	-2.17650	-3.57623	C	5.01714	-0.39906	0.54402
H	1.38183	-1.47940	-4.17913	C	5.01144	2.32407	-0.02554
C	4.20615	-2.36058	-2.52223	H	3.46180	1.88553	-1.44267
H	4.52277	-2.10972	-0.40258	C	5.88474	0.45304	1.21704
H	3.58666	-2.48099	-4.58168	H	5.01506	-1.45908	0.78295
H	5.17712	-2.81059	-2.70231	C	5.88361	1.81800	0.93383
C	-3.04523	-4.26685	0.23260	H	5.00205	3.38621	-0.24732
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C	-4.80302	-2.49921	0.48428	H	6.55809	2.48359	1.46257
C	-1.89757	-3.59218	0.38234	C	0.32794	1.31257	-0.32665
C	-4.00210	-1.31397	0.21554	N	0.94795	1.92405	-1.08851
C	-1.74116	-2.21391	0.98338	C	-0.58176	1.10233	1.90860
C	-2.68104	-1.17938	0.39768	N	-0.74928	1.60111	2.93696
H	-5.14673	-4.54721	0.66724	C	-1.70920	-1.60027	0.29981
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O	-1.39835	4.13377	0.52868	C	-5.04645	-0.03663	0.58092
O	-3.00472	0.60914	-1.83959	C	-6.60220	-2.21249	-0.17705
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N	-1.83420	2.19505	1.63263	C	-6.12479	-0.43187	1.36797
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H	-1.76842	2.17636	3.69848	H	-7.74760	-1.82902	1.60709
C	-2.33658	3.29772	-1.83472	C	-2.47435	1.91268	-1.00248
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C	0.90932	-1.78961	-1.66696
H	0.74212	-2.86878	-1.67770
H	0.49254	-1.41646	-2.61381
C	2.40758	-1.56455	-1.69211
C	3.01310	-0.85748	-2.73217
C	3.22414	-2.13783	-0.71385
C	4.39929	-0.72399	-2.79925
H	2.38880	-0.41413	-3.50504
C	4.60756	-2.02441	-0.78556
H	2.75733	-2.68748	0.10101
C	5.20141	-1.31341	-1.82816
H	4.85059	-0.16965	-3.61680
H	5.22723	-2.48696	-0.02332
H	6.28204	-1.22108	-1.87988
C	-0.68454	-2.11198	0.29664
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O	-0.48025	-3.44030	0.05974
C	-1.29246	-4.35200	0.80078
C	-2.66774	-4.50066	0.17533
H	-1.37115	-4.01105	1.83591
H	-0.74374	-5.29646	0.77380
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H	-3.22850	-3.56702	0.25765
H	-2.57556	-4.77311	-0.87987
P	0.80806	0.82012	1.58696
C	0.32565	-0.29305	2.95815
H	0.99300	-0.10852	3.80402
H	-0.70472	-0.08391	3.23278
H	0.39450	-1.33224	2.63784
C	0.74002	2.49983	2.35181
H	-0.26003	2.90468	2.19878
H	0.95506	2.41608	3.42093
H	1.47798	3.15533	1.88909
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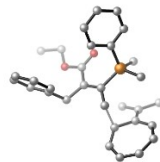
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R2b



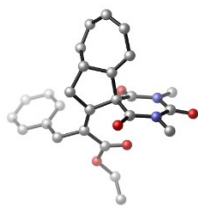
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C	0.26635	1.24885	-0.56872
C	0.26636	-1.24884	-0.56871
C	-0.47317	0.00000	-0.28184
H	3.28651	1.17792	1.00323
H	1.90351	2.52742	-0.45078
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H	-0.27221	-2.01295	-1.12611
C	-1.77422	-0.00000	0.07502
C	-2.56268	-1.26303	0.29308
H	-1.94370	-2.16055	0.27992
H	-3.07506	-1.22393	1.26092
H	-3.34403	-1.37008	-0.46987
C	-2.56269	1.26302	0.29311
H	-3.07480	1.22404	1.26110
H	-1.94377	2.16057	0.27963
H	-3.34427	1.36989	-0.46963

TS2b



C	-1.30111	-0.81388	-1.02011
C	-0.42375	-0.10841	-0.16092
H	-0.91406	-1.71897	-1.47190
H	-1.98110	-0.27768	-1.67069
C	0.59975	-0.71046	0.58139
C	0.96205	-2.16947	0.40332
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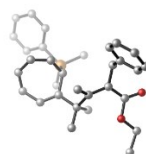
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C	4.82463	1.22286	0.75424	C	2.19727	-1.92953	-1.79562
H	3.01246	2.18875	0.17356	C	3.37326	-2.88251	0.06932
C	4.60700	-0.65522	2.24051	C	3.33685	-2.05697	-2.58418
H	2.62036	-1.21027	2.79104	H	1.29217	-1.49682	-2.21725
C	5.41187	0.21417	1.51293	C	4.51696	-3.01263	-0.71653
H	5.44154	1.89834	0.17076	H	3.38913	-3.18958	1.11165
H	5.05465	-1.45211	2.82628	C	4.50256	-2.60086	-2.04612
H	6.49129	0.10120	1.52722	H	3.31478	-1.73468	-3.62081
C	0.02752	4.80926	-0.66702	H	5.42110	-3.43380	-0.28729
C	-1.30889	5.22960	-1.04735	H	5.39220	-2.70138	-2.65952
C	-2.42414	4.46327	-1.00798	C	1.42918	0.07615	1.45689
C	0.51945	3.56425	-0.77266	O	1.32220	1.28946	1.65386
C	-2.49648	3.07429	-0.59619	O	2.39011	-0.64538	2.07364
C	-0.20343	2.42682	-1.44612	C	3.29550	0.09144	2.89895
C	-1.50848	2.17528	-0.72939	C	4.38346	-0.86969	3.32722
H	-1.43483	6.28422	-1.28043	H	2.75053	0.50185	3.75539
H	-3.37557	4.94932	-1.21027	H	3.69542	0.93379	2.32752
H	-3.43912	2.75344	-0.15297	H	5.10650	-0.35928	3.96763
H	1.52253	3.37178	-0.40017	H	3.95843	-1.70897	3.88311
H	0.67560	5.58270	-0.26006	H	4.90636	-1.26239	2.45172
H	-0.42067	2.71379	-2.48444	P	-0.70580	1.68046	-0.04265
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C	-2.37355	0.63392	1.00599	H	-2.13502	2.84376	1.51454
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C	-3.97989	-0.94525	0.06617	H	-0.39189	3.20156	1.79208
O	-4.89697	-1.71197	0.26987	C	-2.09904	2.12191	-1.12317
O	-1.98693	1.22948	1.99330	H	-3.00843	1.59706	-0.81763
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N	-3.60840	0.01038	1.00873	C	0.68317	2.57637	-0.79782
C	-3.72727	-1.82963	-2.21258	C	0.65261	3.97291	-0.81783
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H	-4.18268	-1.25471	-3.02064	C	1.67073	4.68172	-1.44879
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H	-4.21354	0.91980	2.77450	H	1.76500	0.80605	-1.38632
H	-5.34967	-0.29339	2.10475	C	2.71600	3.99782	-2.06475
H	-3.85625	-0.81957	2.92520	H	1.64665	5.76627	-1.45805
P				H	3.56025	2.06853	-2.51938
				H	3.50916	4.55095	-2.55698
				C	-4.09288	-2.89743	-1.62934
				C	-4.94045	-1.89836	-2.05506



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C	0.31043	0.28394	-1.00975
H	0.40656	1.48008	-2.76116
H	1.60484	1.94673	-1.54186
C	1.20499	-0.70988	-0.92338
C	2.61238	-0.55019	-1.44246
H	3.02885	-1.53436	-1.67267
H	2.58249	0.00121	-2.38893
C	3.55848	0.16812	-0.48829
C	4.89514	0.32594	-0.86898
C	3.14429	0.68580	0.74034
C	5.79876	0.98816	-0.04647
H	5.22723	-0.07550	-1.82376
C	4.05211	1.35051	1.56615
H	2.11203	0.57240	1.06293
C	5.37829	1.50516	1.17854
H	6.83175	1.10138	-0.36074
H	3.71363	1.74450	2.51962
H	6.08135	2.02243	1.82359
C	0.83687	-1.97394	-0.23303
O	-0.30274	-2.32008	0.02665
O	1.90776	-2.70480	0.08200
C	1.65919	-3.94925	0.76310
C	1.24865	-5.03115	-0.21669
H	0.89097	-3.78517	1.52161
H	2.60664	-4.18308	1.25000
H	1.12969	-5.98094	0.31050
H	0.29860	-4.77603	-0.68969
H	2.01111	-5.15730	-0.98874
C	-0.74201	4.35084	0.60689
C	-2.12733	4.58724	0.25227
C	-3.03352	3.63819	-0.11090
C	0.03415	3.38876	0.07268
C	-2.75955	2.22046	-0.20363
C	-0.44946	2.58839	-1.10593
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H	-2.50826	5.59096	0.42705
H	-4.07328	3.94371	-0.19731

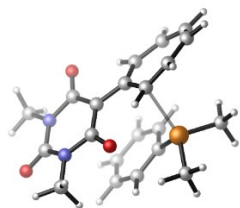
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C	-2.69308	-1.74529	0.14504
C	-3.55926	-0.61114	0.58926
H	-5.56641	-2.10896	-2.91734
H	-5.89907	-0.01426	-1.90237
H	-5.04213	0.83518	0.01684
H	-2.53133	-3.74998	-0.49063
H	-4.14793	-3.83837	-2.17448
H	-1.95597	-2.02098	0.89599
C	-3.31963	-0.02296	1.79897
C	-4.17177	1.12783	2.29362
H	-4.28316	1.92818	1.55197
H	-5.18772	0.80489	2.55535
H	-3.73306	1.57895	3.18722
C	-2.33774	-0.59980	2.79957
H	-2.33074	-0.00396	3.71605
H	-2.61049	-1.62374	3.08578
H	-1.30551	-0.64638	2.42890

M2b



C	-2.60017	1.13910	1.96489
C	-3.42480	-0.00509	2.30205
C	-2.99050	-1.29005	2.34711
C	-1.56913	1.11694	1.10412
C	-1.64612	-1.76343	2.06541
C	-1.21264	-0.08792	0.27613
C	-0.78013	-1.23351	1.17857
H	-4.43325	0.20245	2.65178
H	-3.68148	-2.03142	2.74472
H	-1.32305	-2.62871	2.63925
H	-0.92313	1.98293	0.99199
H	-2.83111	2.07455	2.46887
H	-0.35769	0.16294	-0.36316
C	0.64568	-1.72820	0.93563
P	-2.51189	-0.51649	-0.98666
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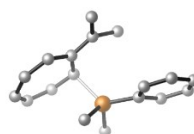
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H	-0.85048	3.27414	-1.86213	H	-1.51807	0.98281	-2.58717
C	-1.10090	0.27172	-0.43522	H	-0.83574	-0.64735	-2.70856
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O	-4.07686	-1.99067	1.24207	C	-4.01776	1.80723	-1.09590
O	-0.20675	0.26310	1.78760	C	-6.42328	0.53639	-0.47658
O	-1.86312	-0.68628	-2.48610	H	-5.27956	-1.27521	-0.36184
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C	-4.00096	-1.96383	-1.48018	C	-6.39394	1.91028	-0.70245
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H	-4.25671	-1.36017	-2.34923	H	-5.16929	3.61556	-1.18398
H	-3.52776	-2.88910	-1.81621	H	-7.30978	2.48846	-0.63877
C	-2.35610	-0.87084	2.97676	C	1.48426	0.39438	1.88453
H	-1.86407	-0.03565	3.46909	C	1.54848	-0.45109	0.83275
H	-3.40713	-0.92098	3.24855	H	0.82977	0.20871	2.73354
H	-1.86024	-1.80285	3.25905	H	2.08346	1.29833	1.91139
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				H	2.28490	1.31969	-1.99275
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				C	3.19997	2.28882	-0.34021
				C	2.84202	3.44353	0.35750
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				C	3.80973	4.30950	0.86716
				H	1.78647	3.66030	0.51377
				C	5.52994	2.88093	-0.02006
				H	4.84238	1.12475	-1.07453
				C	5.15924	4.03108	0.67854
				H	3.50806	5.19863	1.41376
				H	6.58200	2.65803	-0.17390
				H	5.91679	4.70181	1.07239
				C	3.13487	-0.92385	-1.07629
				O	3.72448	-0.71487	-2.15063
				O	3.44009	-2.09271	-0.37118
				C	4.24982	-3.02489	-1.06662
				C	4.44301	-4.21966	-0.15297
TS1'				H	5.20689	-2.56372	-1.33185



