Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Computational Data

Blue Light Enhanced Heck Arylation at Room Temperature Applied to Allenes

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Computational method.

The structures of the reactants, intermediates and transition states have been optimized by using the density functional method (DFT)[1] with the functional M0[2,3] and the basis sets def2-SVP.[4] The electronic energy values where refined by re-optimization with the basis set def2-TZVP.[5] The nature of the critical points was characterized by using vibrational analysis[6] which also furnished the Zero Point Energies (ZPE) and entropies for the calculations of the Free Energies. These have been converted from the gas phase to the 1 M standard state at 1 atm and 298.15 K.[7] The solvent effects (*N*,*N*-dimethylformammide, DMF) were introduced in all calculations using the universal solvation model (SMD) by Truhalr *et al*.[8] The singlet excited states have been optimized with the Time-Dependet DFT.[9] To reduce the calculation times, the methyl group of the tosyl has been substituted by H. The calculations were performed by the quantum package Gaussian 16-A.03[10] The figures were obtained using the graphical program Molden.[11]

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[3] Y. Zhao, D.G. Truhlar, Density functionals with broad applicability in chemistry, *Acc. Chem. Res.* 41 (2008) 157–167, DOI: 10.1021/ar700111a.

[4] A. Schaefer, H. Horn, and R. Ahlrichs, "Fully optimized contracted Gaussian-basis sets for atoms Li to Kr," *J. Chem. Phys.*, 97 (1992) 2571–2577. DOI: 10.1063/1.463096.

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[7] R.F. Ribeiro, A.V. Marenich, C.J. Cramer, D.G. Truhlar, Use of solution-phase vibrational frequencies in continuum models for the free energy of solvation, *J. Phys. Chem. B.* 115 (2011) 14556–14562, DOI: 10.1021/jp205508z.

[8] A. V. Marenich, C. J. Cramer, and D. G. Truhlar, "Universal solvation model based on solute electron density and a continuum model of the solvent defined by the bulk dielectric constant and atomic surface tensions," *J. Phys. Chem. B*, 113 (2009) 6378–6396. DOI: 10.1021/jp810292n .

[9] F. Furche and R. Ahlrichs, "Adiabatic time-dependent density functional methods for excited state properties," *J. Chem. Phys.*, 117 (2002) 7433–7447. DOI: 10.1063/1.1508368

[10] D.J. 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.; Hratch, Gaussian 16, Revision A.03, (2016).

[11] G. Schaftenaar, J.H. Noordik, Molden: A pre- and post-processing program for molecular and electronic structures, J. Comput. Aided. Mol. Des. 14 (2000) 123–134, DOI: 10.1023/A:1008193805436.

Table R. Calculated absolute and relative (in kcal mol^{-1}) energies for the palladium(II) reduction.

Pd(II) Reduction		E(DZ) /au	**ΔE[a]**	E(TZ) /au	**ΔE[b]**	ZPE /au	E^{0K} /au	**ΔE^{0K} c**	δG^{298K}/au	G^{298K} /au	**Δn**	**ΔG^{298K} c**
trans-$(DMF)_2Pd^{II}(AcO)_2$	**0**	-1080.68473		-1081.80391		0.30890	-1081.495006		0.25041	-1081.553494		
Ph_3P		-1035.13659		-1035.99747		0.27170	-1035.725767		0.22551	-1035.771957		
DMF		-248.17312		-248.45568		0.10131	-248.354365		0.07234	-248.383342		
0 + 2 Ph_3P + DMF		-3399.13104	**0.00**	-3402.25452	**0.00**	0.95362	-3401.300903	**0.00**	0.77377	-3401.480748	**0**	**0.00**
$(DMF)_3Pd^0(Ph_3P)$	**I**	-1907.63817		-1909.37966		0.57903	-1908.800638		0.49813	-1908.881536		
$Ph_3P=O$		-1110.30489		-1111.27492		0.27695	-1110.997973		0.23044	-1111.044485		
$(Ac)_2O$		-381.24469		-381.68131		0.09768	-381.583635		0.06439	-381.616920		
I + Ph_3PO + Ac_2O		-3399.18775	**-35.59**	-3402.33590	**-51.07**	0.95366	-3401.382245	**-51.04**	0.79296	-3401.542940	**-1**	**-40.92**

[a] M06/def2-SVP; [b] M06/def2-TZVP; [c] M06/def2-TZVP enegies combined with thermal corrections calculated with the M06/def2-SVP.

Scheme 1. The oxidative addition step step to $(DMF)_3Pd^0(PPh_3)$, **I** (Figure 4 in the article).

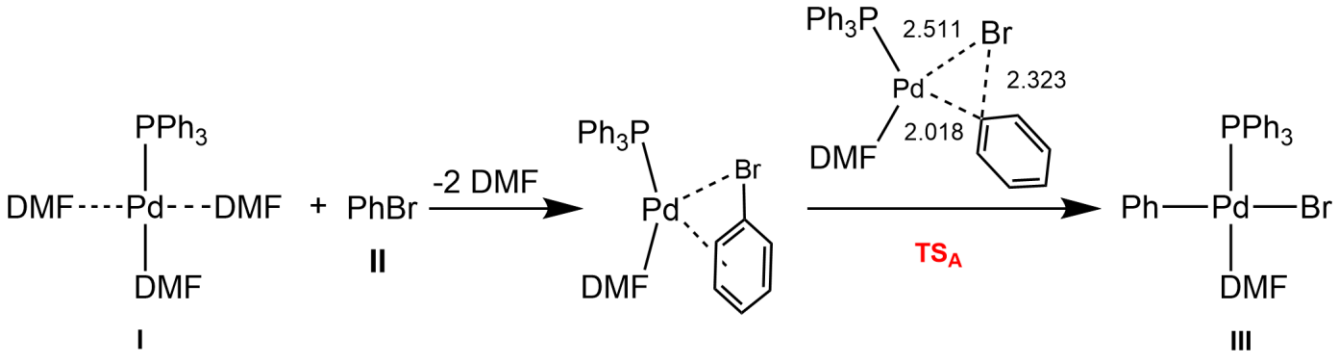


Table 1. Calculated absolute and relative (in kcal mol^{-1}) energies for the oxidative addition step to $(DMF)_3Pd^0(PPh_3)$, **I.**

Scheme 1		E(DZ) /au	**ΔE[a]**	E(TZ) /au	**ΔE[b]**	ZPE /au	E^{0K} /au	**ΔE^{0K} c**	δG^{298K}/au	G^{298K} /au	**Δn**	**ΔG^{298K} c**
$(DMF)_3Pd^0(Ph_3P)$	**I**	-1907.63817		-1909.37966		0.57903	-1908.800638		0.49813	-1908.881536		
Ph-Br	**II**	-2805.04742	**II**	-2805.61567	**II**	0.08986	-2805.525808		0.05896	-2805.556708		
I + II		-4712.68559	**0.00**	-4714.99533	**0.00**		-4714.326445	**0.00**		-4714.438243	**0**	**0.00**
[PhBr * Pd^0Br (DMF)(Ph_3P)]	**C-I**	-4216.32727		-4218.07798		0.46480	-4217.613185		0.39158	-4217.686408		
Dimer of DMF		-496.35029		-496.91239		0.20364	-496.708749		0.15844	-496.753954		
C-I + $(DMF)_2$		-4712.67757	**5.03**	-4714.99038	**3.11**		-4714.321934	**2.83**		-4714.440362	**0**	**-1.33**
TS_A	**TS_A**	-4216.32064		-4218.07188		0.46479	-4217.607094		0.39360	-4217.678285		
TS_A + $(DMF)_2$		-4712.67093	**9.20**	-4714.98428	**6.94**		-4714.315844	**6.65**		-4714.432240	**0**	**3.77**
trans-[Ph-Pd^0-Br (DMF)(Ph_3P)]	**III**	-4216.35406		-4218.09845		0.46555	-4217.632902		0.39621	-4217.702244		
III[1] + $(DMF)_2$		-4712.70435	**-11.77**	-4715.01084	**-9.73**		-4714.341651	**-9.54**		-4714.456198	**0**	**-11.27**

[a] M06/def2-SVP; [b] M06/def2-TZVP; [c] M06/def2-TZVP enegies combined with thermal corrections calculated with the M06/def2-SVP.

Scheme 2. The oxidative addition step step to $(DMF)_2Pd^0(PPh_3)_2$, **I'**.

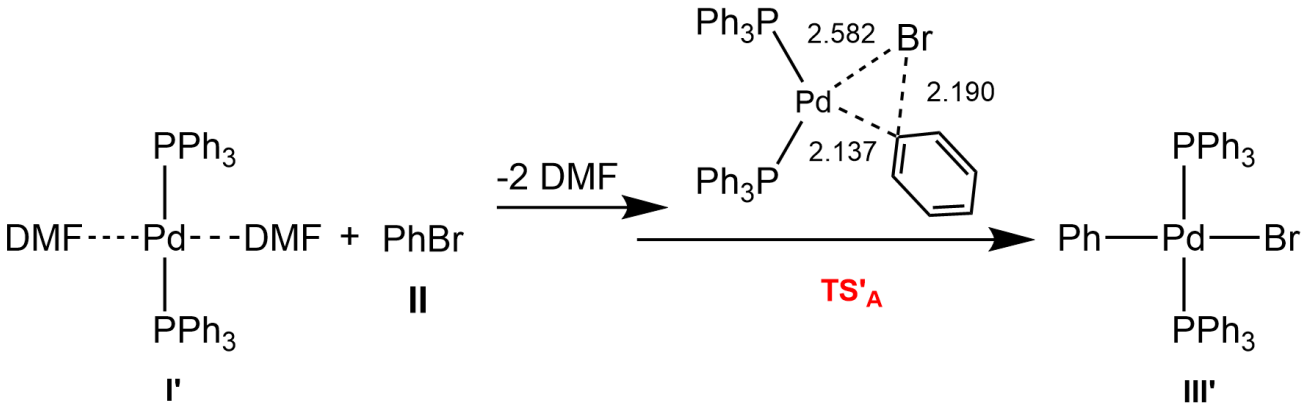
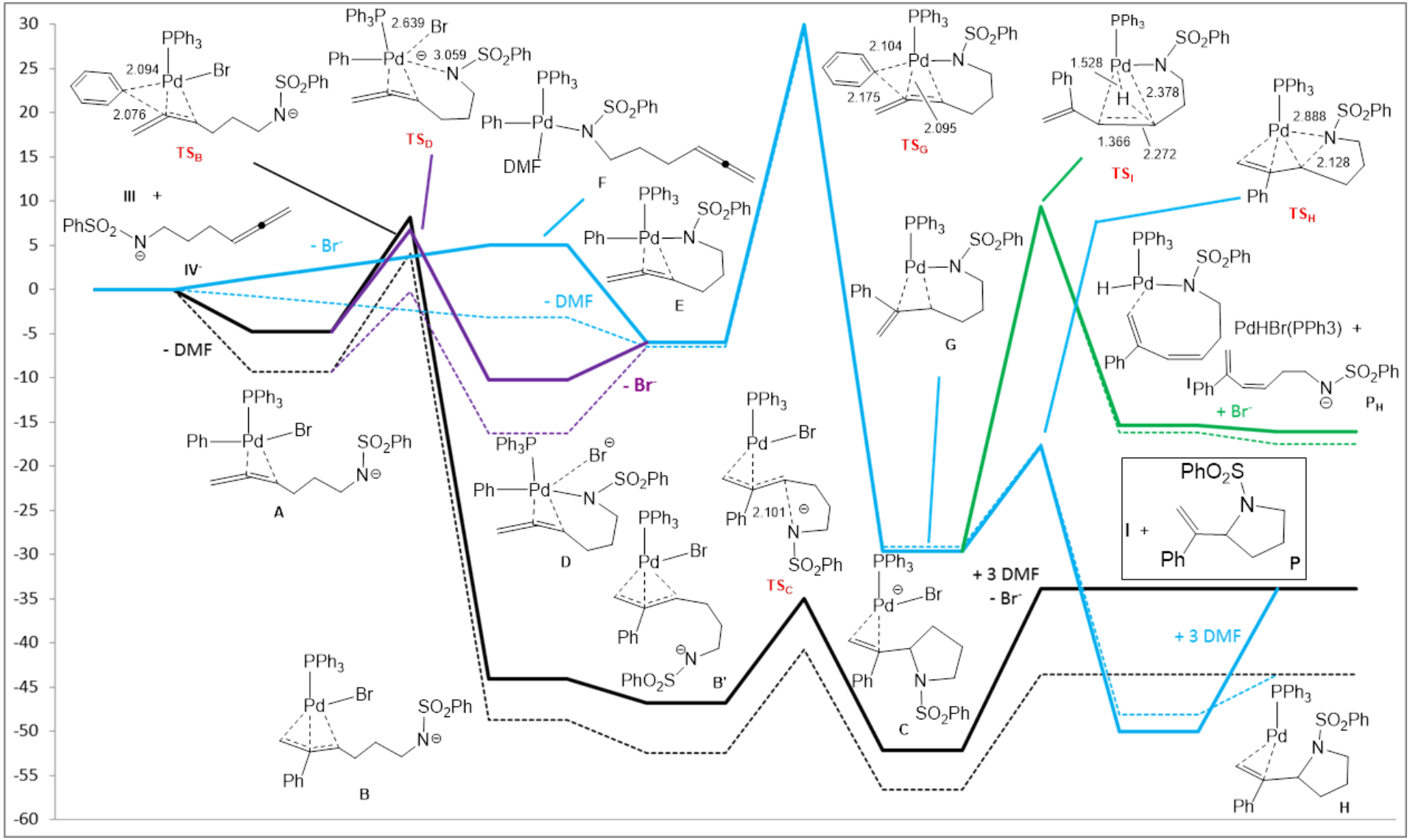


Table 2. Calculated absolute and relative (in kcal mol^{-1}) energies for the oxidative addition step to $(DMF)_2Pd^0(PPh_3)_2$, **I'.**

Scheme 2		E(DZ) /au	**ΔE[a]**	E(TZ) /au	**ΔE[b]**	ZPE /au	E^{0K} /au	**ΔE^{0K} c**	δG^{298K}/au	G^{298K} /au	**Δn**	**ΔG^{298K} c**
trans-$(DMF)_2Pd^0(Ph_3P)_2$	**I'**	-2694.64018		-2696.96564		0.75079	-2696.21485		0.65716	-2696.30848		
Ph-Br	**II**	-2805.04742		-2805.61567		0.08986	-2805.52581		0.05896	-2805.55671		
I' + II		-5499.68760	**0.00**	-5502.58131	**0.00**		-5501.74066	**0.00**		-5501.86519	**0**	**0.00**
Dimer of DMF		-496.35029		-496.91239		0.20364	-496.70875		0.15844	-496.75395		
TS_{OA} to III'	**TS'A**	-5003.31069		-5005.63381		0.63454	-5004.99926		0.55172	-5005.08209		
TS_{OA} to III' + $(DMF)_2$		-5499.66098	**16.70**	-5502.54620	**22.03**		-5501.70801	**20.49**		-5501.83604	**0**	**18.29**
trans-[Ph-Pd^0-Br $(Ph_3P)_2$]	**III'**	-5003.36214		-5005.68584		0.63699	-5005.04886		0.55495	-5005.13090		
III' + $(DMF)_2$		-5499.71243	**-15.58**	-5502.59824	**-10.62**		-5501.75761	**-10.63**		-5501.88485	**0**	**-12.34**

[a] M06/def2-SVP; [b] M06/def2-TZVP; [c] M06/def2-TZVP enegies combined with thermal corrections calculated with the M06/def2-SVP.

Figure 1. Energy profiles in kcal mol-1 (dashed lines are E+ZPE; thick lines are free energies) following the formation of intermediate **III**.



Scheme 3. The favoured pathway (black profiles in Figure 1).

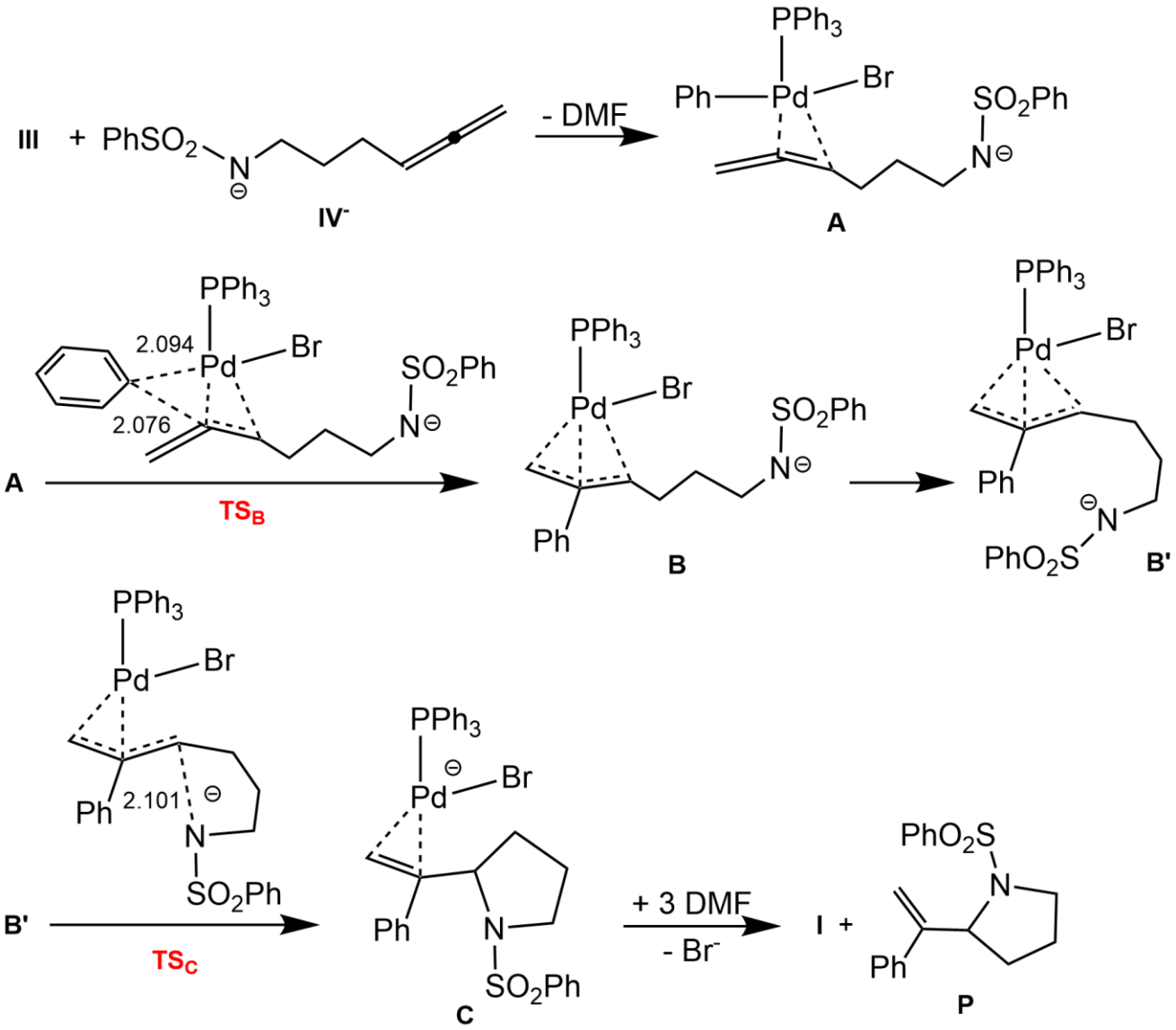


Table 3. Calculated absolute and relative energies for the favoured pathway.