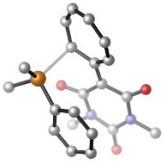
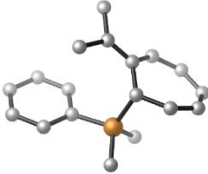
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C	-1.36562	2.09794	0.23723
C	-1.87863	0.34996	-1.46036
C	-0.91536	1.15034	-0.70507
H	-4.75171	2.75070	0.46188
H	-2.68167	3.14403	1.47104
H	-0.58620	2.56767	0.81841
H	-3.57785	0.20814	-2.69445
H	-5.11116	1.56623	-1.58018
H	-1.41382	-0.31138	-2.17772
C	0.48968	0.85971	-0.83999
C	1.47592	1.78608	-0.30280
C	0.96443	-0.38873	-1.40208
C	3.27504	0.13521	-0.68617
O	4.42763	-0.23632	-0.52751
O	1.25545	2.92415	0.10588
O	0.27290	-1.29749	-1.88324
N	2.34609	-0.63269	-1.36638
N	2.81093	1.34880	-0.23206
C	2.80452	-1.91813	-1.88337
H	2.59441	-2.72034	-1.16800
H	2.27617	-2.12992	-2.80986
H	3.87632	-1.85378	-2.04789
C	3.75470	2.25230	0.41782
H	3.46655	2.40206	1.46071
H	4.74181	1.80370	0.35778
H	3.73597	3.21939	-0.08482
P	-1.96959	-1.56740	0.11734
C	-1.82266	-3.29013	-0.49200
H	-2.72549	-3.53495	-1.05625
H	-0.96506	-3.34031	-1.16548
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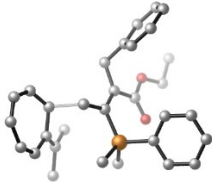
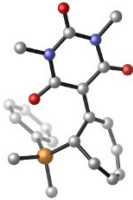
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H	1.11979	-2.13872	3.02415
H	0.59277	-3.57458	2.11247
C	0.55910	-2.56276	-0.35758
H	-0.17803	-3.36108	-0.21550
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TS1b'

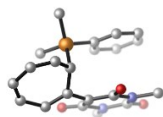


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C	-2.35812	1.50995	0.51647
C	-1.36359	-0.21204	-1.11984
C	-1.35646	1.15058	-0.47225
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H	-3.98112	1.37884	1.79165
H	-2.19670	2.48220	0.97075
H	-2.39505	-1.84951	-1.98427
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H	-0.81759	-0.20050	-2.06092
C	-0.33498	2.01072	-0.75959
P	0.08369	-1.16375	0.08066
C	0.08070	-2.93412	-0.36020
H	-0.96460	-3.24783	-0.40972
H	0.53555	-3.08578	-1.34151
H	0.61135	-3.52715	0.38701
C	-0.66485	-1.06870	1.73408
H	-0.79329	-0.01887	2.01000
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H	-0.05135	-1.59016	2.47118
C	1.82725	-0.68680	0.27615
C	2.82656	-1.23928	-0.53486
C	2.15559	0.36933	1.13792
C	4.13032	-0.75694	-0.47161

H	-4.36388	-1.63502	0.42051	H	2.59333	-2.05191	-1.21675
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C	-0.67696	-0.29199	2.22839	H	4.89696	-1.19742	-1.10097
C	1.73506	-1.62558	1.81858	H	3.70419	1.65827	1.87676
H	0.67018	-2.81901	0.39054	H	5.46862	0.65799	0.44504
C	0.46116	0.09226	2.93337	C	-0.26359	3.38417	-0.12494
H	-1.60706	0.24595	2.38632	H	0.57174	3.95409	-0.53935
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H	2.67725	-2.13897	1.64931	H	-0.11386	3.32903	0.96074
H	0.40317	0.91335	3.64074	C	0.78873	1.76372	-1.73572
H	2.56414	-0.24428	3.24774	H	0.73762	2.48689	-2.56059
TS1'-a				H	1.75730	1.91963	-1.24214
				H	0.81673	0.76524	-2.17217
C	-4.11289	1.51796	-1.15097	M1b'			
C	-3.89408	2.25699	0.01495				
C	-2.65810	2.49063	0.60074	C	3.60253	-0.64072	0.40136
C	-3.20337	0.71755	-1.80972	C	3.76606	0.07212	-0.80036
C	-1.36562	2.09794	0.23723	C	2.88980	1.05276	-1.28653
C	-1.87863	0.34996	-1.46036	C	2.51915	-0.71322	1.24107
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H	-4.75171	2.75070	0.46188	C	1.14753	-0.15804	1.01542
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H	-0.58620	2.56767	0.81841	H	4.68312	-0.09359	-1.35662
H	-3.57785	0.20814	-2.69445	H	3.20435	1.50907	-2.22720
H	-5.11116	1.56623	-1.58018	H	1.27676	2.38174	-1.37681
H	-1.41382	-0.31138	-2.17772	H	2.63516	-1.25517	2.17508
C	0.48968	0.85971	-0.83999	H	4.47126	-1.21367	0.73152
C	1.47592	1.78608	-0.30280	H	0.62340	-0.19612	1.97425
C	0.96443	-0.38873	-1.40208	C	-0.01156	2.04746	0.90377
C	3.27504	0.13521	-0.68617	P	0.17937	-1.37302	0.00266
O	4.42763	-0.23632	-0.52751	C	0.13039	-2.95054	0.89257
O	1.25545	2.92415	0.10588	H	1.16348	-3.27789	1.02493
O	0.27290	-1.29749	-1.88324	H	-0.32370	-2.81146	1.87632
N	2.34609	-0.63269	-1.36638	H	-0.42900	-3.69816	0.32698
N	2.81093	1.34880	-0.23206	C	0.97638	-1.65739	-1.59201
C	2.80452	-1.91813	-1.88337	H	0.93990	-0.73018	-2.16718
H	2.59441	-2.72034	-1.16800	H	2.02552	-1.89957	-1.40781
H	2.27617	-2.12992	-2.80986				

H	3.87632	-1.85378	-2.04789	H	0.46297	-2.46496	-2.11755
C	3.75470	2.25230	0.41782	C	-1.51715	-0.82935	-0.30799
H	3.46655	2.40206	1.46071	C	-2.60389	-1.39021	0.36812
H	4.74181	1.80370	0.35778	C	-1.71696	0.25773	-1.17215
H	3.73597	3.21939	-0.08482	C	-3.88379	-0.87372	0.17897
P	-1.96959	-1.56740	0.11734	H	-2.46149	-2.22875	1.04297
C	-1.82266	-3.29013	-0.49200	C	-2.99638	0.76879	-1.35349
H	-2.72549	-3.53495	-1.05625	H	-0.87111	0.71654	-1.67820
H	-0.96506	-3.34031	-1.16548	C	-4.07934	0.20388	-0.67922
H	-1.70527	-4.00194	0.32949	H	-4.72492	-1.31466	0.70332
C	-3.51730	-1.56323	1.10875	H	-3.14906	1.61023	-2.02121
H	-3.60742	-0.61713	1.64647	H	-5.07640	0.60694	-0.82404
H	-4.36388	-1.63502	0.42051	C	-0.18999	3.44297	0.35914
H	-3.55093	-2.39491	1.81674	H	0.76546	3.90759	0.10422
C	-0.61436	-1.33707	1.29670	H	-0.80957	3.44514	-0.55197
C	0.60003	-2.01651	1.11873	H	-0.69967	4.08233	1.08749
C	-0.67696	-0.29199	2.22839	C	-1.07557	1.67798	1.90539
C	1.73506	-1.62558	1.81858	H	-2.06760	1.77837	1.43812
H	0.67018	-2.81901	0.39054	H	-1.01952	0.65960	2.29316
C	0.46116	0.09226	2.93337	H	-1.06432	2.36009	2.76503
H	-1.60706	0.24595	2.38632	TS2b'			
C	1.67185	-0.55953	2.71644				
H	2.67725	-2.13897	1.64931				
H	0.40317	0.91335	3.64074				
H	2.56414	-0.24428	3.24774				
M1'							
				C	-1.30111	-0.81388	-1.02011
				C	-0.42375	-0.10841	-0.16092
				H	-0.91406	-1.71897	-1.47190
				H	-1.98110	-0.27768	-1.67069
C	2.35312	-3.20605	-0.80206	C	0.59975	-0.71046	0.58139
C	2.67167	-3.00204	0.58539	C	0.96205	-2.16947	0.40332
C	1.86667	-2.35645	1.47741	H	1.14885	-2.62233	1.38111
C	1.53775	-2.43317	-1.54817	H	0.12340	-2.71441	-0.03944
C	0.59199	-1.73301	1.26801	C	2.19988	-2.34336	-0.45876
C	0.94292	-1.11838	-1.13808	C	2.19727	-1.92953	-1.79562
C	0.07996	-1.19868	0.12002	C	3.37326	-2.88251	0.06932
H	3.55174	-3.50900	0.97268	C	3.33685	-2.05697	-2.58418
H	2.18089	-2.39690	2.51981	H	1.29217	-1.49682	-2.21725
H	-0.03915	-1.66163	2.14644	C	4.51696	-3.01263	-0.71653
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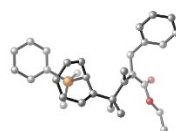
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C	-2.33398	-1.25947	0.79041	C	1.42918	0.07615	1.45689
C	-1.51840	0.45795	-0.80499	O	1.32220	1.28946	1.65386
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O	-5.06064	0.75067	-0.40187	C	3.29550	0.09144	2.89895
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N	-2.84159	0.89536	-0.93822	H	3.69542	0.93379	2.32752
N	-3.62581	-0.71385	0.57267	H	5.10650	-0.35928	3.96763
C	-3.08204	2.04938	-1.79519	H	3.95843	-1.70897	3.88311
H	-4.15546	2.20761	-1.84613	H	4.90636	-1.26239	2.45172
H	-2.58836	2.93275	-1.38379	P	-0.70580	1.68046	-0.04265
H	-2.67294	1.85908	-2.78813	C	-1.12729	2.42922	1.56570
C	-4.76337	-1.27971	1.28886	H	-2.13502	2.84376	1.51454
H	-5.27107	-0.49648	1.85412	H	-1.07090	1.66646	2.34019
H	-5.47623	-1.70904	0.58184	H	-0.39189	3.20156	1.79208
H	-4.37875	-2.04735	1.95371	C	-2.09904	2.12191	-1.12317
P	2.17569	0.27589	-1.06136	H	-3.00843	1.59706	-0.81763
C	2.07881	1.20299	-2.61389	H	-2.24754	3.20140	-1.03518
H	2.30682	0.50912	-3.42782	H	-1.86735	1.88278	-2.16165
H	1.06781	1.59064	-2.73392	C	0.68317	2.57637	-0.79782
H	2.81540	2.00916	-2.60962	C	0.65261	3.97291	-0.81783
C	3.88993	-0.32590	-1.00917	C	1.73100	1.89128	-1.41462
H	4.07778	-0.88235	-0.09172	C	1.67073	4.68172	-1.44879
H	4.05675	-0.98901	-1.85977	H	-0.15855	4.51656	-0.33877
H	4.55585	0.53777	-1.07255	C	2.74448	2.60540	-2.04649
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C	1.30984	2.60956	0.20021	C	2.71600	3.99782	-2.06475
C	2.54726	1.04039	1.57353	H	1.64665	5.76627	-1.45805
C	1.21827	3.47438	1.28625	H	3.56025	2.06853	-2.51938
H	0.83518	2.86243	-0.74077	H	3.50916	4.55095	-2.55698
C	2.44451	1.90781	2.65474	C	-4.09288	-2.89743	-1.62934
H	3.05001	0.08527	1.69723	C	-4.94045	-1.89836	-2.05506
C	1.78459	3.12611	2.50954	C	-5.14047	-0.63722	-1.43056
H	0.69691	4.41922	1.17646	C	-3.13811	-2.85303	-0.60184
H	2.87735	1.63065	3.60994	C	-4.60396	-0.11190	-0.28636
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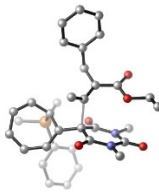
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C	-2.27672	-2.03114	0.31542
C	-1.91379	0.42045	0.85037
C	-1.45966	-1.02166	0.70377
H	-5.64049	-1.29502	-0.14372
H	-4.00149	-2.89968	-0.59569
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C	0.60944	-1.86158	-0.40176
C	0.80000	-0.46315	1.64288
C	2.83107	-1.12421	0.39808
O	4.04520	-1.05992	0.25060
O	0.02343	-2.40567	-1.35012
O	0.36192	0.18486	2.60457
N	2.19595	-0.46864	1.42934
N	2.01935	-1.84769	-0.45267
C	3.06137	0.25060	2.35490
H	3.64619	-0.45116	2.95513
H	3.75047	0.87871	1.78954
H	2.42380	0.85224	2.99661
C	2.65252	-2.50386	-1.58850
H	2.58786	-1.87855	-2.48599
H	3.69694	-2.67641	-1.34253
H	2.13246	-3.43907	-1.78471
P	-1.46952	1.24129	-0.75460
C	-2.40319	2.78795	-0.90590
H	-3.47059	2.56051	-0.86455
H	-2.14931	3.45641	-0.08028
H	-2.15681	3.27142	-1.85293
C	-1.89024	0.17144	-2.14385
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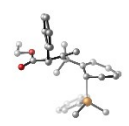
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C	-4.17177	1.12783	2.29362
H	-4.28316	1.92818	1.55197
H	-5.18772	0.80489	2.55535
H	-3.73306	1.57895	3.18722
C	-2.33774	-0.59980	2.79957
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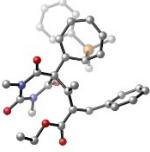
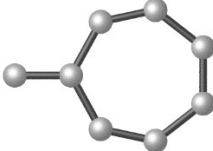
M2b'

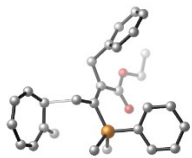


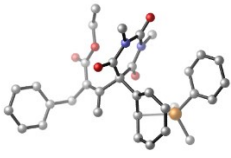
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C	-1.64335	-1.77337	2.05023
C	-1.20530	-0.09160	0.26844
C	-0.77451	-1.23984	1.16830
H	-4.43378	0.18870	2.63171
H	-3.68019	-2.04390	2.72201
H	-1.32156	-2.63984	2.62258
H	-0.92313	1.97989	0.98705
H	-2.83736	2.06448	2.45642
H	-0.34977	0.16185	-0.36855
C	0.65294	-1.73224	0.92823
P	-2.50420	-0.51692	-0.99653
C	-2.89396	-2.28072	-1.06782
H	-1.97980	-2.82524	-1.30766
H	-3.27124	-2.62313	-0.10365
H	-3.63561	-2.44400	-1.85296
C	-1.76407	-0.06669	-2.58943
H	-1.52434	0.99916	-2.58986
H	-0.83612	-0.62711	-2.72844
H	-2.46092	-0.28404	-3.40069
C	-4.04149	0.41895	-0.86425
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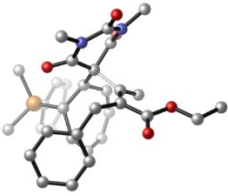
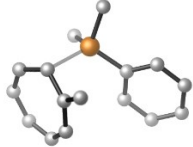
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C	1.15345	1.00889	-1.69294	H	-3.09152	2.30935	-1.32693
C	2.16089	2.79367	0.20444	C	-6.39424	1.89273	-0.67707
H	0.13830	2.99334	0.89439	H	-7.34701	0.02010	-0.20500
C	2.51653	1.28221	-1.64636	H	-5.18022	3.60339	-1.16679
H	0.77305	0.27711	-2.40099	H	-7.31155	2.46719	-0.60382
C	3.01957	2.17307	-0.70030	C	1.48787	0.38985	1.88088
H	2.55442	3.47557	0.95075	C	1.55490	-0.45478	0.82915
H	3.19132	0.77856	-2.33069	H	0.83193	0.20289	2.72846
H	4.08605	2.36771	-0.65754	H	2.08636	1.29418	1.90964
TS2'				C	2.22516	-0.10086	-0.41742
				C	2.15694	1.32878	-0.91394
C	1.72144	-3.39811	2.03364	H	2.29721	1.30610	-2.00199
C	2.91206	-2.76354	2.55271	H	1.15843	1.75324	-0.71873
C	3.11993	-1.42186	2.60915	C	3.18130	2.29794	-0.34529
C	0.91455	-2.88770	1.08586	C	2.79815	3.44749	0.34744
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H	0.34290	-1.45546	-0.35964	H	5.84544	4.75700	1.08749
C	0.33272	0.69030	0.91346	C	3.15808	-0.92417	-1.06631
C	0.14409	1.70387	1.97248	O	3.75825	-0.71502	-2.13485
C	0.46363	1.20652	-0.46143	O	3.46000	-2.09144	-0.35608
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O	0.24108	1.47295	3.16730	H	5.22424	-2.57318	-1.31647
O	0.83880	0.50415	-1.39921	H	3.78161	-3.32389	-1.98988
N	0.04626	2.49109	-0.72182	H	5.08609	-4.97757	-0.60690
N	-0.24958	2.97969	1.56671	H	4.92502	-3.91106	0.80316
C	-0.10766	2.87263	-2.12635	H	3.48965	-4.68070	0.10889
H	-0.95176	2.32607	-2.55945	C	0.57145	-2.56283	-0.36792
H	-0.29133	3.94230	-2.16529	H	-0.15777	-3.36880	-0.22835
H	0.80434	2.61916	-2.66588	H	0.28290	-1.94884	-1.22760
				H	1.53877	-3.00336	-0.59982
				C	1.16634	-2.64444	2.04617
				H	2.21057	-2.88401	1.82973
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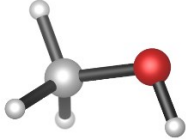
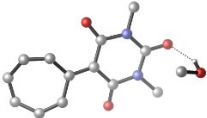
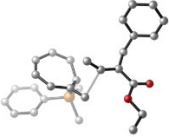
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H	-1.50342	3.57741	3.13838				
P	2.54700	-1.82037	-0.95129				
C	1.73327	-2.10671	-2.54376	C	1.77826	-3.76903	0.90144
H	1.12846	-3.01322	-2.44961	C	2.76797	-3.19688	1.79069
H	1.08557	-1.26130	-2.77699	C	2.74921	-1.96078	2.34631
H	2.48308	-2.25410	-3.32370	C	0.91371	-3.08903	0.11822
C	3.54149	-3.31637	-0.67578	C	1.75064	-0.91767	2.20249
H	4.13503	-3.22715	0.23339	C	0.79443	-1.63935	0.02135
H	2.87824	-4.17753	-0.58202	C	0.88634	-0.73751	1.18127
H	4.19787	-3.44318	-1.53987	H	3.57311	-3.86249	2.09285
C	3.72107	-0.45403	-1.09394	H	3.54286	-1.73935	3.05817
C	3.62320	0.45467	-2.15204	H	1.74551	-0.17634	2.99633
C	4.76235	-0.34295	-0.16737	H	0.25267	-3.65333	-0.53443
C	4.56445	1.47099	-2.27624	H	1.77057	-4.85357	0.82901
H	2.80594	0.38372	-2.86040	H	0.26849	-1.25875	-0.84640
C	5.69574	0.68008	-0.29506	C	-0.07123	0.45888	1.08430
H	4.84222	-1.04441	0.65781	P	2.91482	-1.17147	-1.13789
C	5.59695	1.58572	-1.34862	C	2.34566	-0.99206	-2.87207
H	4.48695	2.17605	-3.09680	H	1.89211	-1.94105	-3.17202
H	6.49908	0.76856	0.42821	H	1.57979	-0.21546	-2.94564
H	6.32675	2.38256	-1.44706	H	3.16821	-0.76043	-3.55376
C	-1.58325	-0.71721	2.04284	C	4.17213	-2.50711	-1.26898
C	-1.38985	-0.16895	0.84895	H	4.75727	-2.54115	-0.34840
H	-0.85180	-0.67374	2.84372	H	3.65521	-3.46317	-1.38346
H	-2.53019	-1.21794	2.22876	H	4.83400	-2.33895	-2.12242
C	-2.02526	-0.22998	-0.39857	C	3.87577	0.33231	-0.78317
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C	-3.44732	-2.27635	-0.75846	H	3.25873	1.45198	-2.52753
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C	-5.85652	-2.50087	-0.91089	H	5.84578	1.57296	1.70013
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H	-6.80222	-2.17378	-1.33318	H	-1.08767	-1.87860	1.72344
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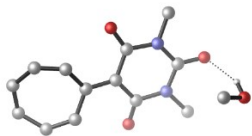
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C	-3.47470	3.10460	-0.65797	H	-3.25816	0.15193	-2.28973
C	-3.85816	3.96757	0.52641	H	-2.53517	-1.32094	-1.64705
H	-4.35449	2.73720	-1.19138	C	-4.39172	-0.78297	-0.74688
H	-2.85927	3.66658	-1.37133	C	-5.18722	-1.73894	-1.38667
H	-4.45694	4.81886	0.19142	C	-4.86863	-0.20403	0.42975
H	-4.44546	3.38746	1.24255	C	-6.42760	-2.10294	-0.87386
H	-2.96630	4.35264	1.02503	H	-4.82428	-2.19972	-2.30330
M2'				C	-6.11041	-0.56638	0.94889
				H	-4.24999	0.53051	0.93864
C	-2.64236	1.43343	2.38528	C	-6.89566	-1.51506	0.30020
C	-3.33368	0.17581	2.58689	H	-7.02931	-2.84636	-1.38854
C	-2.83032	-1.04998	2.28927	H	-6.46425	-0.10672	1.86721
C	-1.75891	1.67382	1.40040	H	-7.86221	-1.79749	0.70595
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C	-1.44687	0.67835	0.31316	O	-2.73086	2.39144	-1.80037
C	-0.79890	-0.54668	0.93345	O	-1.99797	2.67764	0.30249
H	-4.28073	0.21311	3.12101	C	-2.06349	4.08197	0.06393
H	-3.41552	-1.91707	2.58737	C	-1.60465	4.77244	1.33161
H	-1.05271	-2.24369	2.13945	H	-3.08864	4.35756	-0.20203
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H	-0.74707	1.13426	-0.38852	H	-2.24224	4.49089	2.17352
C	0.66659	-0.75460	0.59012	H	-0.57493	4.49325	1.57326
C	1.39085	-1.71109	1.52126	C	0.67129	1.44997	0.15788
C	0.81616	-1.14051	-0.86701	H	0.78602	1.04493	-0.85404
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O	3.88803	-2.88238	-0.72752	H	1.66988	1.64020	0.56520
O	1.12107	-1.83297	2.70049	C	-0.33569	1.11755	2.44276
O	-0.04598	-0.85895	-1.68843	H	-0.69091	0.37992	3.16795
N	1.97960	-1.76624	-1.23684	H	0.56816	1.59297	2.83906
N	2.46676	-2.40020	0.99241	H	-1.09786	1.88774	2.31865
C	2.42034	-1.68837	-2.63378	R2c			
H	3.15838	-0.88479	-2.72419				
H	2.85982	-2.64043	-2.92371	C	-1.88880	0.67377	0.00028
H	1.54812	-1.46500	-3.24180	C	-1.88881	-0.67373	0.00028
C	3.28312	-3.15689	1.94035	C	-0.74255	-1.56654	-0.00014
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H	4.03219	-3.70592	1.37697				