Scheme 3		E(DZ) /au	**ΔE[a]**	E(TZ) /au	**ΔE[b]**	ZPE /au	E^{0K} /au	**ΔE^{0K} c**	δG^{298K}/au	G^{298K} /au	**Δn**	**ΔG^{298K} c**
[Ph-Pd^0-Br (DMF)(Ph_3P)]	**III**	-4216.35406		-4218.09845		0.46555	-4217.632902		0.39621	-4217.702244		
$PhSO_2N^-$-$CH_2CH_2CH_2CHCCH_2$	**IV^-**	-1067.98471		-1068.93295		0.23436	-1068.698591		0.18709	-1068.745856		
III + IV^-		-5284.33876	**0.00**	-5287.03140	**0.00**		-5286.331493	**0.00**		-5286.448100	**0**	**0.00**
Int-A [Ph-Pd^0-Br (Ph_3P)(IV^-)]	**A**	-5036.18903		-5038.59253		0.60059	-5037.991940		0.52013	-5038.072402		
Int-A + DMF		-5284.36215	**-14.67**	-5287.04821	**-10.55**		-5286.346305	**-9.29**		-5286.455744	**0**	**-4.80**
TS_B	**TS_B**	-5036.16303		-5038.57005		0.59943	-5037.970622		0.51818	-5038.051873		
TS_B + DMF		-5284.33615	**1.64**	-5287.02573	**3.56**		-5286.324987	**4.08**		-5286.435215	**0**	**8.09**
Int-B Pd^0-CCC bound	**B**	-5036.25709		-5038.65911		0.60433	-5038.054780		0.52412	-5038.134995		
Int-B + DMF		-5284.43021	**-57.38**	-5287.11479	**-52.33**		-5286.409145	**-48.73**		-5286.518337	**0**	**-44.07**
Int-B' Pd^0-CCC & Tos *endo*	**B'**	-5036.26403		-5038.66511		0.60439	-5038.060715		0.52582	-5038.139290		
Int-B + DMF		-5284.43715	**-61.74**	-5287.12079	**-56.09**		-5286.415080	**-52.45**		-5286.522632	**0**	**-46.77**
TS_C	**TS_C**	-5036.25036		-5038.64611		0.60402	-5038.042094		0.52567	-5038.120440		
TS_C + DMF		-5284.42348	**-53.16**	-5287.10179	**-44.17**		-5286.396458	**-40.77**		-5286.503781	**0**	**-34.94**
Int-C	**C**	-5036.28260		-5038.67329		0.60594	-5038.067344		0.52541	-5038.147877		
Int-C + DMF		-5284.45572	**-73.39**	-5287.12896	**-61.22**		-5286.421709	**-56.61**		-5286.531219	**0**	**-52.16**
Product	**P**	-1299.24017		-1300.41816		0.33261	-1300.085546		0.28331	-1300.134849		
Br^-		-2573.88879		-2574.22346		0.00000	-2574.223457		-0.01618	-2574.239633		
P + Br^- + I - $(DMF)_2$		-5284.41684	**-48.99**	-5287.10889	**48.63**		-5286.40089	**-43.55**		-5286.50206	**0**	**-33.86**

[a] M06/def2-SVP; [b] M06/def2-TZVP; [c] M06/def2-TZVP enegies combined with thermal corrections calculated with the M06/def2-SVP.

Scheme 4. The alternative generation of intermediate **E** (violet and first part of blue profiles).

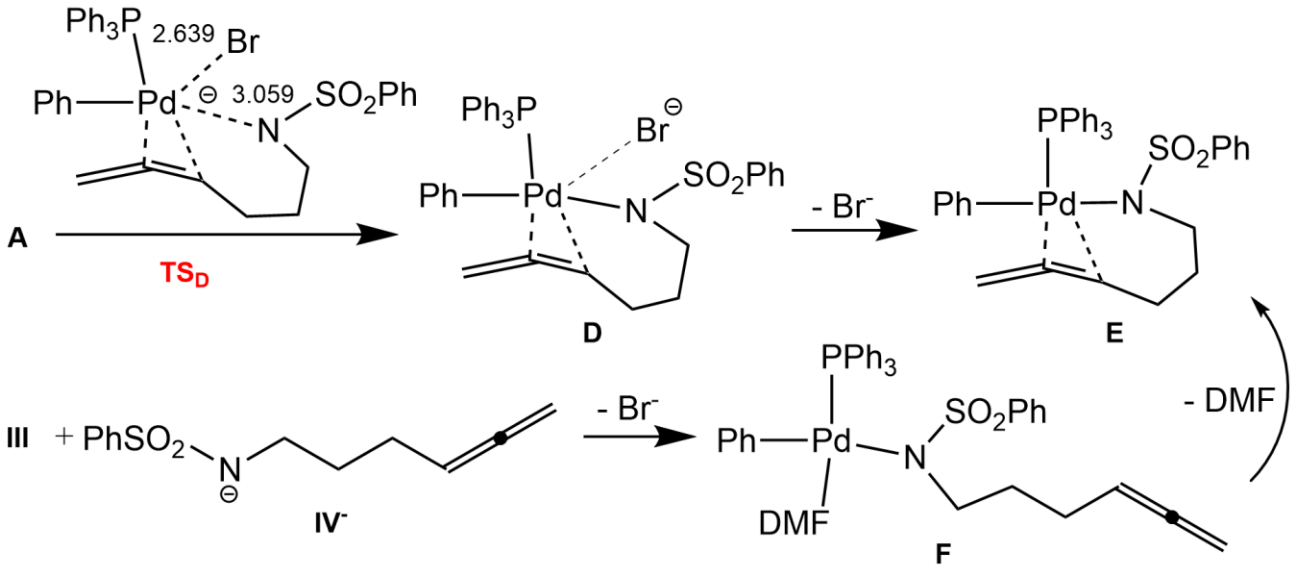


Table 4. Calculated absolute and relative energies for the alternative generation of **E**.

Scheme 4		E(DZ) /au	**ΔE[a]**	E(TZ) /au	**ΔE[b]**	ZPE /au	E^{0K} /au	**ΔE^{0K} [c]**	δG^{298K}/au	G^{298K} /au	**Δn**	**ΔG^{298K}_{c}**
TS_D from A	**TS_D**	-5036.18071		-5038.57799		0.60049	-5037.977504		0.52396	-5038.054036	5.2	
TS_D + DMF		-5284.35383	**-9.46**	-5287.03367	**-1.43**		-5286.331868	**-0.24**		-5286.437377	**0**	**6.73**
Int-D *N bound to Pd*	**D**	-5036.20505		-5038.60455		0.60138	-5038.003168		0.52348	-5038.081074		
Int-D + DMF		-5284.37817	**-24.73**	-5287.06023	**-18.09**		-5286.357533	**-16.34**		-5286.464416	**0**	**-10.24**
Int-E	**E**	-2462.29172		-2464.36569		0.60166	-2463.764032		0.52803	-2463.837661		
Int-E + Br^- + DMF		-5284.35363	**-9.33**	-5287.04482	**-8.43**		-5286.341853	**-6.50**		-5286.460635	**1**	**-5.97**
trans-[Ph-Pd^0-Br (DMF)(Ph_3P)]	**III**	-4216.35406		-4218.09845		0.46555	-4217.632902		0.39621	-4217.702244		
$PhSO_2N^-CH_2CH_2CH_2CHCCH_2$	**IV^-**	-1067.98471		-1068.93295		0.23436	-1068.698591		0.18709	-1068.745856		
III + IV^-		-5284.33876	**0.00**	-5287.03140	**0.00**		-5286.331493	**0.00**		-5286.448100	**0**	**0.00**
Int-F	**F**	-2710.45551		-2712.81565		0.70258	-2712.113075		0.61510	-2712.200551		
Int-F + Br^-		-5284.34430	**-3.47**	-5287.03911	**-4.84**		-5286.336532	**-3.16**		-5286.440183	**0**	**4.97**
Int-E + Br^- + DMF		-5284.35363	**-9.33**	-5287.04482	**-8.43**		-5286.341853	**-6.50**		-5286.460635	**1**	**-5.97**

[a] M06/def2-SVP; [b] M06/def2-TZVP; [c] M06/def2-TZVP enegies combined with thermal corrections calculated with the M06/def2-SVP.

Scheme 5. The alternative pathways (blue and green profiles).

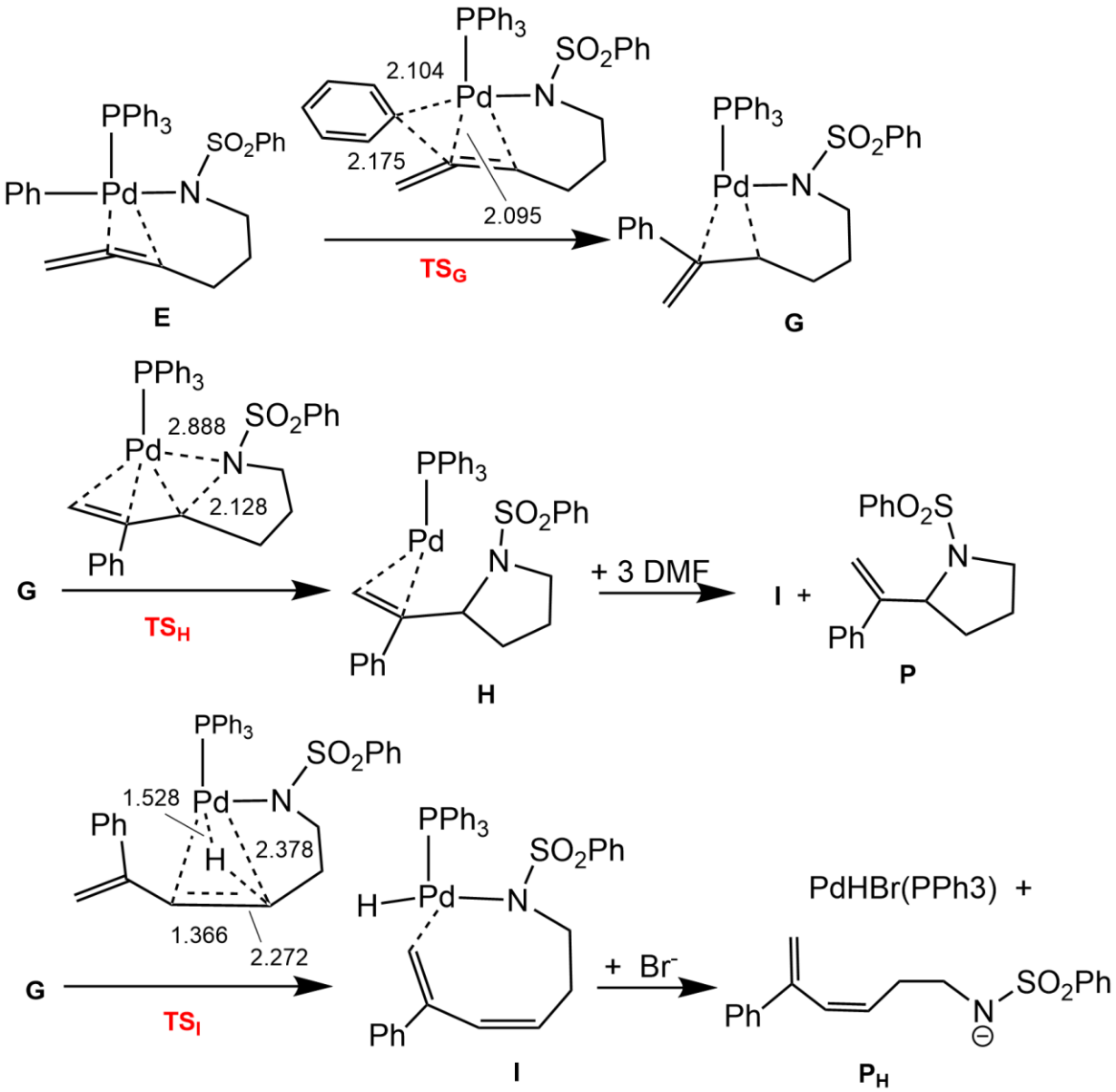


Table 5. Calculated absolute and relative energies for the alternative pathways.

Scheme 5		E(DZ) /au	**ΔE[a]**	E(TZ) /au	**ΔE[b]**	ZPE /au	E^{0K} /au	**ΔE^{0K} c**	δG^{298K}/au	G^{298K} /au	**Δn**	**ΔG^{298K} c**
TS_G from E	**TS_G**	-2462.23374		-2464.30749		0.60046	-2463.707024		0.52702	-2463.780471		
TS_G + Br^- + DMF		-5284.29564	**27.06**	-5286.98662	**28.10**		-5286.284846	**29.27**		-5286.403445	**1**	**29.92**
Int-G Pd on C4	**G**	-2462.33596		-2464.40509		0.60499	-2463.800097		0.52974	-2463.875345		
Int-G + Br^- + DMF		-5284.39786	**-37.09**	-5287.08422	**-33.15**		-5286.377918	**-29.13**		-5286.498319	**1**	**-29.62**
TS_H	**TS_H**	-2462.31799		-2464.38491		0.60333	-2463.781579		0.52848	-2463.856428		
TS_H + Br^- + DMF		-5284.37990	**-25.81**	-5287.06404	**-20.49**		-5286.359400	**-17.51**		-5286.479402	**1**	**-17.75**
Int-H N on C4	**H**	-2462.35936		-2464.43606		0.60570	-2463.830360		0.52813	-2463.907924		
Int-H + Br^- + DMF		-5284.42127	**-51.77**	-5287.11519	**-52.58**		-5286.40818	**-48.12**		-5286.53090	**1**	**-50.06**
P + Br^- + I - $(DMF)_2$		-5284.41684	**-48.99**	-5287.10889	**-48.63**		-5286.40089	**-43.55**		-5286.50206	**0**	**-33.86**
TS_I from G	**TS_I**	-2462.26577		-2464.33852		0.59968	-2463.738836		0.52521	-2463.813305		
TS_I + Br^- + DMF		-5284.32767	**6.96**	-5287.01765	**8.62**		-5286.316657	**9.31**		-5286.436279	**1**	**9.31**
Int-I	**I**	-2462.30548		-2464.38041		0.60092	-2463.779488		0.52775	-2463.852655		
Int-I + Br^- + DMF		-5284.36739	**-17.96**	-5287.05954	**-17.66**		-5286.357309	**-16.20**		-5286.475629	**1**	**-15.38**
$PhSO_2N^-H_2)_2(CH_2)(Ph)CH_2$	**P_H**	-1298.71813		-1299.90655		0.31717	-1299.589371		0.26638	-1299.640162		
$[HPd^0$-Br (DMF)$(Ph_3P)]$	V	-3985.65302		-3987.15274		0.38276	-3986.769978		0.31913	-3986.833614		
P_H + V		-5284.37115	**-20.33**	-5287.05929	**-17.50**		-5286.359349	**-17.48**		-5286.473776	**0**	**-16.11**

[a] M06/def2-SVP; [b] M06/def2-TZVP; [c] M06/def2-TZVP enegies combined with thermal corrections calculated with the M06/def2-SVP.

Scheme 6. The excited states pathways (Figure 6 in the article).