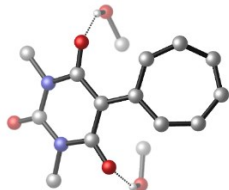
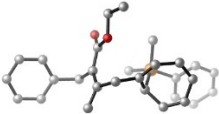
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H	-2.03241	1.60924	-2.64370	C	1.28465	-0.00002	-0.00006
H	-1.71945	-0.12424	-2.85639	H	-2.85670	-1.16829	0.00052
H	-3.36712	0.53059	-3.13460	H	-0.99724	-2.62367	-0.00035
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H	-4.98034	1.45850	-1.24089	H	1.24346	2.14487	-0.00071
C	-3.61244	-1.33037	-0.73716	C	2.63295	-0.00001	0.00047
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H	-1.84805	-2.24500	-1.58211				
C	-5.44216	-2.81735	-0.23454	C	-1.56882	-0.73593	-0.75805
H	-5.49346	-0.70241	0.12586	C	-0.62263	-0.09815	0.07751
C	-4.68636	-3.89362	-0.69485	H	-1.23494	-1.62215	-1.28416
H	-2.80988	-4.52798	-1.53764	H	-2.28412	-0.15256	-1.32340
H	-6.44722	-2.97614	0.14103	C	0.45142	-0.74903	0.69448
H	-5.10467	-4.89467	-0.67622	C	0.77901	-2.19882	0.40791
C	1.49512	1.12693	1.98050	H	1.04386	-2.70614	1.33987
C	1.45975	0.65286	0.73348	H	-0.10066	-2.71303	0.00989
H	1.04307	0.59769	2.81602	C	1.93565	-2.33612	-0.56660
H	2.00127	2.06192	2.18968	C	1.82802	-1.83747	-1.86976
C	2.04038	1.27892	-0.46934	C	3.13844	-2.92582	-0.17659
C	1.23468	2.17356	-1.38135	C	2.89372	-1.93036	-2.75991
H	1.95519	2.56307	-2.11098	H	0.89975	-1.36426	-2.18366
H	0.48150	1.63039	-1.98485	C	4.20844	-3.02196	-1.06470
C	0.52491	3.34206	-0.71676	H	3.23697	-3.29964	0.83913
C	-0.71419	3.79989	-1.17836	C	4.08967	-2.52496	-2.35946
C	1.08945	3.99742	0.38092	H	2.79030	-1.54123	-3.76832
C	-1.38854	4.84518	-0.54792	H	5.13708	-3.48315	-0.74218
H	-1.14652	3.34450	-2.06706	H	4.92192	-2.59844	-3.05211
C	0.42542	5.04282	1.01750	C	1.37696	-0.01143	1.51332
H	2.06450	3.66531	0.72360	O	1.32327	1.19796	1.75253
C	-0.82539	5.46275	0.56613	O	2.37033	-0.77554	2.01688
H	-2.34790	5.18182	-0.93149	C	3.37718	-0.08656	2.76206
H	0.88536	5.53201	1.87107	C	4.48398	-1.08275	3.03336
H	-1.34688	6.27166	1.06792				
C	3.34155	0.97282	-0.87787				
O	3.94111	1.35909	-1.89757				
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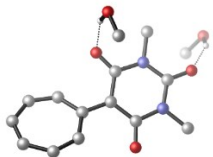
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H	5.43167	-0.75980	-1.24701	H	5.28365	-0.61036	3.60851
H	7.06259	-1.01808	0.66414	H	4.10374	-1.93506	3.60173
H	5.86709	-0.28655	1.75541	H	4.89901	-1.45078	2.09177
H	5.53157	-1.85021	0.97931	P	-0.87361	1.68845	0.30681
TS3'				C	-1.09644	2.39306	1.97522
				H	-2.12772	2.73242	2.07998
				H	-0.86962	1.63518	2.72029
				H	-0.39304	3.21863	2.09551
				C	-2.37918	2.18273	-0.58765
				H	-3.25076	1.63736	-0.21528
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				H	-2.26147	2.01094	-1.65801
				C	0.42998	2.59788	-0.57598
				C	0.38515	3.99434	-0.59360
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				C	1.33552	4.71276	-1.31325
				H	-0.38464	4.53196	-0.04488
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				H	1.29993	5.79700	-1.31976
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				C	-4.63016	-2.59136	-1.22643
				C	-5.54345	-1.56296	-1.31927
				C	-5.62447	-0.42485	-0.47290
				C	-3.50802	-2.70471	-0.39084
				C	-4.84962	-0.05412	0.59051
				C	-2.91097	-1.73648	0.43507
				C	-3.62776	-0.62732	1.11889
				H	-6.32231	-1.65655	-2.07016
				H	-6.47282	0.22923	-0.66887
				H	-5.18758	0.82618	1.13713
				H	-2.92444	-3.61478	-0.51660
				H	-4.79378	-3.43437	-1.89587
				H	-2.10651	-2.12627	1.06041
				C	-3.05801	-0.09773	2.22897
				H	-2.14246	-0.51072	2.64000
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				M2c			
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C	0.84906	-3.36959	0.42134				
C	1.62496	-0.64232	1.75313				
C	0.73132	-2.01709	-0.13659				
C	0.76487	-0.81744	0.73284				
H	3.50720	-3.43746	2.52977				
H	3.48176	-1.10606	2.74278				
H	1.56797	0.28099	2.32455				
H	0.19527	-4.11393	-0.02422				
H	1.68383	-4.79543	1.69327				
H	0.25363	-1.90459	-1.10071				
C	-0.33868	0.21391	0.38285				
C	-0.60895	1.11732	1.57852				
C	0.24110	0.93996	-0.83134				
C	0.87531	2.82596	0.61274				
O	1.50215	3.85965	0.74219				
O	-1.35707	0.79720	2.47031				
O	0.31859	0.40034	-1.91834				
N	0.81651	2.18262	-0.61652				
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C	1.34133	2.94168	-1.75291				
H	1.08030	2.40134	-2.65923				
H	0.89053	3.93540	-1.75421				
H	2.42466	3.05572	-1.67995				
C	0.10050	3.08258	2.88512				
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H	1.11320	3.36714	3.16699				
H	-0.48967	3.98688	2.71819				

H	-3.30215	3.55824	-1.39220	C	-1.89671	0.01627	0.09699
H	-1.63936	3.66648	-1.96969	C	-2.55430	-1.27074	-0.34834
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H	-2.45594	4.06215	0.96520	H	-2.13479	-2.12811	0.20023
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C	0.83180	-0.62215	-2.05530	H	-0.59010	5.26557	-1.68432
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O	4.03645	-2.12679	-2.47186	H	0.48344	4.18940	-0.76613
O	0.43525	-3.51258	-0.18878	H	-0.74376	1.23589	3.12260
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H	3.47512	-0.63358	-4.06935	C	-2.56714	-1.73144	-0.95839
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H	2.34338	0.72130	-3.79299	C	-2.88034	0.57534	-0.02104
C	3.04854	-3.95439	-0.68288	C	-1.09942	-1.76384	1.11833
H	2.73161	-4.78909	-1.31291	C	-1.75654	0.70324	0.85104
H	4.11590	-3.78678	-0.80183	C	-1.13542	-0.41536	1.63623
H	2.80934	-4.18035	0.35533	H	-2.90461	-2.39668	-1.74748
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				H	-0.48162	-2.44099	1.70477

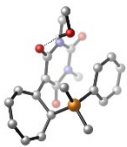
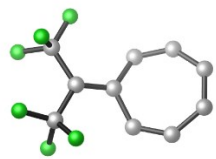
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MeOH				P	-0.01102	0.99689	-0.14934
				C	0.08675	2.76291	0.24268
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H	1.13300	-0.75887	-0.00037	H	0.48322	2.90405	1.25063
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H	-1.02794	-0.54564	-0.89016	H	-0.67594	-0.20857	-2.10226
H	-1.02830	-0.54378	0.89115	H	-1.71774	1.18859	-1.80503
R1-sol				H	-0.06947	1.43653	-2.50407
				C	1.66659	0.32252	-0.17639
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C	-1.90949	-0.05212	0.21847	C	4.21288	-0.80560	-0.19444
H	-6.05515	0.82348	-0.08567	H	4.88247	1.06791	0.62712
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H	-1.80441	-2.16497	0.58625	TS2c'			
C	-0.56388	0.09637	-0.13817				
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C	0.24099	-1.06922	-0.53378	C	-2.77541	-2.23093	-1.38939
C	2.24154	0.37307	-0.65640	C	-2.67539	-1.08553	-2.15112
O	3.44945	0.47626	-0.82997	C	-1.19561	-1.72189	0.49882
O	-0.53200	2.49525	-0.12905	C	-1.87527	0.06242	-1.99931
O	-0.20148	-2.19333	-0.71821	C	-1.17194	-0.22250	0.44522
N	1.61786	-0.85506	-0.70461	C	-1.06846	0.46057	-0.91547
				H	-3.44504	-3.00832	-1.74388
				H	-3.29616	-1.07515	-3.04744
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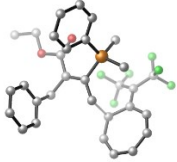
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C	2.48347	-1.99668	-1.01768	H	-0.32274	0.12791	1.04993
H	3.28337	-2.06099	-0.27795	C	-0.12274	1.47008	-0.99788
H	1.86762	-2.88984	-0.99815	P	-2.61243	0.46363	1.36783
H	2.92434	-1.86352	-2.00698	C	-2.46728	2.26702	1.48374
C	2.05061	2.79964	-0.44510	H	-1.58301	2.50797	2.07853
H	1.79739	3.32448	0.47610	H	-2.33146	2.67956	0.48211
H	3.12518	2.67308	-0.53357	H	-3.35852	2.68878	1.95261
H	1.66203	3.37236	-1.28862	C	-2.57847	-0.21143	3.04688
C	3.88010	-0.55055	2.07552	H	-2.52400	-1.30011	2.99053
H	4.11343	-1.01482	3.03630	H	-1.68378	0.16027	3.55214
H	2.86694	-0.87019	1.78570	H	-3.46898	0.09443	3.59881
H	3.86835	0.53877	2.21412	C	-4.19732	0.07535	0.61640
O	4.85877	-0.96332	1.14867	C	-4.69613	0.90941	-0.38904
H	4.67581	-0.48235	0.32777	C	-4.89591	-1.07707	0.98905
R1-sol-1				C	-5.88817	0.58369	-1.02450
				H	-4.14663	1.79343	-0.69547
C	-4.98912	-0.94570	-0.05049	C	-6.08995	-1.39355	0.35157
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C	0.24027	-1.08680	-0.51787	C	4.04799	-2.60932	-0.31427
C	2.23144	0.36766	-0.65308	C	5.24727	-1.05221	1.07367
O	3.43768	0.47881	-0.83229	C	5.24830	-3.21450	-0.67825
O	-0.55960	2.47535	-0.15497	H	3.10669	-2.97788	-0.71552
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				H	5.24286	-4.05968	-1.36008
				H	7.38380	-1.27936	1.11330
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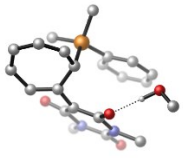
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C	2.01930	2.79644	-0.49169
H	1.75400	3.34072	0.41456
H	3.09551	2.67769	-0.57017
H	1.63137	3.34473	-1.35152
C	3.97092	-0.49734	2.06428
H	4.23187	-0.95333	3.02186
H	2.95015	-0.81941	1.80571
H	3.96309	0.59319	2.19304
O	4.92281	-0.91860	1.11343
H	4.71044	-0.44960	0.29271
R1-2sol			
			
C	-4.22863	0.59654	0.23718
C	-4.19766	-0.76559	0.26292
C	-3.31074	-1.58984	-0.48877
C	-3.37906	1.43108	-0.54569
C	-2.10352	-1.29256	-1.05096
C	-2.15862	1.16656	-1.09550
C	-1.36537	-0.04426	-0.98222
H	-4.97420	-1.27905	0.82269
H	-3.62137	-2.62657	-0.59303
H	-1.59521	-2.10501	-1.55016
H	-3.73589	2.44799	-0.68978
H	-5.02826	1.09493	0.77750
H	-1.68858	1.98048	-1.62804
C	0.03318	-0.00977	-0.93811
C	0.81254	-1.24376	-0.81040
C	0.74527	1.26481	-0.81026
C	2.84445	0.06658	-0.30746
O	4.02024	0.09789	-0.00878
O	0.35376	-2.38053	-0.92533
O	0.22849	2.37469	-0.93802
N	2.09204	1.22191	-0.47434
O	2.71507	2.61670	-0.48635
C	3.23970	3.90136	-0.15357
C	2.78067	4.86168	-1.23019
H	4.33132	3.84276	-0.09651
H	2.87833	4.19785	0.83688
H	3.15621	5.86715	-1.02509
H	3.14942	4.54400	-2.20800
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C	1.44773	2.29774	1.43224
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C	0.65929	1.20449	1.52944
H	4.82940	1.60030	1.39552
H	3.26688	3.25825	0.78427
H	0.96684	3.26467	1.56972
H	2.13094	-1.37846	2.80579
H	4.23476	-0.23681	2.90901
H	0.37946	-0.88999	1.31885
C	-0.76478	1.30986	2.03824
P	1.66986	-0.37987	-0.60383
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H	0.69599	1.66377	-1.29607
H	2.46975	1.78703	-1.34203
H	1.59914	0.87732	-2.62727
C	0.52116	-1.51542	-1.42950
H	0.11537	-2.24183	-0.72274
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H	1.06701	-2.03246	-2.22224
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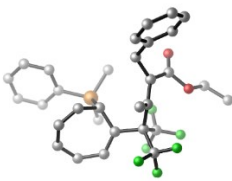
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H	2.20468	3.03224	0.57105	C	5.79562	-2.38236	-0.89639
C	2.89311	-2.38128	-0.29368	H	6.52370	-0.48385	-1.60302
H	2.78899	-3.01024	-1.17755	H	4.78910	-4.14638	-0.17798
H	3.93481	-2.13376	-0.11609	H	6.76502	-2.86541	-0.95859
H	2.46813	-2.90255	0.56739	C	-2.15550	-0.63983	2.49410
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H	0.79261	-1.30937	1.90797	H	-2.83939	-1.44804	2.26520
H	-0.94689	-1.64134	1.70775	C	-1.89557	0.00883	0.12765
O	0.28564	-3.33294	1.73503	C	-2.54686	-1.28727	-0.30443
H	0.25718	-3.33048	0.76696	H	-2.30887	-1.46029	-1.35880
O	-0.02348	3.36620	1.69234	H	-2.13883	-2.13190	0.27103
H	-0.02470	3.34281	0.72422	C	-4.06134	-1.31215	-0.18327
C	-0.18074	2.03402	2.12635	C	-4.73000	-2.31160	0.52423
H	-0.31899	2.05005	3.20974	C	-4.82249	-0.32629	-0.82194
H	-1.05658	1.54586	1.67413	C	-6.12236	-2.32751	0.60636
H	0.70535	1.41644	1.91080	H	-4.15064	-3.08782	1.02062
R1-2sol-1				C	-6.21079	-0.34083	-0.74821
				H	-4.30451	0.44214	-1.38993
C	-5.06799	0.57247	-1.10432	C	-6.86791	-1.34050	-0.02954
C	-5.29847	-0.46377	-0.24446	H	-6.62208	-3.11047	1.16924
C	-4.32539	-1.29289	0.36753	H	-6.78604	0.42927	-1.25392
C	-3.80761	1.02401	-1.56949	H	-7.95177	-1.34828	0.03145
C	-2.95482	-1.26274	0.33488	C	-1.68016	0.93578	-0.90718
C	-2.53371	0.64149	-1.24024	O	-1.79661	0.71618	-2.13090
C	-2.05215	-0.35554	-0.31978	O	-1.26658	2.21166	-0.51794
H	-6.33342	-0.69261	-0.00721	C	-1.31822	3.21131	-1.52749
H	-4.73702	-2.07657	0.99888	C	-0.59325	4.42805	-0.98673
H	-2.47337	-2.02514	0.92951	H	-2.36451	3.44178	-1.76318
H	-3.85932	1.80730	-2.32169	H	-0.85622	2.84323	-2.44855
H	-5.93519	1.09289	-1.50059	H	-0.63428	5.25057	-1.70524
H	-1.75878	1.16999	-1.77578	H	-1.04700	4.76195	-0.04975
C	-0.65310	-0.46327	-0.08891	H	0.45741	4.19039	-0.79087
C	-0.05083	-1.70968	0.37610	H	-0.73129	1.26613	3.13372
				H	-1.14083	2.29808	1.76594
				TS3c'			
				C	3.83214	1.12380	1.61430
				C	3.70758	2.46559	1.21038
				C	2.54296	3.18716	1.04695

C	0.20732	0.69459	-0.27636	C	2.83102	0.20351	1.86022
C	2.17069	-0.62188	0.41568	C	1.20968	2.78036	1.25361
O	3.36953	-0.69053	0.64988	C	1.43283	0.33814	1.73482
O	-0.63542	-2.77264	0.55095	C	0.68281	1.54637	1.59063
O	-0.18671	1.82449	-0.58064	H	4.63723	3.00014	1.03697
N	1.57675	0.53764	-0.04687	H	2.66489	4.22804	0.75665
N	1.33314	-1.70063	0.60400	H	0.47174	3.57016	1.14469
C	2.40959	1.73734	-0.20145	H	3.16888	-0.78746	2.15370
H	3.45430	1.44134	-0.22244	H	4.84716	0.76061	1.75218
H	2.13980	2.22171	-1.13910	H	0.83891	-0.50837	2.06916
H	2.21868	2.43345	0.61922	C	-0.79666	1.47575	1.90472
C	1.91794	-2.96601	1.05017	P	1.35632	-0.74565	-0.71800
H	1.76048	-3.73007	0.28784	C	1.77518	0.77011	-1.66954
H	2.97792	-2.80560	1.21871	H	0.84166	1.30256	-1.86631
H	1.42489	-3.28695	1.96787	H	2.42980	1.42058	-1.08519
O	0.27367	3.53656	1.60872	H	2.25834	0.51806	-2.61813
H	0.11447	3.22492	0.70470	C	0.41490	-1.69575	-1.98710
C	-0.02698	2.45331	2.45858	H	-0.01774	-2.59846	-1.55224
H	0.02963	2.81097	3.48920	H	-0.39506	-1.04574	-2.33329
H	-1.03556	2.05345	2.28666	H	1.06517	-1.96316	-2.82404
H	0.69025	1.62434	2.35151	C	2.95072	-1.65008	-0.64334
C	4.62874	-0.23556	-2.16929	C	4.18960	-1.05967	-0.91738
H	5.05653	0.18244	-3.08328	C	2.92836	-2.97070	-0.17004
H	3.56180	0.03285	-2.14013	C	5.37362	-1.77442	-0.73507
H	4.70181	-1.32974	-2.22428	H	4.23779	-0.03806	-1.28333
O	5.34443	0.29570	-1.07758	C	4.10718	-3.68581	0.00445
H	4.92943	-0.06796	-0.28188	H	1.97637	-3.44242	0.06504
R1-3sol				C	5.33571	-3.08648	-0.27539
C	4.85812	-1.64038	-1.07942	H	6.32631	-1.30301	-0.95656
C	5.14018	-0.33743	-0.76866	H	4.06999	-4.70986	0.36213
C	4.21204	0.68288	-0.45625	H	6.25757	-3.64160	-0.13502
C	3.57875	-2.23759	-1.16231	C	-1.75398	-0.71589	2.34952
C	2.83950	0.67384	-0.40588	C	-1.48528	0.22010	1.40062
C	2.32299	-1.71591	-0.96993	H	-1.51435	-0.52634	3.39100
C	1.90164	-0.38703	-0.63604	H	-2.25685	-1.64837	2.13071
H	6.18729	-0.04981	-0.74316	C	-1.76542	0.04029	-0.00196
H	4.65976	1.63787	-0.19333	C	-2.44749	-1.25189	-0.39628
H	2.40896	1.61922	-0.10439	H	-2.36180	-1.36841	-1.47952
H	3.58845	-3.28701	-1.44589	H	-1.94249	-2.11349	0.06528
H	5.70039	-2.29328	-1.28892	C	-3.92573	-1.30546	-0.05323
H	1.51641	-2.41857	-1.12424	C	-4.47808	-2.34029	0.70144
C	0.50499	-0.11847	-0.50285	C	-4.77755	-0.30396	-0.53275
C	-0.01251	1.21215	-0.74589	C	-5.84356	-2.37587	0.98338
C	-0.40960	-1.15467	-0.06491	H	-3.82861	-3.13066	1.07302

C	-2.25450	0.47875	-0.03557
O	-3.41881	0.75539	0.21516
O	0.64165	2.16105	-1.18824
O	-0.08355	-2.30903	0.22843
N	-1.75252	-0.79955	0.10886
N	-1.36533	1.43619	-0.48641
C	-2.64817	-1.83152	0.64855
H	-3.67671	-1.55618	0.43178
H	-2.40160	-2.77533	0.16669
H	-2.49175	-1.92999	1.72611
C	-1.85889	2.79304	-0.72788
H	-1.69126	3.05905	-1.77181
H	-2.91738	2.81278	-0.48888
H	-1.31383	3.49921	-0.09785
C	0.85498	2.66839	1.94927
H	1.14182	2.93749	2.96804
H	-0.24092	2.72378	1.87927
H	1.15296	1.62124	1.78056
O	1.50292	3.56112	1.07017
H	1.18340	3.36910	0.17508
O	-0.38657	-2.21831	3.04483
H	-0.30610	-2.56144	2.14194
C	0.14414	-0.91353	3.03148
H	0.23547	-0.57656	4.06673
H	1.13975	-0.87114	2.56643
H	-0.50789	-0.19874	2.50327
C	-4.85914	-0.83362	-2.02654
H	-5.40590	-1.52065	-2.67612
H	-3.83405	-1.21863	-1.91306
H	-4.80273	0.14179	-2.52720
O	-5.54591	-0.76637	-0.79737
H	-5.06465	-0.12470	-0.25502
M1²-sol			
			
C	-4.57725	-0.78653	-0.62946
C	-4.62885	0.61707	-0.99610
C	-3.61638	1.32824	-1.53966
C	-3.48801	-1.53017	-0.38142
C	-2.25364	0.92725	-1.83060
C	-2.05377	-1.07934	-0.29860
C	-6.14039	-0.33742	-0.26009
H	-4.35106	0.49331	-1.13673
C	-6.67956	-1.37280	0.50418
H	-6.25188	-3.18708	1.57932
H	-6.78833	0.44461	-0.64543
H	-7.74309	-1.39646	0.72118
C	-1.60960	0.96972	-1.05608
O	-1.89871	0.76994	-2.24858
O	-1.06409	2.21478	-0.73320
C	-1.14738	3.17877	-1.77794
C	-0.39428	4.41649	-1.33564
H	-2.19957	3.40781	-1.98392
H	-0.72610	2.76985	-2.70079
H	-0.46836	5.19445	-2.09976
H	-0.80658	4.81406	-0.40318
H	0.66523	4.18696	-1.18231
H	-0.88266	1.49178	2.99943
H	-1.28078	2.37508	1.52517
R2d			
			
C	3.66481	-0.61977	0.50288
C	3.68314	0.73207	0.44423
C	2.72902	1.56096	-0.24607
C	2.68497	-1.48133	-0.10687
C	1.45540	1.28819	-0.60656
C	1.42127	-1.20238	-0.49541
C	0.68996	0.06378	-0.33564
H	4.53643	1.24649	0.87738
H	3.08096	2.55975	-0.49357
H	0.92543	2.06819	-1.13758
H	3.00029	-2.51271	-0.24574
H	4.50335	-1.11764	0.98151
H	0.85699	-2.01943	-0.93196
C	-0.64996	0.04353	-0.10753
C	-1.37330	-1.27262	0.02814
F	-0.79646	-2.08023	0.93321
F	-2.64826	-1.11262	0.39852
F	-1.39393	-1.96051	-1.13323
C	-1.53986	1.23767	0.08453

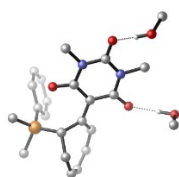
C	-1.52025	-0.09284	-1.32335	F	-2.09355	1.24051	1.30830
H	-5.59668	1.10240	-0.90495	F	-0.90351	2.40990	-0.04320
H	-3.85035	2.34786	-1.83966	F	-2.55274	1.24458	-0.79916
H	-1.71071	1.60647	-2.47910	TS2d			
H	-3.63796	-2.58926	-0.18535				
H	-5.53722	-1.29821	-0.58863				
H	-1.42945	-1.97591	-0.37733				
C	-0.05970	-0.13763	-1.49151				
C	0.68799	1.05698	-1.31397				
C	0.61443	-1.39882	-1.55398				
C	2.78092	-0.25579	-1.23342	C	0.17016	1.40525	-0.77035
O	3.99219	-0.30031	-1.06502	C	-0.39713	0.26068	-0.19958
O	0.20921	2.20614	-1.16727	H	-0.26481	2.36269	-0.51474
O	0.06779	-2.50256	-1.67581	H	0.67125	1.38280	-1.72833
N	2.01698	-1.38549	-1.44077	C	-1.21785	0.27954	0.93380
N	2.08571	0.94125	-1.23642	C	-1.60234	1.60165	1.55248
C	2.68945	-2.67686	-1.50862	H	-1.96749	1.42476	2.56684
H	3.74775	-2.51365	-1.32548	H	-0.72171	2.24973	1.64336
H	2.26567	-3.34654	-0.75915	C	-2.67070	2.33603	0.75928
H	2.53469	-3.12306	-2.49305	C	-3.86521	1.68546	0.42845
C	2.85125	2.16102	-0.99568	C	-2.49300	3.65580	0.34295
H	3.89398	1.95409	-1.21895	C	-4.85209	2.33894	-0.30226
H	2.46318	2.94974	-1.63928	H	-4.01251	0.65855	0.75490
H	2.74743	2.47679	0.04789	C	-3.47888	4.31422	-0.39170
P	-1.57632	-0.41778	1.37112	H	-1.56940	4.17299	0.59588
C	-2.59576	-1.23198	2.62853	C	-4.66065	3.65701	-0.71783
H	-3.64726	-1.02579	2.41820	H	-5.77572	1.82179	-0.54499
H	-2.43000	-2.31109	2.59440	H	-3.31960	5.33935	-0.71138
H	-2.32538	-0.85384	3.61608	H	-5.42914	4.16639	-1.29028
C	-1.84114	1.36205	1.46152	C	-1.73956	-0.94876	1.45933
H	-1.28170	1.84913	0.65670	O	-1.48623	-2.07397	1.02023
H	-2.90872	1.54828	1.31934	O	-2.58389	-0.79217	2.50591
H	-1.50872	1.74505	2.42840	C	-3.11321	-2.00018	3.06094
C	0.15597	-0.80788	1.69224	C	-4.03185	-1.60368	4.19621
C	0.54213	-2.15383	1.70630	H	-2.28639	-2.62902	3.40495
C	1.11058	0.20517	1.83473	H	-3.64301	-2.55161	2.27843
C	1.88334	-2.48414	1.86369	H	-4.46497	-2.49516	4.65561
H	-0.19201	-2.94470	1.57385	H	-3.48102	-1.05130	4.96079
C	2.45174	-0.13984	1.98181	H	-4.84402	-0.97137	3.82998
H	0.83387	1.25737	1.80342	P	-0.11849	-1.29069	-1.10859
C	2.83931	-1.47752	1.98919	C	0.78138	-2.65719	-0.31574
H	2.18336	-3.52681	1.87110	H	1.66993	-2.89057	-0.90188
H	3.19766	0.64348	2.06923	H	1.06018	-2.34352	0.68858
H	3.88898	-1.73511	2.08258	H	0.11597	-3.51528	-0.22955