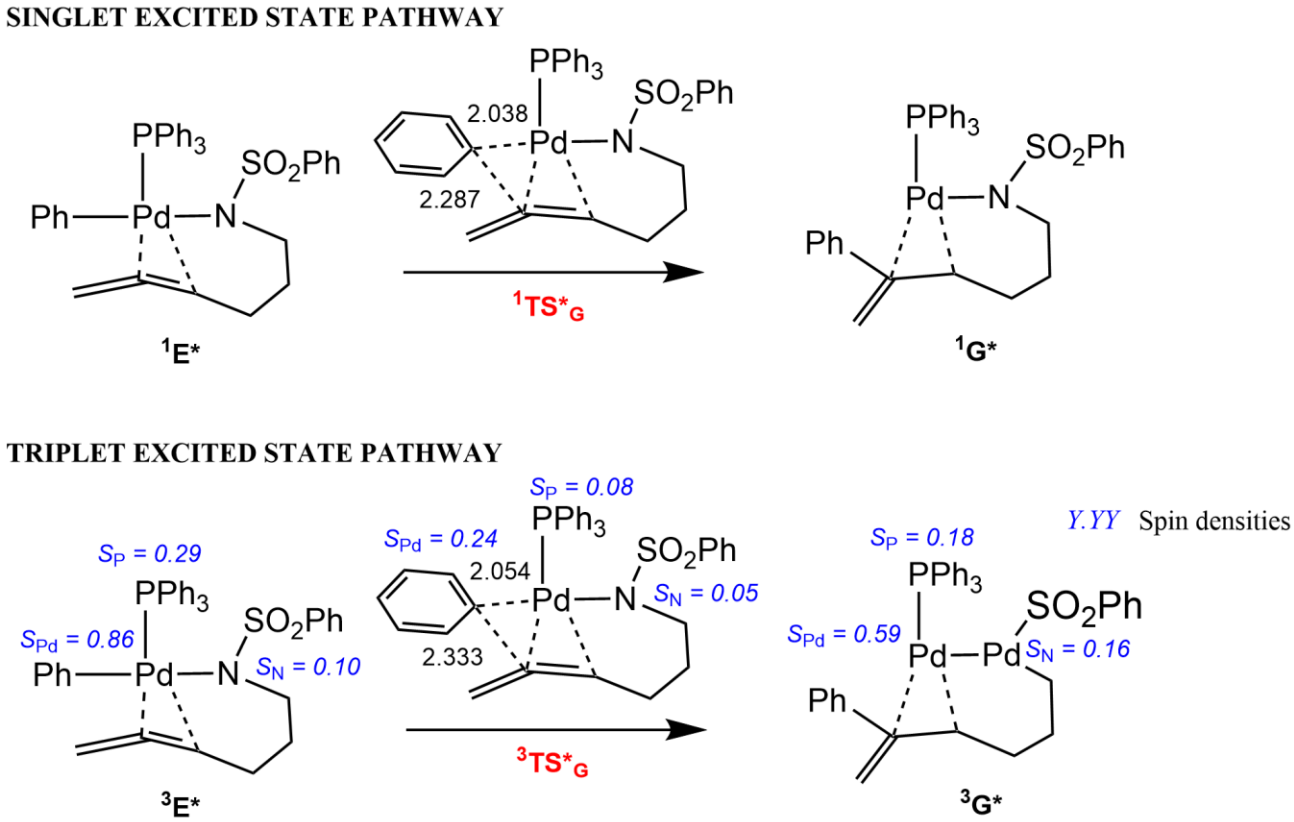


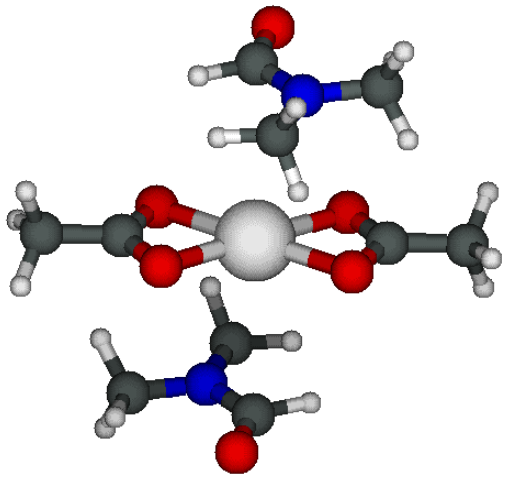
Table 6. Calculated absolute and relative energies for the excited states pathways.

Scheme 6 (EXCITED STATES)		E(DZ) /au	**ΔE[a]**	**ΔE *vs* III + IV$^-$**
^{1}Int-E* at Geom Ground State		*-2462.17483*		**64.02**
^{1}Int-E*	**^{1}E***	-2462.20616	**0.00**	**44.36**
^{1}TS*$_G$	**^{1}TS*$_G$**	-2462.19386	**7.72**	**52.08**
^{1}Int-G*	**^{1}G***	-2462.27963	**-46.10**	**-1.74**
^{3}Int-E* at Geom. ^{1}Int-E*		*-2462.21396*	**-4.89**	**39.47**
^{3}Int-E*	**^{3}E***	-2462.22193	**0.00**	**34.47**
^{3}TS*$_G$	**^{3}TS*$_G$**	-2462.21139	**6.61**	**41.08**
^{3}Int-G*	**^{3}G***	-2462.29743	**-47.38**	**-12.91**

[a] M06/def2-SVP.

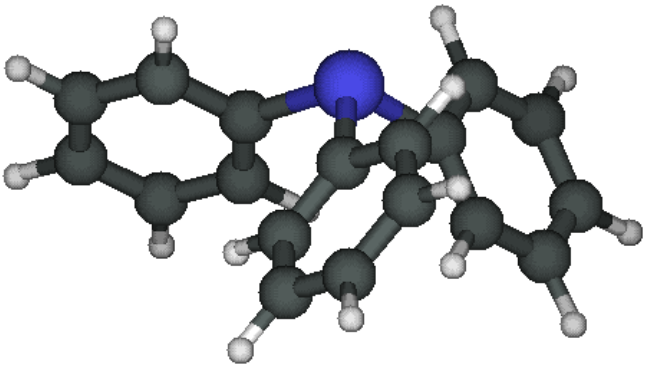
Pictures and **Cartesian coordinates** of optimized structures M06/def2-TZVP.

01 ***trans*-$(DMF)_2Pd^{II}(AcO)_2$**



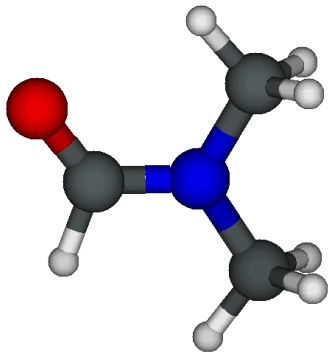
1	46	0	-0.065390	0.005724	0.165183
2	8	0	-0.058067	0.188581	2.209854
3	6	0	1.207096	0.100944	2.215955
4	8	0	1.767572	-0.051293	1.087086
5	6	0	1.979928	0.155465	3.470704
6	1	0	1.571572	0.923558	4.128613
7	1	0	1.888999	-0.806379	3.981969
8	1	0	3.032555	0.348575	3.268729
9	8	0	-0.072705	-0.177177	-1.879478
10	6	0	-1.337863	-0.089498	-1.885602
11	8	0	-1.898358	0.062785	-0.756747
12	6	0	-2.110678	-0.144006	-3.140362
13	1	0	-1.702194	-0.911972	-3.798342
14	1	0	-3.163278	-0.337293	-2.938423
15	1	0	-2.019881	0.817900	-3.651533
16	8	0	1.117441	-3.590953	-0.661562
17	6	0	0.323599	-3.326707	0.218551
18	7	0	-1.012594	-3.231292	0.079764
19	1	0	0.636861	-3.134679	1.264774
20	6	0	-1.875307	-2.983537	1.206445
21	1	0	-2.472201	-2.080442	1.044962
22	1	0	-2.559984	-3.823635	1.360972
23	1	0	-1.278030	-2.850353	2.108918
24	6	0	-1.651956	-3.445940	-1.193420
25	1	0	-2.223404	-4.379934	-1.191293
26	1	0	-2.347703	-2.627914	-1.405643
27	1	0	-0.897300	-3.493593	-1.976787
28	8	0	-1.247395	3.602728	0.989661
29	6	0	-0.452954	3.338090	0.110204
30	7	0	0.883124	3.242515	0.249992
31	1	0	-0.765491	3.145808	-0.936190
32	6	0	1.746602	2.994473	-0.876039
33	1	0	2.431118	3.834701	-1.030586
34	1	0	2.343683	2.091648	-0.713772
35	1	0	1.149906	2.860637	-1.778799
36	6	0	1.521581	3.457611	1.523558
37	1	0	2.217394	2.639824	1.736475
38	1	0	2.092800	4.391749	1.521607
39	1	0	0.766385	3.505271	2.306403

02 PPh_3



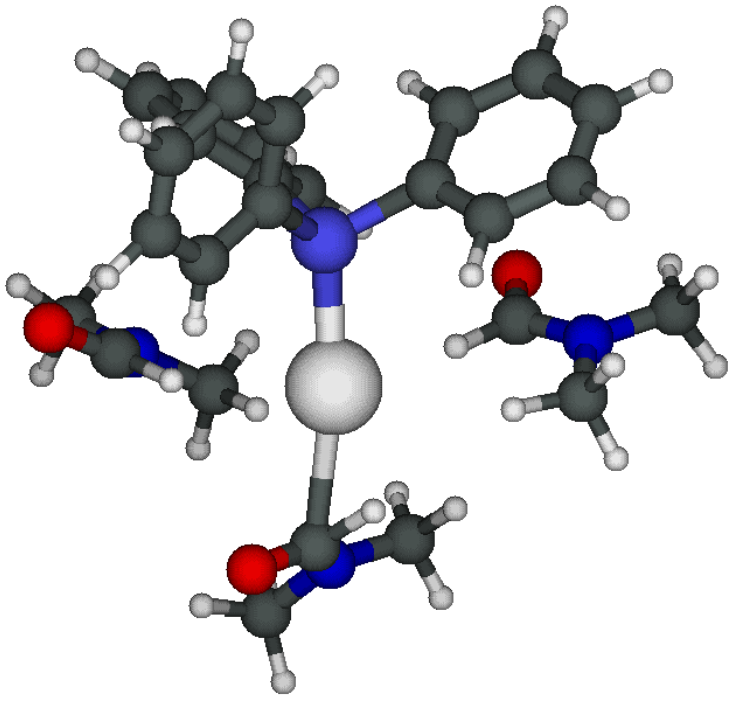
1	6	0	-0.002495	0.020455	0.018939
2	6	0	0.003590	-0.010096	1.412319
3	6	0	1.225148	-0.031771	2.077016
4	6	0	2.413431	-0.027282	1.362578
5	6	0	2.395342	-0.009017	-0.022299
6	6	0	1.182978	0.011447	-0.694819
7	15	0	-1.633375	-0.033272	2.234880
8	6	0	-2.036174	-1.820348	2.226795
9	6	0	-1.137862	-2.832364	1.905043
10	6	0	-1.533897	-4.160528	1.941841
11	6	0	-2.827638	-4.493191	2.308101
12	6	0	-3.730695	-3.492123	2.632047
13	6	0	-3.338838	-2.165906	2.581556
14	6	0	-1.182411	0.248464	3.987902
15	6	0	-1.028724	-0.755219	4.938116
16	6	0	-0.679403	-0.439798	6.242593
17	6	0	-0.471776	0.879033	6.610378
18	6	0	-0.621395	1.887526	5.670232
19	6	0	-0.983706	1.573561	4.372427
20	1	0	-1.178736	-1.794608	4.663711
21	1	0	-0.564614	-1.232208	6.974029
22	1	0	-0.197162	1.122756	7.630475
23	1	0	-0.464209	2.922749	5.951890
24	1	0	-1.111054	2.367289	3.640598
25	1	0	-0.117591	-2.587864	1.626578
26	1	0	-0.824335	-4.940001	1.687001
27	1	0	-3.134390	-5.532624	2.337540
28	1	0	-4.746146	-3.745272	2.915732
29	1	0	-4.051893	-1.382443	2.824965
30	1	0	1.255652	-0.056973	3.161792
31	1	0	3.358924	-0.042962	1.893414
32	1	0	3.325896	-0.006922	-0.578577
33	1	0	1.161312	0.029732	-1.778768
34	1	0	-0.950951	0.047884	-0.511299

03 DMF



1	6	0	0.866614	-0.628827	-0.000041
2	8	0	1.948497	-0.075458	0.000067
3	1	0	0.763658	-1.731702	-0.000100
4	7	0	-0.333753	-0.023058	-0.000151
5	6	0	-1.561821	-0.774314	0.000059
6	6	0	-0.453595	1.412672	0.000009
7	1	0	-2.159297	-0.538226	-0.886004
8	1	0	-1.343949	-1.842618	0.000114
9	1	0	-2.159071	-0.538099	0.886244
10	1	0	-1.000468	1.750096	-0.885659
11	1	0	-0.998879	1.750120	0.886656
12	1	0	0.539114	1.858315	-0.000892

04 $(DMF)_3Pd^0(PPh_3)$, I

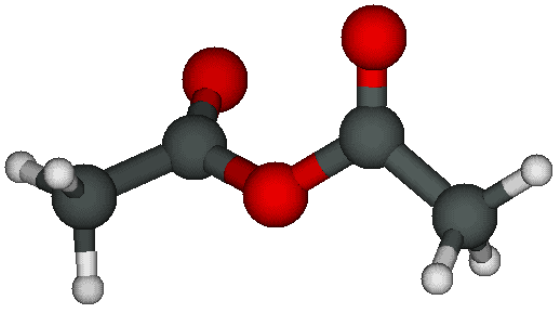


1	46	0	-0.156141	0.111506	0.053966
2	15	0	-0.058097	0.063502	2.311088
3	8	0	1.305681	0.186160	-2.655245
4	6	0	-1.510718	0.776685	3.167445
5	6	0	-2.257175	0.115681	4.135791
6	6	0	-3.374662	0.719326	4.693927
7	6	0	-3.747790	1.993942	4.303584

8	6	0	-2.995548	2.670431	3.353852
9	6	0	-1.891818	2.061874	2.785361
10	1	0	-1.974676	-0.880432	4.458572
11	1	0	-3.953021	0.188242	5.441773
12	1	0	-4.622639	2.462846	4.739746
13	1	0	-3.278147	3.671401	3.046438
14	1	0	-1.318238	2.585064	2.023997
15	6	0	0.073349	-1.631531	2.987524
16	6	0	1.159923	-2.063299	3.740163
17	6	0	1.247842	-3.383413	4.158670
18	6	0	0.248353	-4.284380	3.837760
19	6	0	-0.841400	-3.863066	3.088292
20	6	0	-0.922805	-2.552153	2.656674
21	1	0	1.955349	-1.372893	3.999866
22	1	0	2.104713	-3.704366	4.740574
23	1	0	0.317015	-5.315348	4.166466
24	1	0	-1.628118	-4.563524	2.829560
25	1	0	-1.777633	-2.240618	2.059764
26	6	0	1.339021	0.930444	3.105090
27	6	0	1.302244	1.340677	4.435004
28	6	0	2.406800	1.944346	5.010598
29	6	0	3.560970	2.136903	4.266003
30	6	0	3.607575	1.728102	2.943394
31	6	0	2.498270	1.132779	2.364657
32	1	0	0.406544	1.180369	5.027802
33	1	0	2.368487	2.263668	6.046060
34	1	0	4.425055	2.610050	4.718791
35	1	0	4.507323	1.879062	2.357698
36	1	0	2.522765	0.818780	1.323529
37	6	0	0.130958	-0.016620	-2.418268
38	8	0	3.340666	-2.638594	0.851637
39	6	0	2.221749	-2.599432	0.378264
40	7	0	1.409888	-3.655739	0.179093
41	1	0	1.739233	-1.647281	0.057486
42	6	0	0.138081	-3.519593	-0.483786
43	6	0	1.825195	-4.994730	0.515757
44	1	0	0.143355	-4.039124	-1.448053
45	1	0	-0.662761	-3.946057	0.129540
46	1	0	-0.078469	-2.458805	-0.650117
47	1	0	2.039886	-5.577305	-0.386549
48	1	0	2.720974	-4.952970	1.132944
49	1	0	1.029696	-5.502827	1.068224
50	8	0	-4.082920	-1.562452	1.219152
51	6	0	-3.603979	-0.560282	0.720961
52	7	0	-4.244308	0.604308	0.513239
53	6	0	-3.603946	1.707452	-0.157426
54	6	0	-5.627672	0.782030	0.877321
55	1	0	-3.690013	2.619086	0.441917
56	1	0	-2.541535	1.486921	-0.304581
57	1	0	-4.067568	1.894170	-1.132216
58	1	0	-5.738577	1.670507	1.506195
59	1	0	-6.249616	0.914770	-0.013804
60	1	0	-5.973217	-0.091931	1.426337
61	1	0	-2.542557	-0.507815	0.384681
62	7	0	-0.606259	-1.041832	-2.877637
63	1	0	-0.499760	0.727107	-1.828308
64	6	0	-2.024208	-1.153071	-2.636589
65	6	0	-0.005533	-2.039726	-3.731575
66	1	0	-2.566412	-1.192295	-3.585952

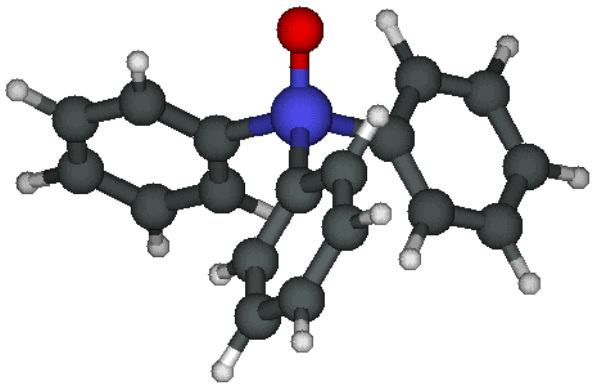
67	1	0	-2.251119	-2.064934	-2.073342
68	1	0	-2.375917	-0.291645	-2.068054
69	1	0	-0.167109	-1.806461	-4.788999
70	1	0	1.066050	-2.091416	-3.541432
71	1	0	-0.456462	-3.011080	-3.520018

05 $(Ac)_2O$



1	6	0	-1.191919	0.083120	-0.157451
2	8	0	0.000007	-0.590859	-0.000046
3	6	0	1.191913	0.083126	0.157441
4	8	0	1.258642	1.155109	0.669745
5	6	0	2.317818	-0.747476	-0.334464
6	1	0	2.278639	-1.739638	0.118467
7	1	0	2.222285	-0.882089	-1.414482
8	1	0	3.267293	-0.269475	-0.105482
9	8	0	-1.258680	1.155110	-0.669733
10	6	0	-2.317790	-0.747502	0.334497
11	1	0	-2.278614	-1.739660	-0.118442
12	1	0	-2.222205	-0.882120	1.414509
13	1	0	-3.267282	-0.269514	0.105559