O	0.72215	3.37147	1.22132	C	0.85264	-0.89773	-2.59728
H	0.57723	3.04522	0.30705	H	1.82198	-0.47212	-2.32955
C	1.16763	4.70670	1.14775	H	1.01089	-1.83729	-3.13371
H	0.43270	5.36235	0.66346	H	0.29896	-0.21069	-3.23784
H	1.32647	5.06850	2.16673	C	-1.71017	-1.83469	-1.78554
H	2.11851	4.79769	0.60409	C	-1.86436	-3.13736	-2.26309
M1'-sol-1				C	-2.75535	-0.91463	-1.90155
				C	-3.06988	-3.52400	-2.84136
C	4.36848	1.08383	-0.83919	H	-1.05384	-3.85668	-2.18379
C	4.76189	-0.30556	-0.99266	C	-3.95893	-1.31042	-2.47777
C	3.94190	-1.32589	-1.32760	H	-2.63791	0.10096	-1.53358
C	3.13802	1.57048	-0.61559	C	-4.11821	-2.61269	-2.94514
C	2.50935	-1.32501	-1.55440	H	-3.19028	-4.53843	-3.20640
C	1.86810	0.80655	-0.34770	H	-4.77216	-0.59617	-2.55721
C	1.56334	-0.44027	-1.15905	H	-5.05856	-2.91827	-3.39201
H	5.82521	-0.51507	-0.91532	C	2.56122	4.09674	-0.70485
H	4.41461	-2.29291	-1.48724	C	3.20750	3.69140	-1.86300
H	2.12867	-2.21910	-2.03795	C	3.67210	2.39751	-2.14316
H	3.02221	2.65149	-0.59642	C	2.07067	3.29235	0.31962
H	5.16622	1.81468	-0.95809	C	3.64419	1.23414	-1.39669
H	1.03616	1.49972	-0.51269	C	2.00623	1.89118	0.40063
C	0.13595	-0.79273	-1.22708	C	2.97665	0.94219	-0.16706
C	-0.26508	-2.08550	-0.75532	H	3.44117	4.45667	-2.59643
C	-0.84096	0.20504	-1.46361	H	4.22877	2.30932	-3.07416
C	-2.63422	-1.37079	-0.85871	H	4.24148	0.43358	-1.81378
O	-3.81726	-1.60120	-0.64729	H	1.51977	3.81176	1.10150
O	0.48315	-2.98989	-0.35939	H	2.38235	5.16396	-0.59685
O	-0.59149	1.38882	-1.79198	H	1.50070	1.53172	1.28824
N	-2.19046	-0.14001	-1.30469	C	3.15851	-0.27715	0.48960
N	-1.65238	-2.32435	-0.67213	C	3.96403	-1.37269	-0.12598
C	-3.18368	0.89474	-1.57626	C	2.81652	-0.41034	1.94087
H	-4.16442	0.42774	-1.56429	F	3.07405	0.71903	2.63659
H	-3.13057	1.68320	-0.81986	F	3.50863	-1.37760	2.55964
H	-2.97664	1.33597	-2.55225	F	1.50486	-0.67835	2.18042
C	-2.06160	-3.62718	-0.16307	F	3.79591	-2.56335	0.47016
H	-3.12598	-3.74409	-0.34556	F	3.62013	-1.59230	-1.42802
H	-1.48857	-4.39982	-0.67290	F	5.29340	-1.13981	-0.15415
H	-1.85790	-3.70316	0.90986	M2d			
P	1.64273	0.34456	1.43591				

C	2.42349	1.61671	2.46174				
H	3.48159	1.68165	2.19933				
H	1.94689	2.58104	2.26989				
H	2.30974	1.35922	3.51609				
C	2.39433	-1.25789	1.78065				
H	1.92758	-2.00798	1.12998				
H	3.45878	-1.19141	1.54359				
H	2.25725	-1.51316	2.83391				
C	-0.11806	0.28619	1.81479				
C	-0.87060	1.45228	1.63798				
C	-0.74587	-0.91385	2.16587				
C	-2.25097	1.41404	1.80481				
H	-0.41050	2.38900	1.33249				
C	-2.12634	-0.93881	2.33916				
H	-0.17534	-1.83439	2.25305				
C	-2.87872	0.21943	2.15175				
H	-2.82181	2.31884	1.62768				
H	-2.62015	-1.87185	2.59058				
H	-3.95785	0.18229	2.25622				
C	-1.93905	4.46686	-1.36628				
H	-2.25460	5.38480	-0.86365				
H	-1.12184	4.71649	-2.05526				
H	-2.78542	4.09733	-1.96202				
O	-1.54029	3.54164	-0.37980				
H	-1.23550	2.74051	-0.85389				
M1'-sol-2							
							
C	-4.87096	0.36235	1.24691	C	-3.09099	0.48932	2.26097
C	-5.17359	-0.84329	0.49650	C	-3.78570	-0.75156	1.99100
C	-4.29915	-1.82691	0.19051	C	-3.18305	-1.91250	1.63057
C	-3.66984	0.91790	1.47037	C	-1.95845	0.87405	1.65278
C	-2.87694	-1.92048	0.45711	C	-1.76727	-2.13730	1.40935
C	-2.33132	0.51456	0.91340	C	-1.33069	0.13587	0.50233
C	-1.97831	-0.95540	0.76687	C	-0.87405	-1.23917	0.94192
H	-6.21755	-0.99701	0.23794	H	-4.84700	-0.78507	2.22418
H	-4.71384	-2.70295	-0.30419	H	-3.80338	-2.80589	1.60088
H	-2.45206	-2.90527	0.29279	H	-1.42136	-3.14357	1.62616
H	-3.63943	1.79461	2.11327	H	-1.43180	1.76308	1.98937
H	-5.72479	0.85009	1.71370	H	-3.51211	1.13191	3.03026
				H	-0.44431	0.68178	0.17431
				C	0.62412	-1.57287	0.75577
				P	-2.30716	0.15446	-1.07881
				C	-2.72434	-1.48170	-1.72779
				H	-1.80685	-2.05244	-1.87028
				H	-3.37188	-2.01308	-1.03035
				H	-3.22547	-1.34775	-2.68949
				C	-1.25294	0.98653	-2.29492
				H	-1.08831	2.01832	-1.97390
				H	-0.27341	0.50034	-2.35437
				H	-1.75107	0.98548	-3.26668
				C	-3.82073	1.12373	-0.91690
				C	-5.07738	0.51926	-0.99235
				C	-3.71706	2.49830	-0.67697
				C	-6.22555	1.29121	-0.84093
				H	-5.16922	-0.54857	-1.16378
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				H	-2.74385	2.97579	-0.59728
				C	-6.12065	2.65969	-0.60753
				H	-7.20111	0.82180	-0.90702
				H	-4.78463	4.32818	-0.33778
				H	-7.01798	3.25825	-0.49017
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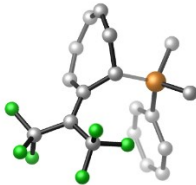
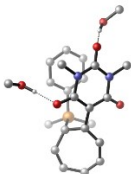
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C	2.26209	-1.33965	0.19744	H	0.58922	2.33781	0.51198
O	3.47621	-1.37439	-0.02717	C	2.61864	2.95095	0.33371
O	-0.71457	-2.45023	-1.35931	C	2.52877	3.75793	1.46853
O	0.03536	0.14918	2.52964	C	3.83046	2.92016	-0.36656
N	1.74791	-0.62582	1.24656	C	3.61860	4.51068	1.90597
N	1.36547	-2.01796	-0.59012	H	1.59272	3.78891	2.02361
C	2.71245	0.04689	2.11124	C	4.91806	3.67153	0.06342
H	3.29581	-0.69087	2.66901	H	3.90160	2.30694	-1.26095
H	3.39164	0.65055	1.50698	C	4.81829	4.46939	1.20361
H	2.14745	0.67152	2.79719	H	3.52951	5.12593	2.79669
C	1.88215	-2.72946	-1.75320	H	5.84990	3.63732	-0.49339
H	2.92091	-2.98642	-1.56503	H	5.67004	5.05295	1.53909
H	1.27698	-3.61959	-1.90967	C	2.27575	0.26592	-1.52432
H	1.81667	-2.10433	-2.65008	O	2.23796	0.89373	-2.59375
P	-1.95864	1.28961	-0.73192	O	3.00164	-0.89796	-1.44123
C	-2.81526	2.88336	-0.83774	C	3.40925	-1.47364	-2.67567
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H	-2.45057	3.55026	-0.05316	H	3.78238	-0.68817	-3.33694
H	-2.62651	3.33444	-1.81348	H	2.53963	-1.93373	-3.16528
C	-2.53197	0.22232	-2.06663	H	4.82510	-2.97179	-3.30064
H	-2.02636	-0.74867	-1.99024	H	5.33135	-2.02986	-1.88442
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H	-2.33694	0.69440	-3.03196	C	1.13006	-2.55642	1.84968
C	-0.18635	1.58149	-0.88882	C	0.70329	-2.39151	-0.56328
C	0.43467	2.44408	0.02238	F	0.66601	-2.26332	3.07082
C	0.57642	0.89504	-1.83935	F	0.73833	-3.82831	1.61563
C	1.81201	2.62511	-0.02896	F	2.45857	-2.57627	1.90164
H	-0.14539	2.95734	0.78534	F	1.84603	-3.05381	-0.70770
C	1.95439	1.08630	-1.88324	F	-0.26804	-3.33234	-0.61733
H	0.10799	0.18230	-2.51367	F	0.47846	-1.63615	-1.65405
C	2.57403	1.94979	-0.98148	TS3d			
H	2.29489	3.28244	0.68645	C	-1.47098	-0.12615	-1.26886
H	2.54988	0.54151	-2.60907	C	-0.68329	0.44300	-0.08698
H	3.65263	2.06806	-0.99325	H	-1.55638	0.58158	-2.10964
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O	5.27505	0.73589	-0.01149	H	0.74944	0.63337	-2.34657
H	4.61328	0.03274	-0.14091	C	1.44658	2.41950	-1.41902

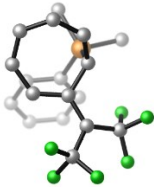
M1'-2sol

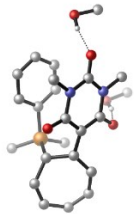
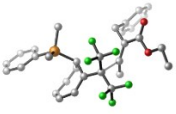


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C	-2.98366	3.23102	-0.14733
C	-2.28401	2.65259	0.86901
C	-2.05229	2.01923	-2.10302
C	-1.14448	1.78077	0.80013
C	-1.70408	0.73557	-1.40752
C	-0.78425	0.93456	-0.20575
H	-3.74536	3.96124	0.11427
H	-2.55260	2.96652	1.87668
H	-0.49882	1.79040	1.67117
H	-1.77171	2.07345	-3.15139
H	-2.94626	3.90326	-2.19863
H	-1.18505	0.09477	-2.11963
C	0.45514	0.17046	-0.19590
C	1.64202	0.72097	0.38350
C	0.46037	-1.14848	-0.72326
C	2.86047	-1.33214	-0.24254
O	3.90421	-1.98643	-0.25947
O	1.71435	1.82485	0.93396
O	-0.53572	-1.75884	-1.16300
N	1.68339	-1.83531	-0.75000
N	2.81215	-0.07083	0.29771
C	1.67585	-3.18722	-1.29959
H	2.69901	-3.55037	-1.31112
H	1.04937	-3.83544	-0.68371
H	1.26229	-3.16472	-2.30812
C	4.06612	0.42196	0.87183
H	4.32799	-0.17216	1.75125
H	4.86747	0.32951	0.13700
H	3.93357	1.46068	1.15905
P	-3.17782	-0.33135	-1.00404
C	-3.31233	-1.61706	-2.27339
H	-3.45884	-1.12119	-3.23682
H	-2.39047	-2.19723	-2.29521
H	-4.17405	-2.25298	-2.06016
C	-4.74682	0.57613	-1.13237
H	-4.80906	1.36101	-0.38020

C	0.29352	3.20346	-1.53759
C	2.67249	3.06116	-1.23191
C	0.36418	4.59160	-1.46392
H	-0.66477	2.71260	-1.68961
C	2.74786	4.45076	-1.15918
H	3.57299	2.46026	-1.14036
C	1.59364	5.22007	-1.27113
H	-0.54028	5.18460	-1.56341
H	3.71077	4.93131	-1.01631
H	1.65047	6.30246	-1.21424
C	1.55260	0.72874	1.00930
O	1.09813	0.95047	2.11428
O	2.85285	0.76385	0.74169
C	3.73700	0.96650	1.85428
C	5.12466	0.60777	1.37250
H	3.41009	0.32697	2.67762
H	3.65927	2.01021	2.17527
H	5.84465	0.71525	2.18676
H	5.13552	-0.42601	1.02116
H	5.43139	1.25846	0.54982
P	-1.56511	0.88061	1.35495
C	-1.22969	2.55459	2.02317
H	-2.15831	2.96591	2.42475
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C	-1.61117	-0.20418	2.82398
H	-0.62865	-0.18448	3.29279
H	-2.37348	0.15910	3.51856
H	-1.83649	-1.22539	2.51034
C	-3.30531	1.01087	0.82442
C	-4.25728	0.04710	1.15835
C	-3.67576	2.09752	0.02370
C	-5.56620	0.16767	0.69492
H	-3.98197	-0.80859	1.76649
C	-4.98214	2.21729	-0.43545
H	-2.93602	2.84726	-0.24829
C	-5.92861	1.25028	-0.10040
H	-6.30067	-0.58779	0.95478
H	-5.26201	3.06256	-1.05539
H	-6.94790	1.34166	-0.46126
C	-2.80655	-2.89784	-2.29503
C	-3.28584	-3.00218	-0.92894
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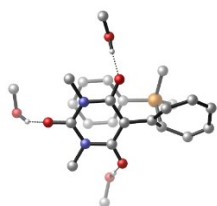
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C	-3.14330	-1.08860	0.63410	C	-0.22649	-2.16311	-0.59874
C	-2.65200	-2.38596	0.80822	H	-4.34163	-3.22286	-0.78967
C	-3.64119	-0.37158	1.72730	H	-2.98990	-3.17681	1.12261
C	-2.67234	-2.96248	2.07438	H	-0.65261	-3.18053	1.19662
H	-2.22860	-2.92469	-0.03151	H	-1.37829	-2.35927	-3.71544
C	-3.65276	-0.95416	2.98892	H	-3.39860	-3.40293	-3.05572
H	-4.00499	0.64412	1.60132	H	0.03164	-1.12746	-2.42421
C	-3.17190	-2.25040	3.16133	C	1.15808	-1.75774	-0.24353
H	-2.28959	-3.96812	2.21095	C	1.59942	-2.23017	1.12460
H	-4.03467	-0.39559	3.83668	F	0.81599	-1.74283	2.10689
H	-3.18188	-2.70371	4.14727	F	1.58012	-3.57365	1.27056
O	3.58988	3.77245	1.49622	F	2.85611	-1.85293	1.43121
H	2.84982	3.14336	1.50865	C	2.25636	-2.10011	-1.22535
C	3.79132	4.09624	0.13953	F	3.38803	-1.40145	-1.01049
H	2.92355	4.60443	-0.30181	F	2.61383	-3.40205	-1.15002
H	4.65012	4.76961	0.07844	F	1.93054	-1.88605	-2.51286
H	4.01043	3.20887	-0.47159	TS1d'			
C	7.11333	-1.51426	0.23632				
H	8.13114	-1.11631	0.22376				
H	6.61279	-1.14083	1.14052				
H	7.17525	-2.60832	0.31070				
O	6.46923	-1.09257	-0.94382				
H	5.56105	-1.43157	-0.88887				
M1'-2sol-1							
				C	1.01637	3.57306	-0.14793
C	4.99816	0.00144	-0.43791	C	1.30367	3.12806	-1.46892
C	5.00706	-1.41078	-0.77836	C	0.68589	2.05810	-2.08564
C	3.97965	-2.09840	-1.32285	C	0.47409	2.83652	0.85605
C	3.93195	0.78325	-0.20958	C	-0.27725	1.14519	-1.60987
C	2.63739	-1.64885	-1.64308	C	0.26529	1.35498	0.83817
C	2.48409	0.37427	-0.13085	C	-0.64595	0.86646	-0.29083
C	1.93801	-0.59373	-1.16568	H	1.93959	3.75929	-2.08262
H	5.95680	-1.92603	-0.66368	H	0.91949	1.93878	-3.14414
H	4.18060	-3.13130	-1.59982	H	-0.78150	0.55907	-2.37149
H	2.08103	-2.31192	-2.29846	H	0.17704	3.33622	1.77294
H	4.11112	1.84112	-0.03386	H	1.22314	4.61982	0.07224
H	5.97381	0.48254	-0.40047	H	-0.18791	1.09175	1.79504
H	1.88846	1.28978	-0.21142	C	-1.77372	0.12240	0.06438
				P	1.86808	0.39961	0.92492
				C	2.09150	-0.02959	2.67215
				H	2.13907	0.90571	3.23636
				H	1.23819	-0.61127	3.02280
				H	3.01924	-0.58702	2.81385

C	0.48552	-0.49031	-1.39644	C	3.32977	1.38163	0.49423
C	-0.31795	-1.64870	-1.14598	H	3.31758	1.63696	-0.56413
C	-0.11588	0.77847	-1.56089	H	3.31422	2.30446	1.07588
C	-2.33353	-0.23457	-1.33170	H	4.21491	0.79110	0.74074
O	-3.56087	-0.12058	-1.25362	C	1.92103	-1.10726	-0.06591
O	0.09752	-2.77319	-0.84138	C	1.71255	-2.35755	0.52433
O	0.50650	1.85815	-1.68553	C	2.19108	-1.01359	-1.43601
N	-1.51969	0.84470	-1.57078	C	1.78065	-3.50828	-0.25379
N	-1.72121	-1.45337	-1.19356	H	1.48959	-2.43898	1.58265
C	-2.13688	2.15655	-1.74404	C	2.25360	-2.16885	-2.20703
H	-3.19197	2.00782	-1.95520	H	2.33822	-0.04424	-1.90172
H	-2.01349	2.75674	-0.83765	C	2.04853	-3.41363	-1.61700
H	-1.64207	2.66550	-2.57130	H	1.61927	-4.47736	0.20553
C	-2.60507	-2.58450	-0.92568	H	2.45844	-2.09505	-3.26950
H	-3.34709	-2.65994	-1.72243	H	2.09442	-4.31310	-2.22215
H	-1.98825	-3.47719	-0.88783	C	-2.91614	-0.03215	-0.86782
H	-3.12811	-2.43893	0.02395	F	-3.08090	1.04008	-1.66478
P	1.97909	-0.27185	1.53306	F	-2.81258	-1.09224	-1.71455
C	2.96964	0.55928	2.80112	F	-4.09048	-0.20244	-0.22253
H	4.02586	0.34682	2.62353	C	-1.86221	-0.59968	1.34662
H	2.80442	1.63741	2.74060	F	-2.70495	-1.64121	1.32159
H	2.67139	0.20147	3.78817	F	-0.64961	-1.12332	1.73756
C	2.23326	-2.05361	1.64365	F	-2.23334	0.15410	2.41967
H	1.61988	-2.53943	0.87496	M1d'			
H	3.28792	-2.25936	1.44689				
H	1.95938	-2.40342	2.64148	C	1.01637	3.57306	-0.14793
C	0.23927	0.11243	1.79545	C	1.30367	3.12806	-1.46892
C	-0.16060	1.45163	1.71202	C	0.68589	2.05810	-2.08564
C	-0.70850	-0.90047	1.97357	C	0.47409	2.83652	0.85605
C	-1.51139	1.77271	1.79202	C	-0.27725	1.14519	-1.60987
H	0.55545	2.25372	1.54825	C	0.26529	1.35498	0.83817
C	-2.05733	-0.56772	2.06485	C	-0.64595	0.86646	-0.29083
H	-0.40854	-1.94405	1.99666	H	1.93959	3.75929	-2.08262
C	-2.45895	0.76337	1.96292	H	0.91949	1.93878	-3.14414
H	-1.80573	2.81209	1.69382	H	-0.78150	0.55907	-2.37149
H	-2.81136	-1.33832	2.18245	H	0.17704	3.33622	1.77294
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H	-0.32105	5.94486	-0.09081	C	-1.77372	0.12240	0.06438
H	0.74567	5.30137	-1.35423				
H	-1.00941	5.03093	-1.44548				
O	-0.01789	3.93691	0.03170				
H	0.14335	3.18997	-0.58087				
C	-5.96916	-1.72281	0.46278				

H	-6.50757	-2.22233	1.27167	P	1.86808	0.39961	0.92492
H	-5.63773	-2.48807	-0.25258	C	2.09150	-0.02959	2.67215
H	-6.66845	-1.05273	-0.05346	H	2.13907	0.90571	3.23636
O	-4.88277	-1.02385	1.03026	H	1.23819	-0.61127	3.02280
H	-4.39756	-0.61817	0.28891	H	3.01924	-0.58702	2.81385
M1'-2sol-2				C	3.32977	1.38163	0.49423
				H	3.31758	1.63696	-0.56413
C	-5.09980	-0.50679	-0.29127	H	3.31422	2.30446	1.07588
C	-5.09070	0.89867	-0.65581	H	4.21491	0.79110	0.74074
C	-4.08577	1.54252	-1.28822	C	1.92103	-1.10726	-0.06591
C	-4.04340	-1.31886	-0.13345	C	1.71255	-2.35755	0.52433
C	-2.78245	1.05152	-1.69491	C	2.19108	-1.01359	-1.43601
C	-2.58118	-0.96183	-0.17216	C	1.78065	-3.50828	-0.25379
C	-2.07508	-0.01120	-1.24375	H	1.48959	-2.43898	1.58265
H	-6.01256	1.44655	-0.48102	C	2.25360	-2.16885	-2.20703
H	-4.27624	2.57612	-1.57032	H	2.33822	-0.04424	-1.90172
H	-2.25715	1.69200	-2.39527	C	2.04853	-3.41363	-1.61700
H	-4.24382	-2.36665	0.07742	H	1.61927	-4.47736	0.20553
H	-6.08380	-0.95562	-0.16871	H	2.45844	-2.09505	-3.26950
H	-2.02766	-1.89797	-0.30246	H	2.09442	-4.31310	-2.22215
C	-0.63750	-0.14481	-1.53501	C	-2.91614	-0.03215	-0.86782
C	0.18890	1.00448	-1.42906	F	-3.08090	1.04008	-1.66478
C	-0.04681	-1.44320	-1.63897	F	-2.81258	-1.09224	-1.71455
C	2.19451	-0.42846	-1.51210	F	-4.09048	-0.20244	-0.22253
O	3.42197	-0.54050	-1.45818	C	-1.86221	-0.59968	1.34662
O	-0.20288	2.17990	-1.25193	F	-2.70495	-1.64121	1.32159
O	-0.66161	-2.51328	-1.70897	F	-0.64961	-1.12332	1.73756
N	1.36368	-1.51244	-1.63015	F	-2.23334	0.15410	2.41967
N	1.58390	0.80395	-1.47113	TS2d'			
C	1.94944	-2.84466	-1.73470				
H	3.02553	-2.75290	-1.61856	C	-2.74126	0.76431	2.17356
H	1.52849	-3.48278	-0.95729	C	-3.55295	-0.42386	2.18500
H	1.70655	-3.27830	-2.70672	C	-3.13561	-1.66071	1.79150
C	2.44038	1.97375	-1.29704	C	-1.72361	1.00115	1.32234
H	3.43117	1.73335	-1.67352	C	-1.84491	-2.05133	1.29101
H	2.00440	2.80466	-1.84938	C	-1.37703	0.11917	0.15918
H	2.49822	2.24599	-0.23702	C	-0.94776	-1.27455	0.61497
P	-1.92028	-0.34409	1.44915	H	-4.53566	-0.34489	2.64272
C	-2.88486	-1.08416	2.79274	H	-3.82364	-2.48354	1.97756