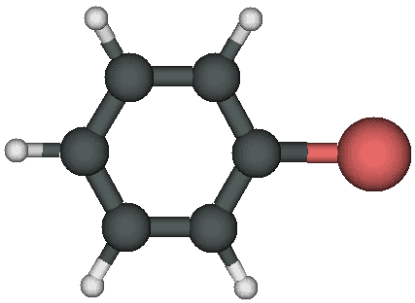
06 $O=PPh_3$



1	6	0	0.009325	-0.195199	0.025048
2	6	0	-0.035577	0.038149	1.397427
3	6	0	1.148829	0.253594	2.092897
4	6	0	2.362153	0.238584	1.423958
5	6	0	2.398841	0.007919	0.058902
6	6	0	1.221645	-0.209732	-0.640973
7	15	0	-1.658757	0.016868	2.193721
8	6	0	-2.017206	-1.720010	2.541124
9	6	0	-1.028783	-2.693925	2.629590
10	6	0	-1.367047	-4.004571	2.924061

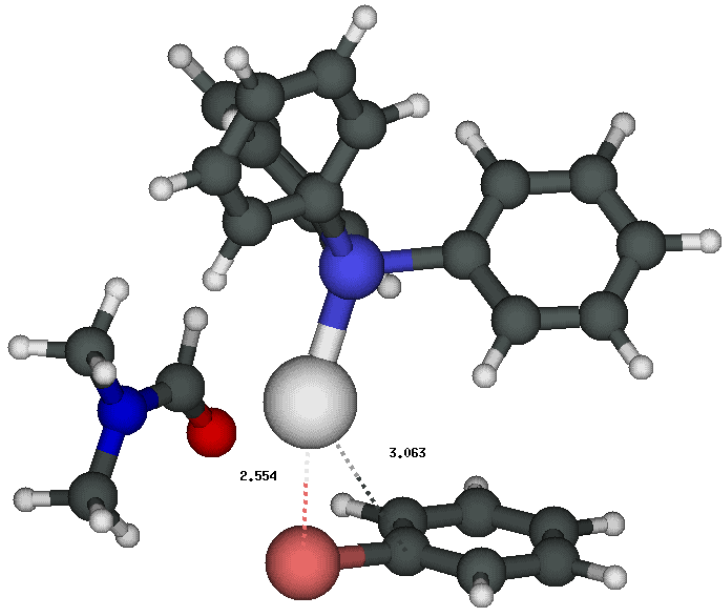
11	6	0	-2.692722	-4.348796	3.131310
12	6	0	-3.683309	-3.382647	3.045308
13	6	0	-3.347367	-2.072746	2.752212
14	6	0	-1.432130	0.811527	3.801306
15	6	0	-1.176999	0.103102	4.969890
16	6	0	-0.992585	0.776898	6.166524
17	6	0	-1.060777	2.159702	6.201616
18	6	0	-1.312801	2.872861	5.039341
19	6	0	-1.497354	2.202040	3.843734
20	1	0	-1.122183	-0.980539	4.951046
21	1	0	-0.797153	0.218554	7.074873
22	1	0	-0.918284	2.685241	7.139120
23	1	0	-1.367058	3.955206	5.066093
24	1	0	-1.698171	2.758430	2.933620
25	1	0	0.011905	-2.431453	2.467923
26	1	0	-0.592145	-4.759827	2.989041
27	1	0	-2.956151	-5.375600	3.358688
28	1	0	-4.721140	-3.651676	3.205498
29	1	0	-4.121306	-1.315444	2.679148
30	1	0	1.129001	0.435588	3.162611
31	1	0	3.281646	0.410986	1.971553
32	1	0	3.348701	-0.000995	-0.463638
33	1	0	1.249279	-0.389938	-1.709550
34	1	0	-0.913285	-0.361232	-0.522220
35	8	0	-2.710668	0.666059	1.374385

07 C_6H_5Br, II



1	6	0	0.010523	-0.000000	0.005918
2	6	0	0.007540	0.000000	1.389535
3	6	0	1.219394	0.000000	2.061560
4	6	0	2.412024	-0.000000	1.356316
5	6	0	2.395016	-0.000000	-0.029125
6	6	0	1.191209	-0.000000	-0.715460
7	1	0	-0.927251	0.000000	1.937460
8	1	0	1.226097	0.000000	3.145709
9	1	0	3.356812	-0.000000	1.887584
10	1	0	3.324853	-0.000000	-0.586643
11	1	0	1.173735	-0.000000	-1.798859
12	35	0	-1.645228	0.000000	-0.925135

08 Cpl [(DMF)Pd(PPh_3) C_6H_5Br]



1	46	0	-0.837130	-1.056786	0.206719
2	15	0	-0.343923	-0.311761	2.262810
3	8	0	2.443188	-0.692758	-1.719406
4	6	0	-1.417703	0.955893	3.028050
5	6	0	-1.491235	1.173650	4.400773
6	6	0	-2.290727	2.183796	4.907845
7	6	0	-3.019164	2.993515	4.049780
8	6	0	-2.952044	2.785678	2.682212
9	6	0	-2.160705	1.767257	2.176291
10	1	0	-0.922712	0.551928	5.084336
11	1	0	-2.344238	2.340901	5.979351
12	1	0	-3.643987	3.784259	4.449588
13	1	0	-3.523413	3.412236	2.006619
14	1	0	-2.116329	1.588413	1.104710
15	6	0	-0.260301	-1.659283	3.501972
16	6	0	0.524661	-1.591559	4.651133
17	6	0	0.554294	-2.648657	5.544644
18	6	0	-0.197040	-3.788355	5.301356
19	6	0	-0.978032	-3.868513	4.160575
20	6	0	-1.005605	-2.811000	3.266066
21	1	0	1.127710	-0.710414	4.846969
22	1	0	1.171946	-2.584566	6.433492
23	1	0	-0.166555	-4.617704	5.999098
24	1	0	-1.559711	-4.761006	3.957517
25	1	0	-1.603548	-2.876080	2.359833
26	6	0	1.324585	0.431991	2.381981
27	6	0	1.537509	1.785587	2.613335
28	6	0	2.821331	2.312538	2.571147
29	6	0	3.904165	1.492449	2.308139
30	6	0	3.701129	0.137836	2.080244
31	6	0	2.422255	-0.384572	2.106741
32	1	0	0.700046	2.443170	2.823769
33	1	0	2.971714	3.371269	2.750980
34	1	0	4.906282	1.904893	2.278921
35	1	0	4.543799	-0.511450	1.869926
36	1	0	2.269642	-1.441143	1.898999
37	6	0	1.806879	0.266983	-1.323414
38	7	0	0.858636	0.927401	-2.011240

39	1	0	1.977760	0.721681	-0.327974
40	6	0	0.161915	2.052505	-1.444285
41	6	0	0.458372	0.520704	-3.332953
42	1	0	0.297736	2.944158	-2.064605
43	1	0	-0.911418	1.842389	-1.374900
44	1	0	0.541992	2.260217	-0.442427
45	1	0	0.697492	1.297664	-4.066056
46	1	0	0.973534	-0.399009	-3.603805
47	1	0	-0.622994	0.351039	-3.362382
48	6	0	-0.280900	-3.856215	-0.904293
49	6	0	1.093810	-3.749084	-0.800751
50	6	0	1.770294	-4.715671	-0.073696
51	6	0	1.079576	-5.757185	0.527050
52	6	0	-0.297052	-5.841521	0.400913
53	6	0	-0.994068	-4.884827	-0.321518
54	1	0	1.620933	-2.915953	-1.255336
55	1	0	2.847552	-4.646621	0.025545
56	1	0	1.617535	-6.506076	1.096368
57	1	0	-0.840697	-6.654563	0.868161
58	1	0	-2.071974	-4.938002	-0.416851
59	35	0	-1.242362	-2.496177	-1.863545

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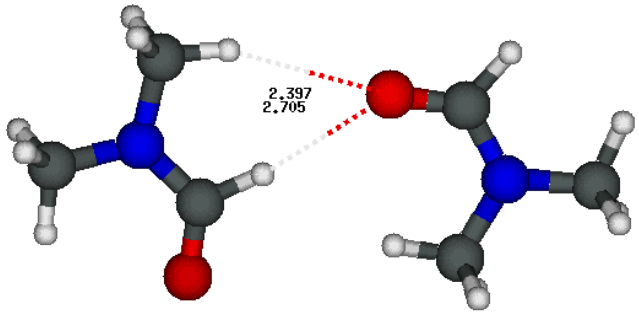
09 (DMF)$_2$



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4	7	0	-1.080035	0.003791	-0.843540
5	6	0	-1.051844	-0.122640	-2.278268
6	6	0	-2.377752	-0.049309	-0.218410
7	1	0	-1.628585	0.680282	-2.747362
8	1	0	-0.023275	-0.069971	-2.635462
9	1	0	-1.483350	-1.078994	-2.588985
10	1	0	-3.013519	0.758600	-0.592691
11	1	0	-2.868402	-1.001272	-0.441854
12	1	0	-2.269845	0.052009	0.859612
13	6	0	-1.841973	0.435388	3.976057
14	8	0	-3.055644	0.467814	4.061340
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19	1	0	0.925183	1.316552	5.206452
20	1	0	0.881733	-0.452432	5.293098
21	1	0	-2.518842	0.573403	6.392002
22	1	0	-1.085908	-0.327034	6.940010
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24	1	0	-1.312339	0.374802	3.004906

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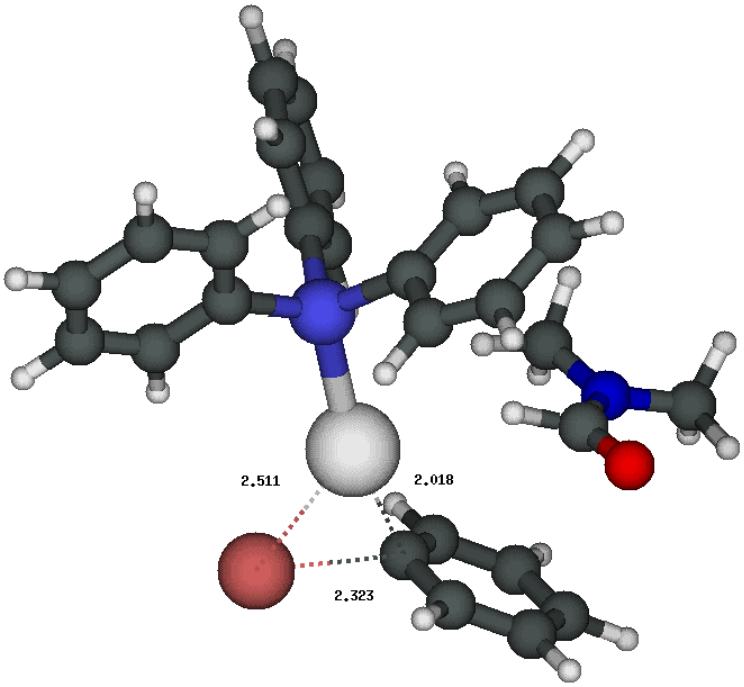
10 TS_A



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4	6	0	-1.092195	1.080084	2.776049
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6	6	0	-2.025407	2.615157	4.379557
7	6	0	-2.433181	3.449580	3.348782
8	6	0	-2.175508	3.102170	2.033707
9	6	0	-1.509943	1.919997	1.749383
10	1	0	-1.040178	0.791667	4.908656
11	1	0	-2.229043	2.884634	5.409764
12	1	0	-2.957517	4.371502	3.573852
13	1	0	-2.497867	3.748713	1.225455
14	1	0	-1.313445	1.635331	0.717513
15	6	0	-0.926193	-1.696794	3.453879
16	6	0	-0.471722	-1.936833	4.747159
17	6	0	-1.104400	-2.874494	5.546434
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19	6	0	-2.657711	-3.342789	3.779241
20	6	0	-2.019628	-2.413206	2.975938
21	1	0	0.382542	-1.391985	5.135634
22	1	0	-0.740580	-3.056737	6.551446
23	1	0	-2.690651	-4.310308	5.693307
24	1	0	-3.509460	-3.893340	3.396099
25	1	0	-2.367600	-2.241645	1.960560
26	6	0	1.489059	-0.197147	2.975895
27	6	0	1.984135	1.050180	3.335984
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29	6	0	4.169772	0.109368	3.675342
30	6	0	3.682852	-1.140544	3.318329
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33	1	0	3.694641	2.181106	3.955460

34	1	0	5.212375	0.229307	3.946945
35	1	0	4.343704	-2.000011	3.308636
36	1	0	1.987584	-2.266495	2.656909
37	6	0	3.283442	0.384185	-0.274744
38	7	0	2.939285	1.636486	-0.632637
39	1	0	2.469324	-0.113585	0.296885
40	6	0	1.702026	2.233253	-0.202388
41	6	0	3.828952	2.469264	-1.402473
42	1	0	1.886586	3.083427	0.463898
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44	1	0	1.102701	1.488592	0.327625
45	1	0	4.185118	3.314952	-0.805418
46	1	0	4.683370	1.879996	-1.730336
47	1	0	3.306667	2.865642	-2.278434
48	6	0	0.203479	-0.975758	-1.987942
49	6	0	-0.069994	0.234064	-2.614657
50	6	0	0.865740	0.743682	-3.502465
51	6	0	2.021669	0.031510	-3.790795
52	6	0	2.247204	-1.201075	-3.195196
53	6	0	1.328517	-1.728028	-2.300407
54	1	0	-0.985338	0.774595	-2.398562
55	1	0	0.683984	1.703309	-3.974985
56	1	0	2.742114	0.432244	-4.494728
57	1	0	3.146889	-1.761032	-3.425509
58	1	0	1.491412	-2.696338	-1.840673
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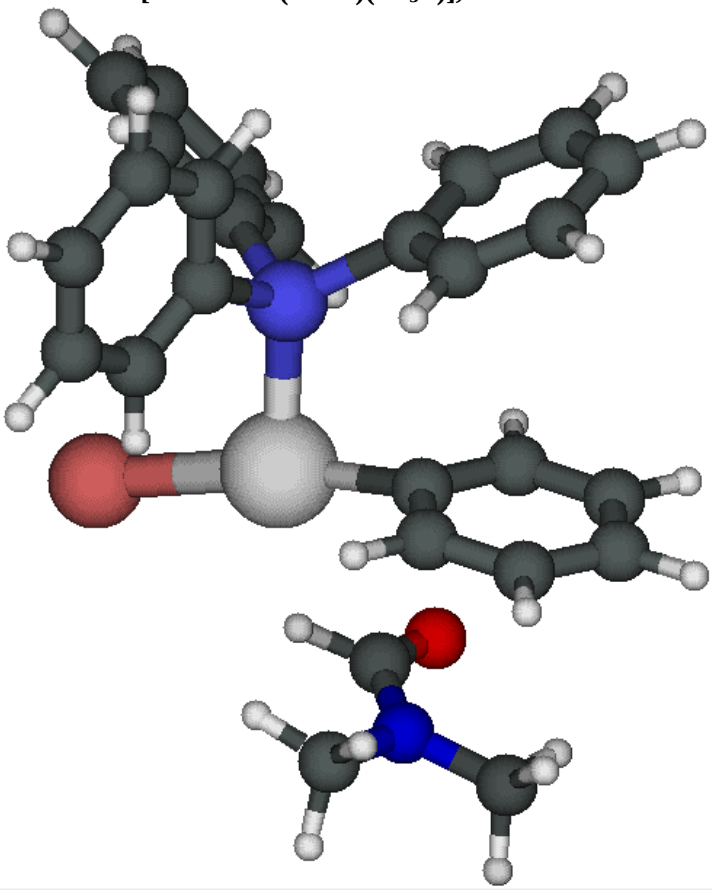
11 ***trans*-[Ph-Pd-Br (DMF)(Ph_3P)], lll**