H	-3.93478	-0.81177	2.66708	H	-1.57441	-3.08691	1.47118
H	-2.79126	-2.17181	2.75920	H	-1.08768	1.87054	1.46560
H	-2.51068	-0.71689	3.75009	H	-2.96131	1.51953	2.92498
C	-2.04644	1.45106	1.55798	H	-0.53190	0.56971	-0.35924
H	-1.52716	1.90295	0.70709	C	0.43785	-1.65435	0.31749
H	-3.10528	1.71788	1.51297	P	-2.67100	0.11259	-1.17749
H	-1.60157	1.80228	2.49135	C	-2.84959	-1.52133	-1.92657
C	-0.19976	-0.85401	1.62178	H	-1.88200	-1.82584	-2.32796
C	0.09927	-2.22241	1.63102	H	-3.15008	-2.24359	-1.16537
C	0.82636	0.09680	1.65949	H	-3.59111	-1.46724	-2.72646
C	1.42568	-2.63614	1.68865	C	-2.04991	1.24684	-2.44844
H	-0.69180	-2.96645	1.57569	H	-1.87169	2.22944	-2.00527
C	2.15022	-0.33218	1.70019	H	-1.10673	0.85668	-2.83543
H	0.61397	1.16382	1.63137	H	-2.78150	1.33911	-3.25304
C	2.45134	-1.69255	1.71282	C	-4.30244	0.72313	-0.70400
H	1.65738	-3.69621	1.69864	C	-5.39273	-0.14813	-0.63122
H	2.96204	0.38843	1.70348	C	-4.46856	2.08094	-0.41308
H	3.49181	-1.99932	1.73576	C	-6.64384	0.33937	-0.27058
O	0.61246	3.30045	1.08589	H	-5.26901	-1.20623	-0.83936
H	0.36265	3.01719	0.18184	C	-5.72108	2.56046	-0.04497
C	1.21300	4.57360	1.01045	H	-3.62607	2.76474	-0.45671
H	0.53212	5.32859	0.59753	C	-6.80677	1.69095	0.02561
H	1.48609	4.87867	2.02350	H	-7.48962	-0.33734	-0.21678
H	2.12765	4.56685	0.40097	H	-5.84795	3.61263	0.18527
C	5.59675	0.81945	0.53001	H	-7.78312	2.06797	0.31162
H	6.35857	1.02715	1.28552	C	1.38679	0.14818	2.14680
H	4.80472	1.57692	0.62981	C	1.67466	-0.00308	0.86523
H	6.05407	0.93685	-0.46089	H	0.64672	-0.44191	2.67389
O	5.11801	-0.48826	0.74381	H	1.93533	0.90460	2.70385
H	4.51334	-0.67874	0.00635	C	2.36738	0.59767	-0.15538

M1'-3sol

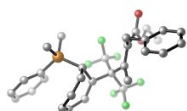


C	5.00605	0.84911	-0.39734
C	5.16130	-0.49598	-0.92428
C	4.21196	-1.20194	-1.57599
C	3.86282	1.46866	-0.06772
C	2.83467	-0.84121	-1.86046
C	2.47279	0.88737	-0.05198
C	2.03199	0.05419	-1.24259
H	6.15797	-0.92465	-0.86320
H	4.51706	-2.16142	-1.98857
H	2.35691	-1.43822	-2.63129
H	3.92216	2.50819	0.24469
H	5.92412	1.42469	-0.29568
H	1.77927	1.73235	0.01249
C	0.58007	0.07113	-1.50685
C	-0.12777	-1.15978	-1.45037
C	-0.12920	1.29628	-1.50388
C	-2.25641	0.07280	-1.46244
O	-3.48555	0.07708	-1.39457
O	0.38699	-2.29129	-1.32954
O	0.40059	2.42755	-1.44828
N	-1.53264	1.23739	-1.55040
N	-1.53220	-1.09712	-1.47984
C	-2.27400	2.49536	-1.58616
H	-3.25326	2.30485	-2.01764
H	-2.38121	2.90921	-0.57902
H	-1.71219	3.19928	-2.19873
C	-2.26160	-2.35940	-1.38291
H	-3.30881	-2.16085	-1.59370
H	-1.84690	-3.05967	-2.10830
H	-2.14978	-2.78567	-0.38118
P	2.06940	-0.06079	1.48910
C	2.95455	0.70351	2.87274
H	4.02771	0.67522	2.67284
H	2.63321	1.74300	2.97311
H	2.72560	0.16310	3.79297
C	2.54016	-1.79761	1.35247
H	1.98478	-2.24397	0.52032

C	3.59359	0.06203	-0.69065
O	4.20236	0.52139	-1.65160
O	4.04582	-1.02690	-0.01977
C	5.15502	-1.69173	-0.61639
C	5.39016	-2.96601	0.16635
H	6.03130	-1.03460	-0.59823
H	4.92737	-1.90054	-1.66731
H	6.24773	-3.50701	-0.24198
H	5.58884	-2.73887	1.21662
H	4.50884	-3.60820	0.11584
C	0.95192	-2.83515	1.08880
C	0.71294	-1.82285	-1.14173
F	1.98640	-2.08133	-1.43601
F	0.35641	-0.72196	-1.86281
F	-0.00431	-2.83668	-1.70818
F	0.40639	-4.02124	0.69121
F	2.27492	-2.99547	0.97426
F	0.68050	-2.73852	2.40297

H	3.61167	-1.85617	1.15042
H	2.30059	-2.31620	2.28345
C	0.29447	0.05195	1.76702
C	-0.30279	1.31872	1.78618
C	-0.48744	-1.10336	1.85019
C	-1.68662	1.42311	1.85799
H	0.28264	2.23281	1.71655
C	-1.87290	-0.98260	1.93194
H	-0.04761	-2.09541	1.82192
C	-2.47751	0.27332	1.92017
H	-2.13274	2.41197	1.84373
H	-2.47527	-1.88403	1.99085
H	-3.56067	0.36120	1.93348
O	-0.24630	-3.96294	0.72453
H	-0.05562	-3.40093	-0.05449
C	-0.49848	-5.27057	0.26211
H	0.36346	-5.69843	-0.26597
H	-0.71430	-5.90047	1.12865
H	-1.36652	-5.31112	-0.41060
C	-0.77420	5.35212	0.05474
H	-1.08297	5.99342	0.88381
H	0.09717	5.81221	-0.42871
H	-1.59512	5.32376	-0.67579
O	-0.48396	4.07475	0.57602
H	-0.18807	3.51330	-0.16890
C	-5.51158	-1.11631	0.55869
H	-6.22056	-1.42236	1.33210
H	-4.54627	-1.60432	0.75992
H	-5.87561	-1.48251	-0.41006
O	-5.41260	0.28919	0.59402
H	-4.77339	0.51990	-0.09918

M2d'



C	1.91241	-2.88225	1.36528
C	3.02762	-2.13744	1.91776
C	3.05536	-0.79847	2.10378
C	1.00201	-2.41780	0.49343
C	1.99775	0.14770	1.80385
C	1.06618	-1.06737	-0.18157

C	1.03987	0.03996	0.85982
H	3.86119	-2.71824	2.30373
H	3.91761	-0.38346	2.62034
H	1.97634	1.01410	2.45600
H	0.13608	-3.02654	0.25031
H	1.78067	-3.89746	1.73280
H	0.17335	-0.95642	-0.81761
C	-0.17977	0.97800	0.75895
P	2.42360	-1.02618	-1.45100
C	2.05286	0.14495	-2.78053
H	1.04842	-0.04029	-3.16513
H	2.10930	1.17030	-2.41888
H	2.79408	-0.01209	-3.56760
C	2.41973	-2.66466	-2.21868
H	2.64812	-3.43332	-1.48017
H	1.41921	-2.84797	-2.61994
H	3.14681	-2.68711	-3.03267
C	4.08312	-0.64338	-0.86781
C	4.38421	0.67161	-0.49543
C	5.04888	-1.64809	-0.76239
C	5.64834	0.96941	0.00139
H	3.63424	1.45270	-0.56447
C	6.31186	-1.33893	-0.26958
H	4.82104	-2.66999	-1.04788
C	6.60835	-0.03409	0.11798
H	5.88237	1.98586	0.29805
H	7.06232	-2.11728	-0.18619
H	7.59279	0.20290	0.50739
C	-1.54689	-0.84582	1.68393
C	-1.43403	0.01315	0.64279
H	-0.83649	-0.89488	2.49912
H	-2.37801	-1.54098	1.70767
C	-2.19382	-0.16528	-0.57521
C	-2.61144	-1.56069	-0.98641
H	-2.74274	-1.54998	-2.07558
H	-1.80973	-2.27816	-0.75373
C	-3.90000	-2.09949	-0.38441
C	-3.92390	-3.27515	0.36732
C	-5.10473	-1.41517	-0.58815
C	-5.11317	-3.75957	0.91205
H	-2.99254	-3.81302	0.53697
C	-6.29325	-1.89685	-0.05074
H	-5.08943	-0.50609	-1.18322
C	-6.30350	-3.07086	0.70384

H	-5.10725	-4.67290	1.49994
H	-7.21936	-1.35534	-0.22041
H	-7.23230	-3.44293	1.12508
C	-2.78641	0.88805	-1.29938
O	-3.40315	0.82274	-2.37111
O	-2.65008	2.10440	-0.65518
C	-3.01673	3.25791	-1.39505
C	-3.23692	4.38557	-0.40536
H	-3.91905	3.04634	-1.97316
H	-2.21686	3.50690	-2.10666
H	-3.51331	5.30512	-0.92844
H	-4.04027	4.12335	0.28753
H	-2.33273	4.57023	0.17806
C	0.14592	1.96700	-0.40472
C	-0.33836	1.87928	2.00188
F	-0.15737	1.49656	-1.61512
F	-0.37534	3.18322	-0.27997
F	1.49694	2.18223	-0.44307
F	0.65095	2.80300	2.06252
F	-1.49151	2.53875	1.97459
F	-0.28269	1.20901	3.15684
TS3d'			
C	-1.47098	-0.12615	-1.26886
C	-0.68329	0.44300	-0.08698
H	-1.55638	0.58158	-2.10964
H	-2.49231	-0.37287	-0.97608
C	0.72924	0.36187	-0.19291
C	1.36373	0.90531	-1.48837
H	2.36079	0.49536	-1.63864
H	0.74944	0.63337	-2.34657
C	1.44658	2.41950	-1.41902
C	0.29352	3.20346	-1.53759
C	2.67249	3.06116	-1.23191
C	0.36418	4.59160	-1.46392
H	-0.66477	2.71260	-1.68961
C	2.74786	4.45076	-1.15918
H	3.57299	2.46026	-1.14036
C	1.59364	5.22007	-1.27113
H	-0.54028	5.18460	-1.56341
H	3.71077	4.93131	-1.01631
H	1.65047	6.30246	-1.21424
C	1.55260	0.72874	1.00930
O	1.09813	0.95047	2.11428

O	2.85285	0.76385	0.74169
C	3.73700	0.96650	1.85428
C	5.12466	0.60777	1.37250
H	3.41009	0.32697	2.67762
H	3.65927	2.01021	2.17527
H	5.84465	0.71525	2.18676
H	5.13552	-0.42601	1.02116
H	5.43139	1.25846	0.54982
P	-1.56511	0.88061	1.35495
C	-1.22969	2.55459	2.02317
H	-2.15831	2.96591	2.42475
H	-0.47130	2.49860	2.80087
H	-0.86042	3.19040	1.21462
C	-1.61117	-0.20418	2.82398
H	-0.62865	-0.18448	3.29279
H	-2.37348	0.15910	3.51856
H	-1.83649	-1.22539	2.51034
C	-3.30531	1.01087	0.82442
C	-4.25728	0.04710	1.15835
C	-3.67576	2.09752	0.02370
C	-5.56620	0.16767	0.69492
H	-3.98197	-0.80859	1.76649
C	-4.98214	2.21729	-0.43545
H	-2.93602	2.84726	-0.24829
C	-5.92861	1.25028	-0.10040
H	-6.30067	-0.58779	0.95478
H	-5.26201	3.06256	-1.05539
H	-6.94790	1.34166	-0.46126
C	-2.80655	-2.89784	-2.29503
C	-3.28584	-3.00218	-0.92894
C	-2.50091	-2.96831	0.17088
C	-1.68054	-2.27645	-2.67381
C	-1.06174	-2.78554	0.27424
C	-0.79654	-1.42593	-1.79286
C	-0.22649	-2.16311	-0.59874
H	-4.34163	-3.22286	-0.78967
H	-2.98990	-3.17681	1.12261
H	-0.65261	-3.18053	1.19662
H	-1.37829	-2.35927	-3.71544
H	-3.39860	-3.40293	-3.05572
H	0.03164	-1.12746	-2.42421
C	1.15808	-1.75774	-0.24353
C	1.59942	-2.23017	1.12460
F	0.81599	-1.74283	2.10689

F	1.58012	-3.57365	1.27056
F	2.85611	-1.85293	1.43121
C	2.25636	-2.10011	-1.22535
F	3.38803	-1.40145	-1.01049
F	2.61383	-3.40205	-1.15002
F	1.93054	-1.88605	-2.51286