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4	6	0	-1.684006	-0.320662	3.029395
5	6	0	-1.846478	-0.509744	4.401540
6	6	0	-3.108258	-0.713795	4.928002
7	6	0	-4.214566	-0.739092	4.091688
8	6	0	-4.058661	-0.558269	2.728374
9	6	0	-2.796567	-0.349360	2.196702
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11	1	0	-3.228554	-0.857346	5.995546
12	1	0	-5.202229	-0.904583	4.506932
13	1	0	-4.921189	-0.582696	2.072539
14	1	0	-2.668715	-0.204850	1.127832
15	6	0	1.039304	-1.198544	3.222632
16	6	0	2.292625	-0.826141	3.692129
17	6	0	3.122457	-1.765375	4.286092
18	6	0	2.706968	-3.078072	4.416769
19	6	0	1.452394	-3.454302	3.957219
20	6	0	0.624837	-2.522959	3.361351
21	1	0	2.633602	0.198501	3.599691
22	1	0	4.097625	-1.462736	4.649878
23	1	0	3.357389	-3.810899	4.880396
24	1	0	1.118465	-4.480416	4.061155
25	1	0	-0.349029	-2.830581	2.994527
26	6	0	0.510896	1.621220	2.840070
27	6	0	-0.166476	2.374074	3.790578
28	6	0	0.286042	3.642529	4.119930
29	6	0	1.415057	4.160441	3.509811
30	6	0	2.094188	3.412133	2.559549
31	6	0	1.638281	2.153426	2.218125
32	1	0	-1.055697	1.984222	4.272453
33	1	0	-0.251879	4.227439	4.857179
34	1	0	1.764455	5.153388	3.768968
35	1	0	2.974091	3.816844	2.073021
36	1	0	2.151931	1.580014	1.450882
37	6	0	1.313573	-0.374488	-2.735279
38	7	0	0.753236	-1.497577	-3.213045
39	1	0	0.546214	0.304425	-2.286973
40	6	0	-0.670743	-1.710396	-3.201357
41	6	0	1.556436	-2.547017	-3.789732
42	1	0	-1.056172	-1.793536	-4.222323
43	1	0	-0.915755	-2.632058	-2.664147
44	1	0	-1.172959	-0.876026	-2.707362
45	1	0	1.323266	-2.676333	-4.851121
46	1	0	2.610444	-2.297355	-3.684048
47	1	0	1.354660	-3.492657	-3.276457
48	6	0	0.686545	-1.864806	0.194679
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51	6	0	1.717925	-4.424155	-0.146378
52	6	0	2.572765	-3.348461	0.051189
53	6	0	2.059376	-2.072257	0.234180
54	1	0	-1.247702	-2.795265	0.015577
55	1	0	-0.327168	-5.058077	-0.306786
56	1	0	2.121344	-5.421743	-0.279755
57	1	0	3.646641	-3.503559	0.068275
58	1	0	2.737433	-1.240023	0.403269
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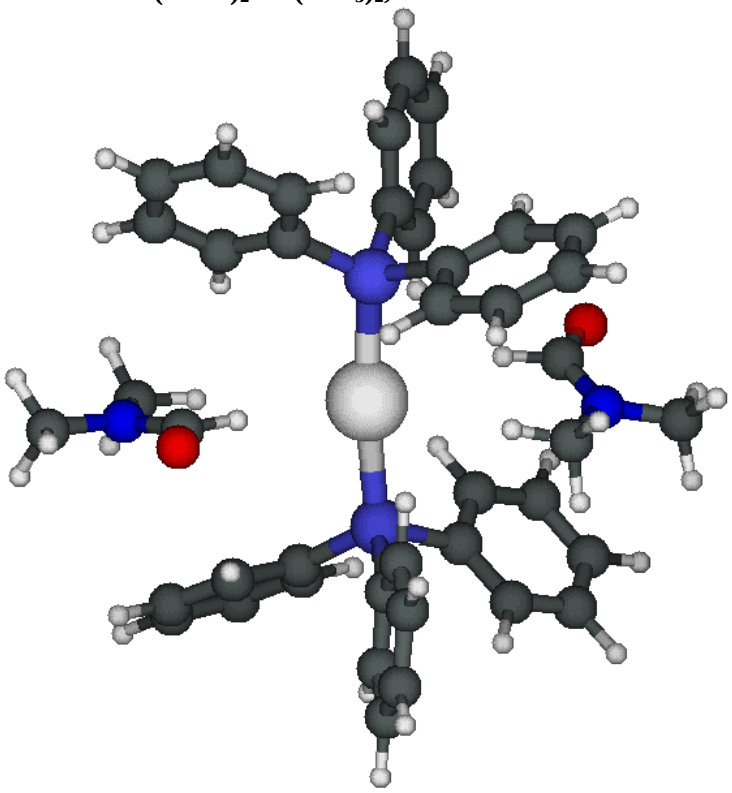
12 ***trans*-$(DMF)_2Pd^0(PPh_3)_2$, l'**



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12	1	0	-3.893803	-3.244941	4.835420
13	1	0	-4.636781	-1.596184	3.143144
14	1	0	-2.987296	-0.151954	2.022008
15	6	0	1.491414	-0.341842	2.707188
16	6	0	2.392737	0.511128	3.333104
17	6	0	3.693534	0.096454	3.585970
18	6	0	4.101915	-1.176593	3.229928
19	6	0	3.207794	-2.036677	2.606136
20	6	0	1.919618	-1.617361	2.334191
21	1	0	2.089320	1.512265	3.621797
22	1	0	4.387057	0.775574	4.069576
23	1	0	5.116329	-1.500385	3.433464
24	1	0	3.521031	-3.034568	2.320136
25	1	0	1.231904	-2.287513	1.823783
26	6	0	-0.439709	1.767781	3.055104
27	6	0	-0.609178	1.843903	4.435612
28	6	0	-0.782172	3.070372	5.051456
29	6	0	-0.784599	4.233948	4.295152
30	6	0	-0.615774	4.168013	2.922752
31	6	0	-0.447978	2.938252	2.305282

32	1	0	-0.601804	0.937082	5.033527
33	1	0	-0.915232	3.120718	6.126319
34	1	0	-0.921679	5.194120	4.779791
35	1	0	-0.618751	5.074817	2.328526
36	1	0	-0.321652	2.876906	1.226420
37	6	0	1.247909	1.629422	-2.818549
38	6	0	2.462621	1.424708	-3.461455
39	6	0	3.358354	2.472998	-3.620632
40	6	0	3.042597	3.738071	-3.156776
41	6	0	1.824895	3.955973	-2.527594
42	6	0	0.943258	2.907262	-2.346877
43	1	0	2.728055	0.439684	-3.829900
44	1	0	4.308537	2.295013	-4.112258
45	1	0	3.744401	4.555007	-3.281779
46	1	0	1.571428	4.942994	-2.157577
47	1	0	0.005097	3.074990	-1.822791
48	6	0	0.817165	-1.219066	-3.123044
49	6	0	0.915548	-1.425519	-4.497343
50	6	0	1.487007	-2.584262	-4.991702
51	6	0	1.964225	-3.551463	-4.118682
52	6	0	1.868219	-3.357602	-2.751239
53	6	0	1.294057	-2.196896	-2.256305
54	1	0	0.544225	-0.672054	-5.186207
55	1	0	1.559319	-2.735964	-6.062824
56	1	0	2.407949	-4.460736	-4.508374
57	1	0	2.234163	-4.113797	-2.065914
58	1	0	1.203472	-2.041405	-1.182880
59	6	0	-1.334265	0.566532	-3.556248
60	6	0	-1.420065	1.621416	-4.455819
61	6	0	-2.531940	1.754343	-5.275277
62	6	0	-3.562369	0.833022	-5.209297
63	6	0	-3.480665	-0.228500	-4.319059
64	6	0	-2.377608	-0.356388	-3.495823
65	1	0	-0.616329	2.346446	-4.526734
66	1	0	-2.587273	2.583125	-5.972352
67	1	0	-4.429458	0.938751	-5.851332
68	1	0	-4.282258	-0.956944	-4.263964
69	1	0	-2.318332	-1.190030	-2.799436
70	8	0	3.006417	3.589722	0.882537
71	6	0	2.856928	2.453722	0.474877
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73	1	0	1.872167	1.935891	0.482926
74	6	0	3.569401	0.288757	-0.377401
75	6	0	5.188545	2.115985	-0.127275
76	1	0	3.883437	0.082985	-1.405870
77	1	0	4.121381	-0.384049	0.289408
78	1	0	2.498514	0.077470	-0.285975
79	1	0	5.584446	1.915413	-1.126929
80	1	0	5.232938	3.185831	0.068637
81	1	0	5.819660	1.593564	0.600588
82	8	0	-1.539304	-3.925279	0.581142
83	6	0	-2.072769	-2.904881	0.187865
84	7	0	-3.398401	-2.700059	0.075746
85	6	0	-3.937560	-1.439598	-0.365350
86	6	0	-4.350088	-3.708451	0.466112
87	1	0	-4.591819	-1.013940	0.403442
88	1	0	-3.125097	-0.734101	-0.561043
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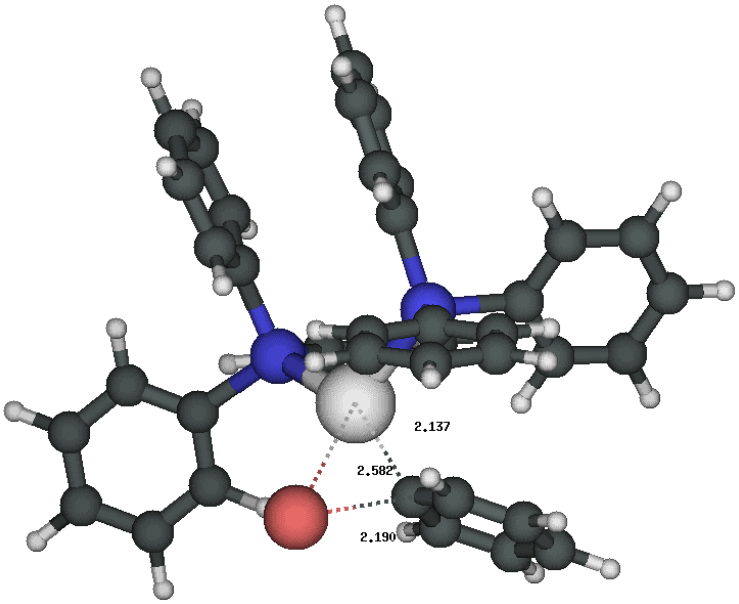
13 **TS'$_A$**



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5	6	0	-2.352088	0.668482	3.878920
6	6	0	-3.401513	1.521797	4.190360
7	6	0	-3.432516	2.806216	3.677023
8	6	0	-2.410576	3.238430	2.842578
9	6	0	-1.374274	2.382952	2.519211
10	1	0	-2.351126	-0.337976	4.283329
11	1	0	-4.199134	1.175293	4.838130
12	1	0	-4.253581	3.470882	3.920664
13	1	0	-2.429145	4.242267	2.433266
14	1	0	-0.593703	2.715390	1.838638
15	6	0	-0.282112	-1.583188	3.302927
16	6	0	-0.065884	-1.738630	4.671032
17	6	0	-0.316126	-2.952448	5.285696
18	6	0	-0.786683	-4.025980	4.542456
19	6	0	-1.002449	-3.882082	3.182827
20	6	0	-0.745499	-2.666753	2.566780
21	1	0	0.295467	-0.901558	5.261413
22	1	0	-0.145016	-3.062664	6.350720
23	1	0	-0.981726	-4.976135	5.026994
24	1	0	-1.368190	-4.716361	2.593729
25	1	0	-0.904340	-2.556438	1.497932
26	6	0	1.497139	0.608296	3.315683
27	6	0	1.514912	1.710134	4.162553
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31	6	0	2.682681	-0.094832	3.102308
32	1	0	0.604716	2.267945	4.353691
33	1	0	2.692344	2.964565	5.438500

34	1	0	4.782397	1.698041	5.056003
35	1	0	4.764390	-0.276494	3.561025
36	1	0	2.685549	-0.956704	2.438625
37	6	0	2.964699	-1.707496	-1.062836
38	6	0	3.917854	-2.052262	-2.018324
39	6	0	4.402410	-3.347153	-2.089946
40	6	0	3.942619	-4.312966	-1.207664
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42	6	0	2.504686	-2.687178	-0.187068
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44	1	0	5.142683	-3.603950	-2.839391
45	1	0	4.321075	-5.327149	-1.268199
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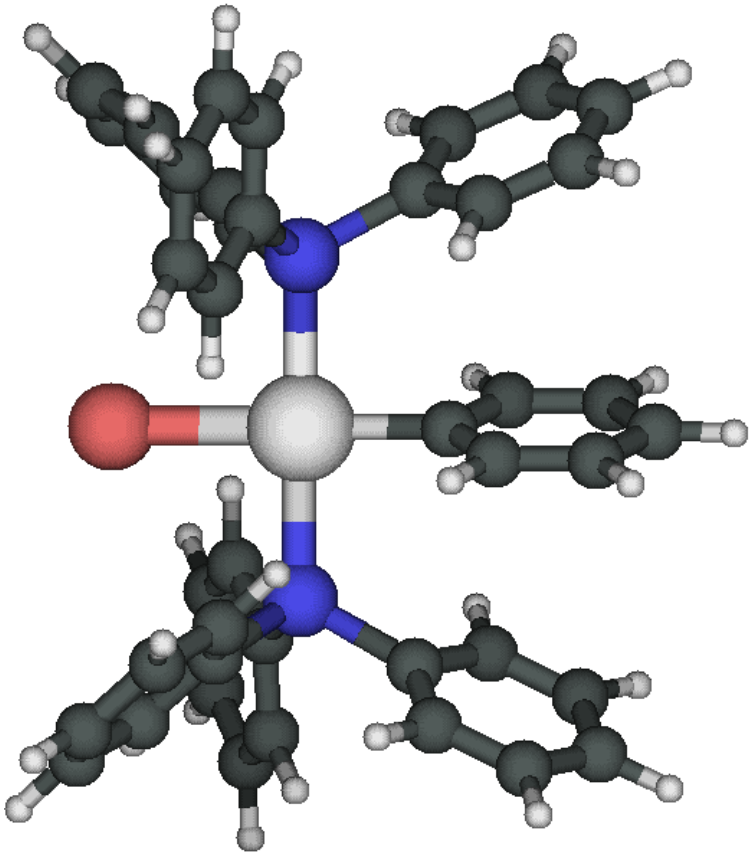
47	1	0	1.746482	-2.428478	0.548173
48	6	0	2.406763	0.615109	-2.610659
49	6	0	3.279386	1.624620	-3.000053
50	6	0	3.300852	2.065352	-4.315748
51	6	0	2.458850	1.497660	-5.255696
52	6	0	1.584333	0.489108	-4.876034
53	6	0	1.552032	0.060381	-3.562453
54	1	0	3.954432	2.073372	-2.278784
55	1	0	3.986135	2.854375	-4.605124
56	1	0	2.479350	1.841431	-6.283685
57	1	0	0.919191	0.041719	-5.606239
58	1	0	0.854729	-0.719039	-3.265750
59	6	0	3.565632	0.922214	-0.024190
60	6	0	4.884847	0.503742	0.105889
61	6	0	5.807046	1.293529	0.775808
62	6	0	5.422108	2.509838	1.315180
63	6	0	4.108610	2.936601	1.187702
64	6	0	3.186114	2.143501	0.528488
65	1	0	5.201863	-0.445392	-0.313263
66	1	0	6.832348	0.954848	0.875299
67	1	0	6.144548	3.124595	1.840374
68	1	0	3.800209	3.885901	1.611454
69	1	0	2.152827	2.472011	0.439762
70	6	0	-2.014370	-0.562202	-0.305334
71	6	0	-1.882115	-1.812099	-0.915182
72	6	0	-2.705337	-2.857113	-0.512315
73	6	0	-3.691697	-2.650798	0.436404
74	6	0	-3.865310	-1.378670	0.978135
75	6	0	-3.054001	-0.329599	0.596744
76	1	0	-1.147343	-1.965065	-1.699402
77	1	0	-2.580259	-3.834143	-0.967347
78	1	0	-4.342522	-3.464239	0.735280
79	1	0	-4.645744	-1.201396	1.711719
80	1	0	-3.200528	0.660311	1.015843
81	35	0	-1.576917	1.110129	-1.649746

14 ***trans*-[Ph-Pd-Br ($Ph_3P)_2$], lll'**



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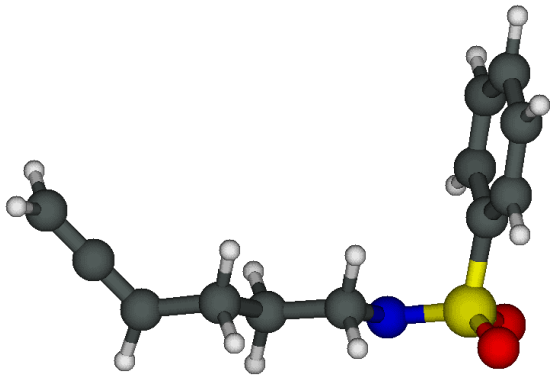
4	6	0	-2.970287	-1.243534	-1.319473
5	6	0	-3.913844	-2.237480	-1.100230
6	6	0	-4.289321	-3.082564	-2.133820
7	6	0	-3.731029	-2.937018	-3.391822
8	6	0	-2.786425	-1.946414	-3.617683
9	6	0	-2.401525	-1.112256	-2.584853
10	1	0	-4.353027	-2.371109	-0.118149
11	1	0	-5.021553	-3.860724	-1.950276
12	1	0	-4.026221	-3.599498	-4.197617
13	1	0	-2.340163	-1.831552	-4.598985
14	1	0	-1.641771	-0.353658	-2.757054
15	6	0	-3.087031	-0.660904	1.557346
16	6	0	-4.460871	-0.585268	1.783073
17	6	0	-4.988864	-0.964550	3.003439
18	6	0	-4.150285	-1.411351	4.014343
19	6	0	-2.784270	-1.478431	3.802136
20	6	0	-2.253564	-1.104620	2.577512
21	1	0	-5.120950	-0.222332	1.001033
22	1	0	-6.058557	-0.906257	3.169261
23	1	0	-4.565633	-1.702934	4.972441
24	1	0	-2.125873	-1.820255	4.592631
25	1	0	-1.183023	-1.162004	2.404522
26	6	0	-3.229260	1.453092	-0.330815
27	6	0	-3.831692	1.761853	-1.543842
28	6	0	-4.393413	3.013875	-1.749337
29	6	0	-4.358464	3.966909	-0.747463
30	6	0	-3.765013	3.663584	0.470040

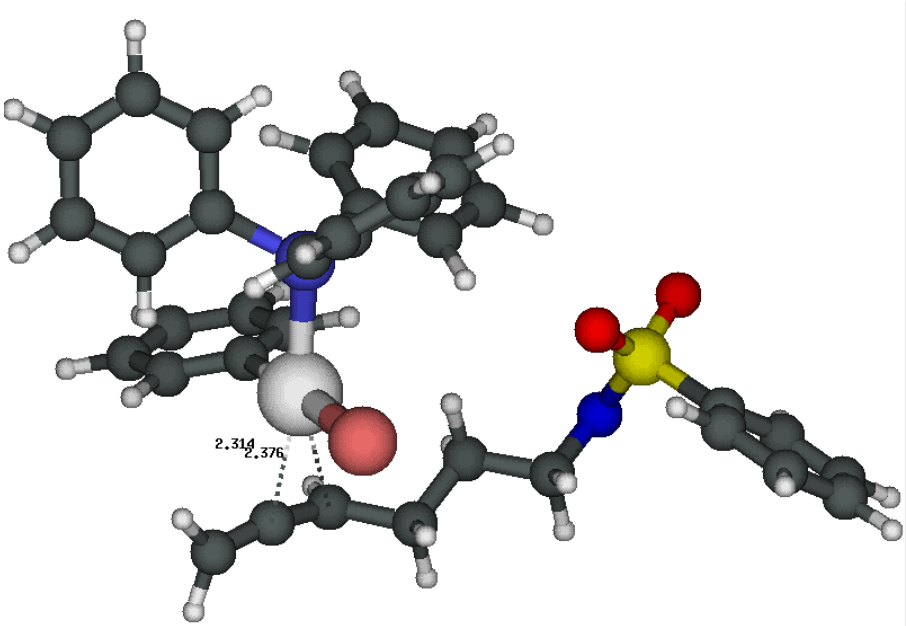
31	6	0	-3.204653	2.417478	0.676314
32	1	0	-3.869690	1.028066	-2.341010
33	1	0	-4.863206	3.239574	-2.700047
34	1	0	-4.796376	4.945141	-0.910282
35	1	0	-3.736202	4.403434	1.262298
36	1	0	-2.737707	2.193181	1.630841
37	6	0	3.226437	1.463881	0.267335
38	6	0	3.855001	1.806503	1.457664
39	6	0	4.419712	3.064152	1.615551
40	6	0	4.361101	3.988785	0.588510
41	6	0	3.741895	3.651024	-0.606975
42	6	0	3.179519	2.399010	-0.766294
43	1	0	3.911387	1.095089	2.273736
44	1	0	4.910012	3.316714	2.548994
45	1	0	4.800429	4.971795	0.714514
46	1	0	3.695043	4.368452	-1.418774
47	1	0	2.693292	2.146597	-1.704112
48	6	0	2.956449	-1.193002	1.357458
49	6	0	3.891625	-2.203362	1.181895
50	6	0	4.255856	-3.009307	2.250222
51	6	0	3.694052	-2.808485	3.499025
52	6	0	2.757732	-1.801069	3.681191
53	6	0	2.384667	-1.005279	2.614379
54	1	0	4.333232	-2.380123	0.207646
55	1	0	4.982016	-3.800446	2.101159
56	1	0	3.980225	-3.440621	4.331991
57	1	0	2.309156	-1.642776	4.655394
58	1	0	1.632921	-0.231819	2.753123
59	6	0	3.098673	-0.718960	-1.537603
60	6	0	4.475002	-0.652305	-1.750380
61	6	0	5.016692	-1.078320	-2.949188
62	6	0	4.189325	-1.562947	-3.951832
63	6	0	2.820865	-1.620670	-3.752982
64	6	0	2.276444	-1.200344	-2.549627
65	1	0	5.126607	-0.260271	-0.975250
66	1	0	6.088293	-1.027060	-3.104715
67	1	0	4.615298	-1.891446	-4.893167
68	1	0	2.171104	-1.991847	-4.537377
69	1	0	1.204097	-1.251302	-2.386871
70	6	0	-0.003427	1.901874	-0.009259
71	6	0	0.227232	2.611685	1.165103
72	6	0	0.230179	4.000614	1.168723
73	6	0	0.005112	4.702791	-0.005863
74	6	0	-0.224844	4.004754	-1.181996
75	6	0	-0.231103	2.615929	-1.181580
76	1	0	0.412947	2.081285	2.096688
77	1	0	0.411440	4.535565	2.095838
78	1	0	0.009026	5.787287	-0.004694
79	1	0	-0.402616	4.542930	-2.107937
80	1	0	-0.418377	2.089600	-2.115023
81	35	0	0.001742	-2.707363	0.016985

15 Ph-SO_2-N--$CH_2CH_2CH_2$-CH=C=CH_2 IV$^-$



1	7	0	0.127342	-1.435293	-0.602445
2	6	0	-0.831568	-0.910916	0.346848
3	6	0	-2.209292	-0.861001	-0.278345
4	1	0	-0.885318	-1.518876	1.266042
5	1	0	-0.571722	0.111423	0.686197
6	6	0	-3.260154	-0.312143	0.671164
7	1	0	-2.173803	-0.246247	-1.185925
8	1	0	-2.493955	-1.870144	-0.601768
9	6	0	-4.629490	-0.318173	0.065131
10	1	0	-3.270000	-0.923272	1.582792
11	1	0	-2.995957	0.705087	0.977921
12	6	0	-5.371348	0.733103	-0.119827
13	1	0	-5.013240	-1.286109	-0.259349
14	6	0	-6.107868	1.788344	-0.298734
15	1	0	-6.812102	2.126947	0.456783
16	1	0	-6.050756	2.375310	-1.211706
17	16	0	1.595203	-1.482047	-0.110682
18	6	0	2.154601	0.223501	-0.018050
19	8	0	1.778909	-1.991831	1.240872
20	8	0	2.429098	-2.095848	-1.125401
21	6	0	2.404764	0.836404	1.198887
22	6	0	2.788069	2.170270	1.240773
23	6	0	2.921869	2.891707	0.067455
24	6	0	2.666713	2.279250	-1.152677
25	6	0	2.279322	0.952477	-1.194956
26	1	0	2.303507	0.259917	2.111190
27	1	0	2.983627	2.645054	2.196135
28	1	0	3.223975	3.932544	0.099689
29	1	0	2.770248	2.841487	-2.074317
30	1	0	2.073097	0.471183	-2.145444

16 Int. A



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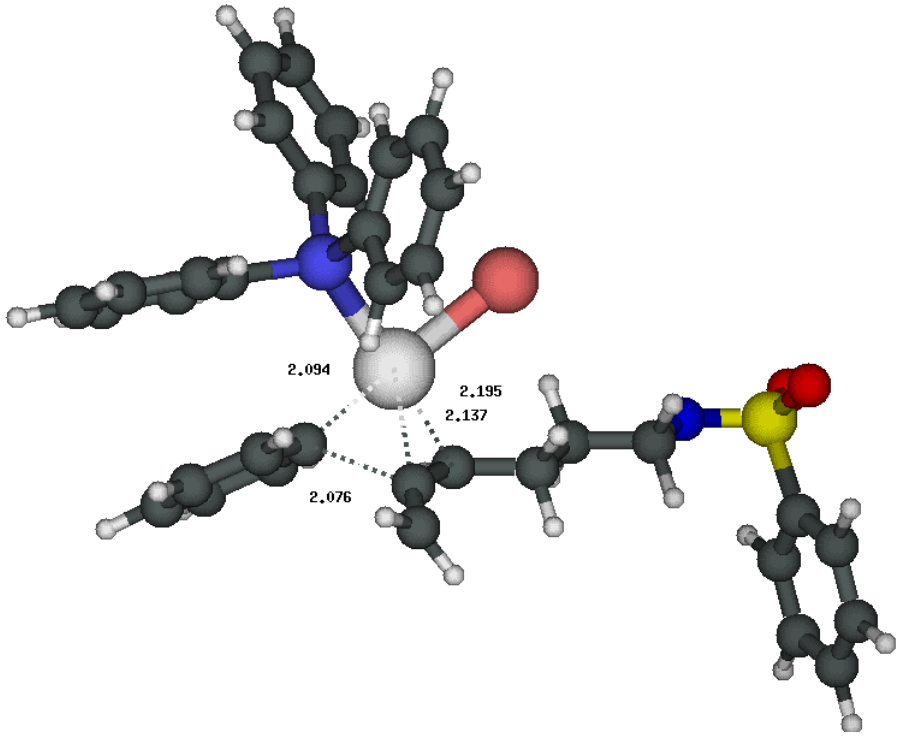
2	15	0	-0.010120	-0.038173	2.441373
3	35	0	2.622916	0.201826	-0.027492
4	6	0	-0.991327	1.367218	3.038692
5	6	0	-0.547225	2.645339	2.698667
6	6	0	-1.305885	3.758915	3.012683
7	6	0	-2.524840	3.606884	3.657309
8	6	0	-2.977653	2.340528	3.987057
9	6	0	-2.216919	1.223695	3.677918
10	1	0	0.392226	2.792030	2.170367
11	1	0	-0.937509	4.744120	2.740117
12	1	0	-3.124790	4.477312	3.898280
13	1	0	-3.933850	2.215293	4.482508
14	1	0	-2.599442	0.238257	3.918951
15	6	0	-0.700848	-1.562964	3.150769
16	6	0	-0.885369	-2.674791	2.339597
17	6	0	-1.317559	-3.874919	2.882270
18	6	0	-1.565043	-3.969335	4.240359
19	6	0	-1.363280	-2.868764	5.061144
20	6	0	-0.923221	-1.674142	4.522737
21	1	0	-0.673037	-2.601414	1.277989
22	1	0	-1.455858	-4.737515	2.240657
23	1	0	-1.906554	-4.906148	4.665894
24	1	0	-1.541407	-2.945268	6.127669
25	1	0	-0.741292	-0.825219	5.174698
26	6	0	1.576887	0.044463	3.342662
27	6	0	2.430325	-1.050027	3.219978
28	6	0	3.635377	-1.078584	3.894203
29	6	0	4.012000	-0.006542	4.690704
30	6	0	3.171738	1.085003	4.814414
31	6	0	1.955556	1.110947	4.146690
32	1	0	2.148846	-1.887170	2.588623
33	1	0	4.288233	-1.938268	3.793656
34	1	0	4.959894	-0.026307	5.216545
35	1	0	3.454941	1.923933	5.440001
36	1	0	1.305611	1.968968	4.269146
37	6	0	-1.975521	-0.107762	0.149756

38	6	0	-2.804258	0.974880	0.423869
39	6	0	-4.184297	0.862896	0.311921
40	6	0	-4.759248	-0.334892	-0.081033
41	6	0	-3.942291	-1.415241	-0.373624
42	6	0	-2.562038	-1.300305	-0.264169
43	1	0	-2.379886	1.928277	0.726522
44	1	0	-4.809641	1.722275	0.533324
45	1	0	-5.836667	-0.424259	-0.165449
46	1	0	-4.377411	-2.356956	-0.692707
47	1	0	-1.945445	-2.159538	-0.512589
48	6	0	0.108669	-0.257063	-2.176940
49	6	0	-0.332373	0.991678	-2.038538
50	6	0	0.462606	-1.442296	-2.577548
51	1	0	0.448646	-1.686430	-3.637249
52	1	0	0.790885	-2.216387	-1.891668
53	6	0	0.464447	2.254317	-2.142199
54	1	0	-1.413460	1.126520	-1.995715
55	6	0	0.033028	3.279182	-1.108540
56	1	0	1.531200	2.032300	-2.052441
57	1	0	0.296701	2.661909	-3.148825
58	6	0	0.777452	4.595881	-1.211017
59	1	0	-1.043650	3.471354	-1.208895
60	1	0	0.181095	2.867755	-0.102156
61	7	0	0.242951	5.594083	-0.302332
62	1	0	1.852706	4.398463	-1.058982
63	1	0	0.689442	4.966434	-2.244156
64	16	0	1.090598	5.921867	0.948275
65	6	0	2.497654	6.887857	0.385319
66	8	0	0.345488	6.817318	1.814557
67	8	0	1.698009	4.778895	1.618410
68	6	0	3.786073	6.380483	0.432696
69	6	0	4.847437	7.131842	-0.053641
70	6	0	4.623218	8.390127	-0.584053
71	6	0	3.331562	8.898480	-0.633087
72	6	0	2.272674	8.148414	-0.156084
73	1	0	3.951792	5.397569	0.858264
74	1	0	5.854046	6.729958	-0.014219
75	1	0	5.452730	8.978101	-0.960731
76	1	0	3.151650	9.884504	-1.047422
77	1	0	1.261086	8.539025	-0.198646

17 **TS_B**



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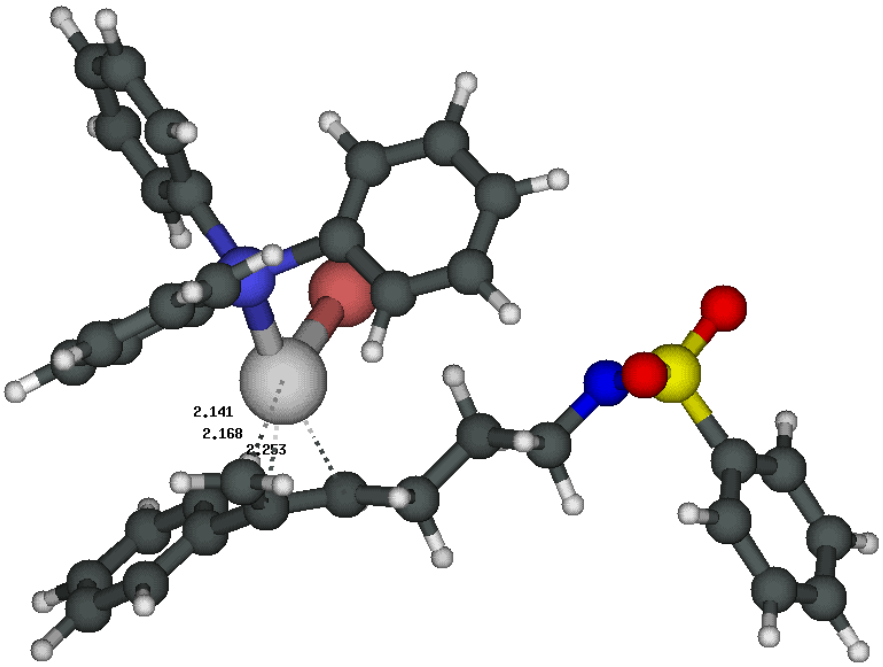
4	6	0	0.771203	1.427648	3.262897
5	6	0	1.307054	2.482322	2.534535
6	6	0	1.834588	3.586916	3.185288
7	6	0	1.832567	3.644108	4.567868
8	6	0	1.293244	2.598821	5.303528
9	6	0	0.757647	1.501108	4.655659
10	1	0	1.318910	2.433564	1.451353
11	1	0	2.246758	4.405584	2.606422
12	1	0	2.246587	4.507513	5.076431
13	1	0	1.283269	2.642827	6.386675
14	1	0	0.319196	0.696393	5.238277
15	6	0	-1.611358	-0.045948	3.277463
16	6	0	-2.404009	1.099725	3.226644
17	6	0	-3.645524	1.122212	3.832513
18	6	0	-4.116480	-0.003626	4.493561
19	6	0	-3.335325	-1.144450	4.548937
20	6	0	-2.086063	-1.167099	3.945279
21	1	0	-2.045079	1.983057	2.704696
22	1	0	-4.251884	2.019907	3.784555
23	1	0	-5.091555	0.012037	4.967084
24	1	0	-3.693939	-2.025131	5.069877
25	1	0	-1.484053	-2.067167	4.003130
26	6	0	0.869555	-1.490111	2.915653
27	6	0	0.473952	-2.682761	2.311877
28	6	0	1.115464	-3.869663	2.613852
29	6	0	2.175387	-3.876143	3.508456
30	6	0	2.586110	-2.692917	4.097255
31	6	0	1.935749	-1.503672	3.804817
32	1	0	-0.339982	-2.678138	1.590106
33	1	0	0.795087	-4.790954	2.140847
34	1	0	2.686328	-4.804196	3.738593

35	1	0	3.421940	-2.690035	4.787833
36	1	0	2.277602	-0.584179	4.266039
37	6	0	-2.129872	0.116688	-0.168580
38	6	0	-2.678045	1.333051	-0.561623
39	6	0	-4.019124	1.612273	-0.318763
40	6	0	-4.825968	0.674826	0.297940
41	6	0	-4.282267	-0.543822	0.692817
42	6	0	-2.947655	-0.815079	0.471616
43	1	0	-2.069018	2.076574	-1.065039
44	1	0	-4.429017	2.568085	-0.627040
45	1	0	-5.874295	0.886901	0.475234
46	1	0	-4.905379	-1.283312	1.185124
47	1	0	-2.539051	-1.771922	0.783894
48	6	0	-1.026484	-0.726670	-1.712266
49	6	0	-0.170304	0.247144	-2.186890
50	6	0	-1.469305	-1.934964	-2.004184
51	1	0	-1.902957	-2.609658	-1.276409
52	1	0	-1.451050	-2.259764	-3.041874
53	6	0	1.018071	-0.104349	-3.029354
54	1	0	-0.560309	1.257202	-2.316933
55	6	0	1.868150	1.095172	-3.389572
56	1	0	1.623234	-0.867235	-2.528329
57	1	0	0.636517	-0.572931	-3.950248
58	6	0	3.089674	0.718989	-4.198502
59	1	0	1.266620	1.815416	-3.958504
60	1	0	2.188100	1.601567	-2.471550
61	7	0	3.832395	1.908040	-4.560012
62	1	0	3.695068	0.012224	-3.605005
63	1	0	2.755539	0.147214	-5.087576
64	16	0	5.092631	1.676462	-5.428638
65	6	0	4.503868	1.181758	-7.053488
66	8	0	5.773558	2.938114	-5.644802
67	8	0	5.943432	0.572472	-5.006787
68	6	0	4.655534	-0.117115	-7.511272
69	6	0	4.143520	-0.483635	-8.748724
70	6	0	3.480412	0.446890	-9.529512
71	6	0	3.323507	1.747839	-9.069355
72	6	0	3.827853	2.112139	-7.834297
73	1	0	5.183429	-0.836143	-6.895497
74	1	0	4.266337	-1.501547	-9.102519
75	1	0	3.083475	0.161637	-10.497388
76	1	0	2.804326	2.479955	-9.678249
77	1	0	3.703052	3.125974	-7.468141

18 Int. B



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5	6	0	1.672695	2.212814	2.702259
6	6	0	2.370039	3.172089	3.420641
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9	6	0	0.893644	1.245871	4.760422
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12	1	0	2.876838	3.916170	5.365452
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14	1	0	0.311550	0.496466	5.289131
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24	1	0	-3.776251	-1.361140	5.388725
25	1	0	-1.569460	-1.675820	4.354448
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27	6	0	-0.044357	-2.723029	2.307568
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30	6	0	2.368227	-3.073669	3.615221
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33	1	0	-0.010166	-4.846709	1.992363
34	1	0	2.137155	-5.158013	3.159170
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56	1	0	-1.408237	-2.475233	-1.073366
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67	8	0	0.238653	-6.871792	0.610752
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74	1	0	-1.838733	-9.050986	-3.247305
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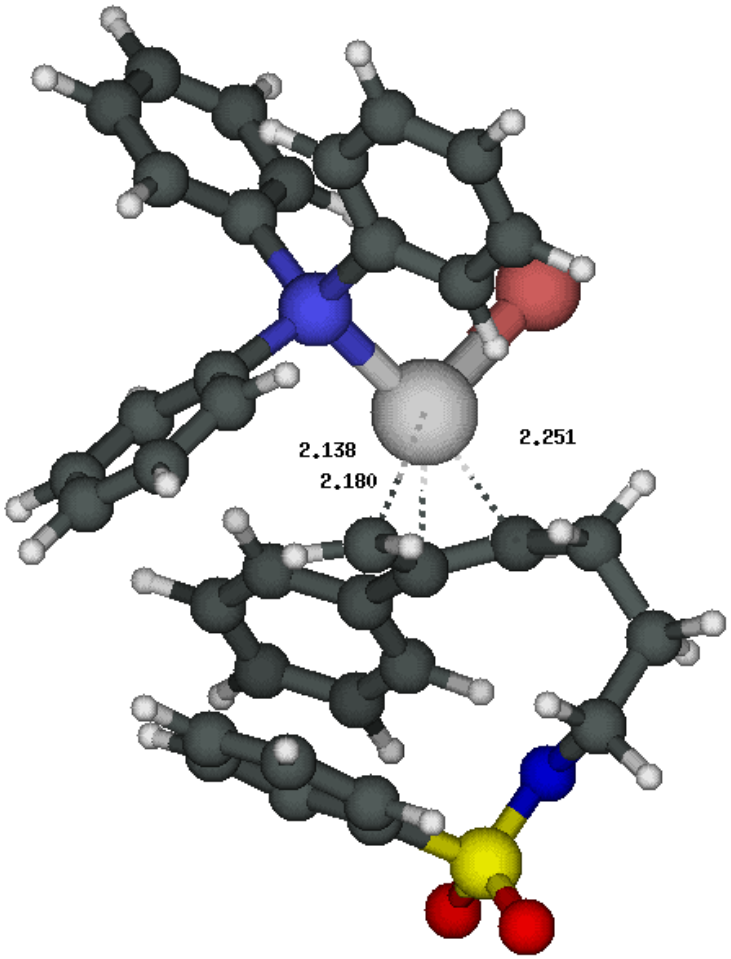
19 Int. B’



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6	6	0	2.666937	2.830315	3.431694
7	6	0	2.313832	3.148433	4.731902
8	6	0	1.235354	2.514595	5.330202
9	6	0	0.512804	1.565024	4.630124
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11	1	0	3.506558	3.326946	2.958502
12	1	0	2.876170	3.895422	5.280897
13	1	0	0.953282	2.762720	6.347180
14	1	0	-0.333583	1.080437	5.105872
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23	1	0	-5.493925	0.394580	3.914129
24	1	0	-4.387942	-1.817470	3.922287
25	1	0	-2.011180	-2.017382	3.338142
26	6	0	0.556994	-1.633302	2.985367

27	6	0	0.551922	-2.714594	2.108903
28	6	0	0.937203	-3.972247	2.542009
29	6	0	1.342290	-4.157668	3.853484
30	6	0	1.357222	-3.084899	4.731213
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32	1	0	0.247188	-2.562972	1.075823
33	1	0	0.927250	-4.807387	1.850902
34	1	0	1.651575	-5.139962	4.192484
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36	1	0	0.977106	-0.998772	4.999652
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46	1	0	-2.244252	3.798337	-4.473268
47	1	0	-1.771848	1.453102	-3.869532
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53	6	0	-0.516676	-1.824802	-2.286781
54	1	0	-0.033726	0.220547	-2.868196
55	6	0	-1.149198	-2.337070	-3.581961
56	1	0	0.540721	-2.109607	-2.277081
57	1	0	-0.984128	-2.346478	-1.445929
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67	8	0	-5.395510	-1.771005	-4.612516
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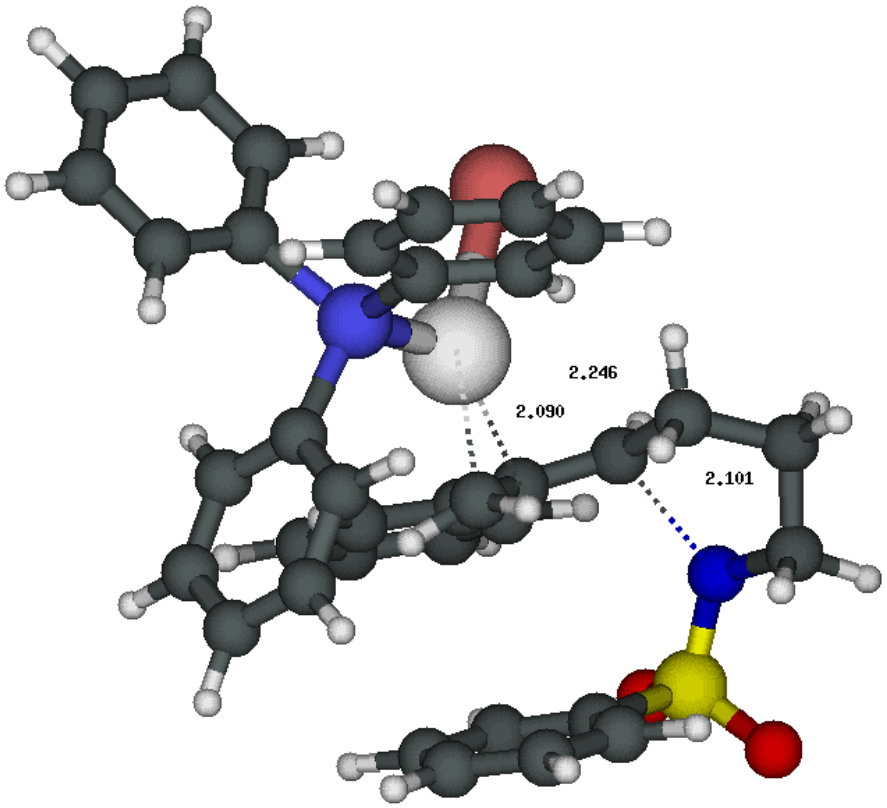
20 TS_C



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7	6	0	3.264392	2.171486	4.654571
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9	6	0	0.968402	1.483318	4.503493
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12	1	0	4.060265	2.672231	5.194517
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17	6	0	-3.128997	2.520689	3.055510
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27	6	0	0.026076	-2.796313	2.166197
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36	1	0	0.122889	-1.081390	5.084970
37	6	0	-1.433926	1.644889	-2.108537
38	6	0	-1.539932	2.757131	-1.262963
39	6	0	-1.436361	4.047595	-1.748110
40	6	0	-1.215503	4.277166	-3.097983
41	6	0	-1.104454	3.191029	-3.949283
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44	1	0	-1.523110	4.882690	-1.061198
45	1	0	-1.132477	5.288615	-3.479284
46	1	0	-0.941739	3.347159	-5.010515
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51	1	0	-2.574971	0.844637	0.255870
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56	1	0	-0.127895	-2.438646	-1.663630
57	1	0	-1.811258	-2.459859	-1.137831
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68	6	0	-5.409133	-1.011965	-1.626730
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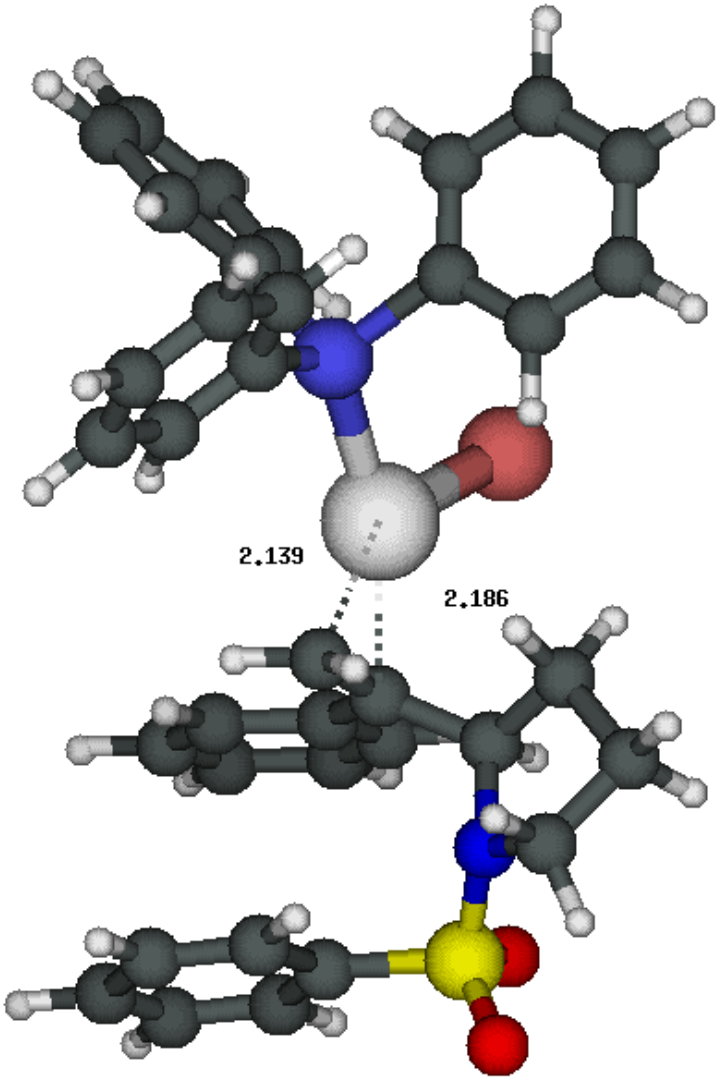
21 Int. C



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7	6	0	1.824973	3.670142	4.473706
8	6	0	0.707231	3.075409	5.035038
9	6	0	0.125452	1.972971	4.428203
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16	6	0	-2.688203	0.580206	2.822049
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19	6	0	-3.109652	-1.247856	4.852372
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24	1	0	-3.270621	-1.969543	5.645696
25	1	0	-1.055288	-1.789706	4.604566
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28	6	0	1.553804	-3.715700	2.962398
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38	6	0	0.393659	1.388781	-3.385316
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40	6	0	0.026565	3.751738	-3.669293
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62	1	0	-2.786860	-3.629219	-3.974894
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69	6	0	-4.943156	1.494247	-3.537902
70	6	0	-4.654129	2.641222	-4.264105
71	6	0	-3.613934	2.644039	-5.178297
72	6	0	-2.854551	1.501006	-5.371056
73	1	0	-4.406202	-0.551468	-3.157446
74	1	0	-5.756429	1.493914	-2.821438
75	1	0	-5.242984	3.538628	-4.112151
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77	1	0	-2.033137	1.493647	-6.077408

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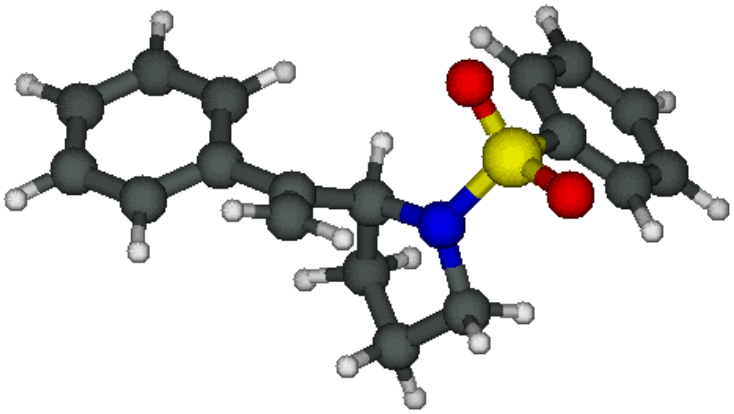
22 P



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2	6	0	0.069964	0.121817	1.423462
3	16	0	1.455848	-0.011373	-0.865757
4	6	0	-1.315135	-0.362970	1.803787
5	6	0	-1.631773	-1.363805	0.708314
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7	1	0	0.293625	1.130909	1.771611
8	1	0	0.833837	-0.557806	1.820986
9	1	0	-2.027977	0.466061	1.779258
10	1	0	-1.334757	-0.795363	2.803868
11	1	0	-1.052712	-2.281025	0.860041
12	1	0	-2.687090	-1.631141	0.643569
13	6	0	-2.166186	0.241128	-1.168714
14	1	0	-0.806593	-1.395159	-1.295129
15	6	0	2.044066	-1.662334	-0.628498
16	6	0	1.664090	-2.661328	-1.516125
17	6	0	2.074416	-3.963061	-1.288942
18	6	0	2.857809	-4.263372	-0.185851
19	6	0	3.241149	-3.261430	0.690912
20	6	0	2.836224	-1.955758	0.474064
21	1	0	1.067402	-2.418692	-2.387496
22	1	0	1.786186	-4.745060	-1.981558
23	1	0	3.179136	-5.284169	-0.013655
24	1	0	3.864176	-3.494875	1.546309
25	1	0	3.147943	-1.165075	1.145700
26	8	0	1.156266	0.150201	-2.256555
27	8	0	2.368093	0.878962	-0.213169
28	6	0	-2.084572	1.566530	-1.119581
29	6	0	-3.316018	-0.440295	-1.803500
30	1	0	-2.842069	2.197409	-1.570867
31	1	0	-1.243735	2.061616	-0.647852
32	6	0	-4.608627	0.060425	-1.646775
33	6	0	-5.690292	-0.554515	-2.251489
34	6	0	-5.505108	-1.690290	-3.023734
35	6	0	-4.229124	-2.205644	-3.180903
36	6	0	-3.147348	-1.592140	-2.572374
37	1	0	-4.765183	0.937145	-1.027304
38	1	0	-6.686037	-0.148751	-2.111111
39	1	0	-6.352156	-2.174660	-3.496071
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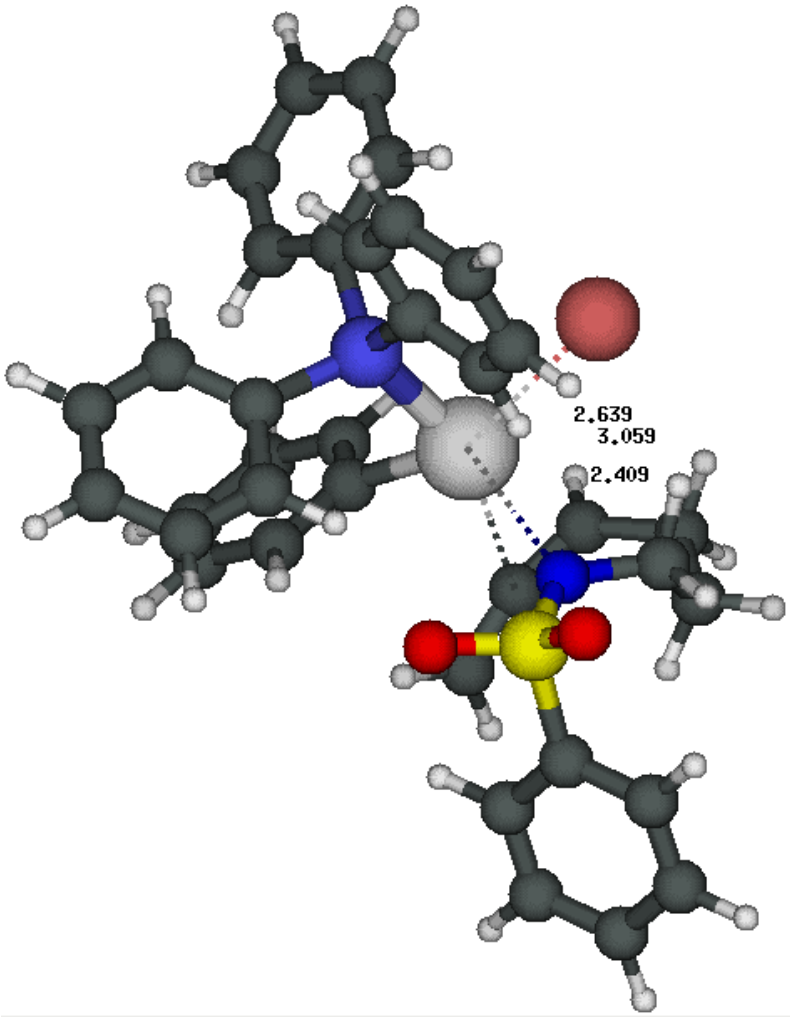
41	1	0	-2.156010	-2.007327	-2.719886

23 **TS_D**



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5	1	0	-0.067761	-1.028018	1.558894
6	1	0	1.386476	-0.055474	1.679063
7	6	0	-1.941633	0.862108	1.926001
8	1	0	-0.112164	1.134195	2.939167
9	1	0	-0.174420	2.009255	1.422186
10	6	0	-2.727042	1.083873	0.660895
11	1	0	-2.178762	-0.132180	2.314961
12	1	0	-2.369972	1.576142	2.642875
13	46	0	-2.485445	-0.532637	-1.057897
14	6	0	-2.279811	1.771885	-0.385656
15	6	0	2.219846	1.940886	-0.473582
16	8	0	2.887434	-0.537044	-0.331943
17	8	0	1.637238	0.210437	-2.308774
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19	6	0	-1.815129	2.708099	-1.158460
20	1	0	-1.837477	3.741991	-0.820510
21	1	0	-1.405452	2.518506	-2.144038
22	15	0	-2.334685	-2.315298	-2.532340
23	6	0	-3.943077	-3.145746	-2.676251
24	6	0	-1.743923	-1.970089	-4.226841
25	6	0	-1.098663	-3.589261	-2.101482

26	6	0	-3.396604	0.451235	-2.594860
27	6	0	-4.769965	0.583305	-2.415220
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31	6	0	-2.816759	0.994578	-3.731249
32	1	0	-5.250243	0.168859	-1.531871
33	1	0	-6.619605	1.325585	-3.205272
34	1	0	-5.573984	2.253717	-5.253573
35	1	0	-3.123803	2.050101	-5.570857
36	1	0	-1.744468	0.928810	-3.887582
37	6	0	-4.949798	-2.573967	-3.453924
38	6	0	-6.214783	-3.134500	-3.488345
39	6	0	-6.494359	-4.266939	-2.740834
40	6	0	-5.504807	-4.832631	-1.953823
41	6	0	-4.238309	-4.274592	-1.916532
42	1	0	-4.752611	-1.678074	-4.032967
43	1	0	-6.984772	-2.680263	-4.101765
44	1	0	-7.485316	-4.705839	-2.768212
45	1	0	-5.718803	-5.713912	-1.359751
46	1	0	-3.478686	-4.714817	-1.281609
47	6	0	-2.367291	-2.394032	-5.393079
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49	6	0	-0.610245	-1.410831	-6.706829
50	6	0	0.029099	-1.008433	-5.543347
51	6	0	-0.533543	-1.284183	-4.310794
52	1	0	-3.293501	-2.955170	-5.353116
53	1	0	-2.301922	-2.438751	-7.532223
54	1	0	-0.173651	-1.187515	-7.673785
55	1	0	0.969479	-0.470345	-5.594201
56	1	0	-0.025415	-0.946292	-3.408257
57	6	0	-1.120458	-4.821006	-2.750755
58	6	0	-0.116278	-5.746371	-2.524945
59	6	0	0.930477	-5.438411	-1.669639
60	6	0	0.970077	-4.202914	-1.044783
61	6	0	-0.042090	-3.279233	-1.254103
62	1	0	-1.921493	-5.061002	-3.443309
63	1	0	-0.147256	-6.706951	-3.026748
64	1	0	1.720288	-6.161146	-1.497401
65	1	0	1.794893	-3.952424	-0.386352
66	1	0	-0.001695	-2.306690	-0.769052
67	6	0	1.639120	2.978613	-1.192490
68	6	0	1.860495	4.292976	-0.820613
69	6	0	2.662811	4.581347	0.274789
70	6	0	3.253122	3.548875	0.984976
71	6	0	3.035637	2.230819	0.610954
72	1	0	1.013685	2.746585	-2.047363
73	1	0	1.406297	5.098010	-1.388377
74	1	0	2.833742	5.611186	0.567718
75	1	0	3.890747	3.769116	1.834310
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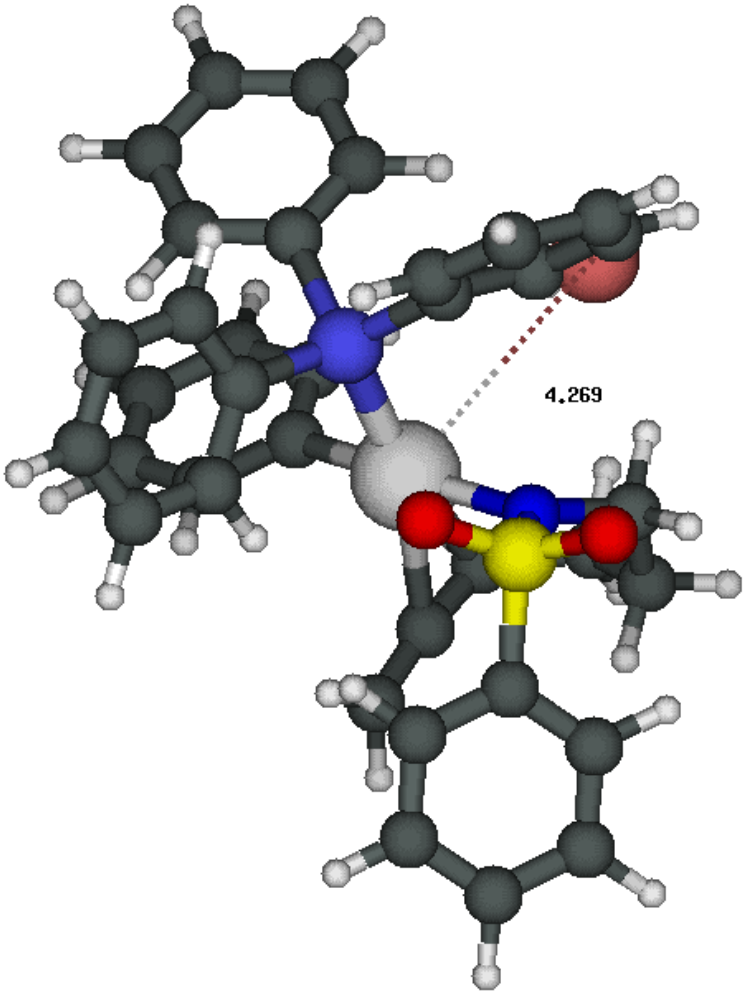
24 Int. D



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4	6	0	-0.480046	1.074483	2.049916
5	1	0	-0.545240	-1.000519	1.562557
6	1	0	1.084603	-0.353776	1.690036
7	6	0	-1.976219	1.247483	1.888719
8	1	0	-0.273692	0.937221	3.116517
9	1	0	0.051109	1.984196	1.745085
10	6	0	-2.465451	1.774253	0.575025
11	1	0	-2.482453	0.290320	2.076729
12	1	0	-2.356242	1.947421	2.644825
13	46	0	-1.790246	0.326088	-1.141340
14	6	0	-1.779109	2.468494	-0.331342
15	6	0	2.083350	1.760375	-0.817499
16	8	0	2.523029	-0.681423	-0.138027
17	8	0	1.337460	-0.231892	-2.255756
18	1	0	-3.547019	1.748946	0.443533
19	6	0	-1.190776	3.356600	-1.078204
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21	1	0	-0.709919	3.104229	-2.018005
22	15	0	-1.614648	-1.515974	-2.566821
23	6	0	-3.181741	-2.399437	-2.902512
24	6	0	-1.011873	-1.069744	-4.220162
25	6	0	-0.506542	-2.789086	-1.881434

26	6	0	-3.606714	0.632768	-1.976000
27	6	0	-4.731703	0.054312	-1.390458
28	6	0	-5.998471	0.304549	-1.899128
29	6	0	-6.161865	1.130608	-3.002700
30	6	0	-5.049007	1.712017	-3.587210
31	6	0	-3.779174	1.467160	-3.074327
32	1	0	-4.613423	-0.606842	-0.530461
33	1	0	-6.864843	-0.153753	-1.431582
34	1	0	-7.152071	1.321108	-3.402144
35	1	0	-5.163824	2.363053	-4.448172
36	1	0	-2.921744	1.935725	-3.550723
37	6	0	-3.943220	-2.083588	-4.026608
38	6	0	-5.180600	-2.669943	-4.227485
39	6	0	-5.682029	-3.573781	-3.303966
40	6	0	-4.938501	-3.882489	-2.177771
41	6	0	-3.698417	-3.299049	-1.975188
42	1	0	-3.574864	-1.368725	-4.754146
43	1	0	-5.756937	-2.413802	-5.109588
44	1	0	-6.652277	-4.031689	-3.460445
45	1	0	-5.326185	-4.576681	-1.440204
46	1	0	-3.160951	-3.526336	-1.061604
47	6	0	-0.940718	-2.006805	-5.249274
48	6	0	-0.488775	-1.634624	-6.503086
49	6	0	-0.112874	-0.321992	-6.743908
50	6	0	-0.188054	0.617303	-5.728763
51	6	0	-0.633844	0.243537	-4.472135
52	1	0	-1.246830	-3.033337	-5.073461
53	1	0	-0.434029	-2.371793	-7.296011
54	1	0	0.236658	-0.030799	-7.728125
55	1	0	0.101993	1.645432	-5.914125
56	1	0	-0.681843	0.972297	-3.668491
57	6	0	0.529690	-3.374212	-2.598103
58	6	0	1.360017	-4.302964	-1.991531
59	6	0	1.163435	-4.655942	-0.666391
60	6	0	0.134470	-4.070427	0.054229
61	6	0	-0.690988	-3.135025	-0.545124
62	1	0	0.714280	-3.093622	-3.628179
63	1	0	2.169137	-4.748605	-2.559393
64	1	0	1.817205	-5.380809	-0.194118
65	1	0	-0.025067	-4.330411	1.095808
66	1	0	-1.477282	-2.666876	0.046811
67	6	0	2.024739	2.541901	-1.960461
68	6	0	2.410037	3.873153	-1.908926
69	6	0	2.850346	4.423773	-0.717213
70	6	0	2.917456	3.637258	0.424573
71	6	0	2.539666	2.307187	0.375570
72	1	0	1.676706	2.101149	-2.888289
73	1	0	2.366281	4.481108	-2.805845
74	1	0	3.150573	5.464734	-0.677204
75	1	0	3.273258	4.061951	1.356599
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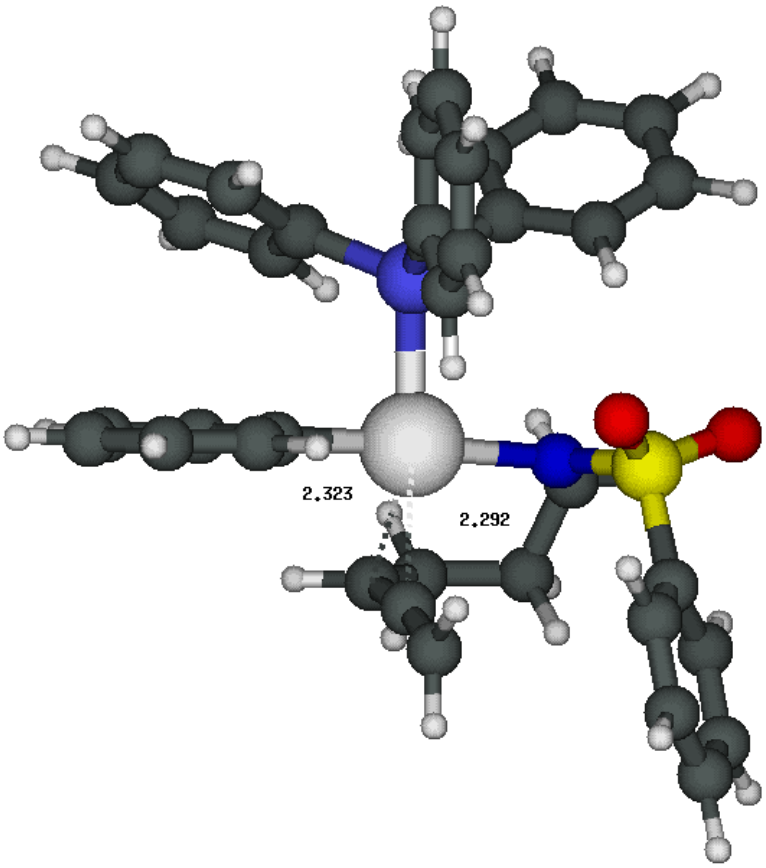
25 Int. E



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4	6	0	-0.495247	1.372503	2.028965
5	1	0	-0.678416	-0.747629	1.798791
6	1	0	0.982506	-0.182356	1.872083
7	6	0	-1.955388	1.672662	1.762991
8	1	0	-0.354546	1.341207	3.114119
9	1	0	0.127240	2.194143	1.658191
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11	1	0	-2.573103	0.814711	2.061165
12	1	0	-2.284697	2.498361	2.406956
13	46	0	-1.880137	0.244860	-0.983988
14	6	0	-1.607516	2.494982	-0.643847
15	6	0	2.071415	1.679615	-0.830613
16	8	0	2.429843	-0.708096	0.004718
17	8	0	1.197540	-0.375954	-2.112483
18	1	0	-3.430440	2.194013	0.241583
19	6	0	-0.982586	3.154997	-1.573783
20	1	0	-0.806526	4.223633	-1.470248
21	1	0	-0.610496	2.677709	-2.475115
22	15	0	-2.204802	-2.019729	-1.499419
23	6	0	-3.944240	-2.474614	-1.237908
24	6	0	-1.779448	-2.480570	-3.202795
25	6	0	-1.244749	-3.235927	-0.526606
26	6	0	-3.645064	0.582500	-1.925707
27	6	0	-4.863483	0.598490	-1.252622
28	6	0	-6.045664	0.885266	-1.919804
29	6	0	-6.031034	1.167126	-3.277719
30	6	0	-4.823177	1.174314	-3.955038

31	6	0	-3.639747	0.888645	-3.282964
32	1	0	-4.904171	0.370992	-0.190748
33	1	0	-6.983465	0.885658	-1.372992
34	1	0	-6.954730	1.385424	-3.802120
35	1	0	-4.794574	1.403320	-5.015514
36	1	0	-2.707534	0.904877	-3.840022
37	6	0	-4.800939	-2.802430	-2.281336
38	6	0	-6.147089	-3.026021	-2.035503
39	6	0	-6.646856	-2.930659	-0.748192
40	6	0	-5.799991	-2.593619	0.297061
41	6	0	-4.461124	-2.352427	0.051230
42	1	0	-4.427244	-2.872711	-3.296845
43	1	0	-6.806447	-3.276665	-2.858711
44	1	0	-7.698905	-3.110599	-0.558497
45	1	0	-6.186911	-2.503039	1.305612
46	1	0	-3.812456	-2.044313	0.868199
47	6	0	-1.955471	-3.788650	-3.651900
48	6	0	-1.591217	-4.135093	-4.939303
49	6	0	-1.037354	-3.183177	-5.783880
50	6	0	-0.841189	-1.888196	-5.336965
51	6	0	-1.208971	-1.537683	-4.047332
52	1	0	-2.377366	-4.538966	-2.989537
53	1	0	-1.734143	-5.152551	-5.284829
54	1	0	-0.749841	-3.457948	-6.792517
55	1	0	-0.394241	-1.147766	-5.990378
56	1	0	-1.027569	-0.533561	-3.678061
57	6	0	-1.819468	-4.178812	0.319366
58	6	0	-1.022860	-5.083205	1.004455
59	6	0	0.351929	-5.059110	0.850135
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61	6	0	0.139985	-3.225986	-0.685902
62	1	0	-2.893856	-4.227641	0.444759
63	1	0	-1.486133	-5.813421	1.658345
64	1	0	0.972880	-5.766811	1.387706
65	1	0	2.006366	-4.108788	-0.135285
66	1	0	0.602894	-2.505532	-1.352482
67	6	0	2.142061	2.340068	-2.045968
68	6	0	2.624603	3.639050	-2.100535
69	6	0	3.031623	4.278475	-0.942170
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71	6	0	2.503322	2.310656	0.329341
72	1	0	1.817182	1.833289	-2.946643
73	1	0	2.680716	4.152082	-3.054160
74	1	0	3.404567	5.295528	-0.984547
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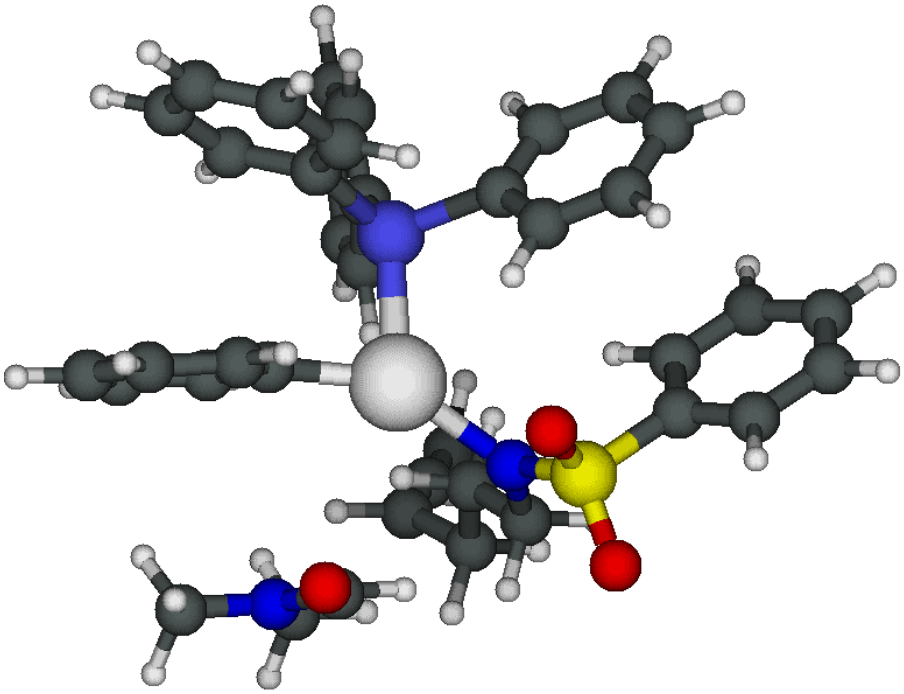
76	1	0	2.476723	1.784416	1.277442

26 Int. F



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4	6	0	-1.241384	-0.925721	3.128681
5	6	0	-1.248993	-1.151759	4.504944
6	6	0	-2.276453	-1.873983	5.083681
7	6	0	-3.302606	-2.378547	4.298659
8	6	0	-3.298566	-2.163787	2.931355
9	6	0	-2.269724	-1.441995	2.348679
10	1	0	-0.451951	-0.759492	5.128278
11	1	0	-2.276029	-2.043910	6.154109
12	1	0	-4.105220	-2.944935	4.757084
13	1	0	-4.094627	-2.560698	2.310725
14	1	0	-2.256301	-1.282735	1.275656
15	6	0	1.607568	-0.434224	3.140659
16	6	0	2.652731	0.469729	3.295915
17	6	0	3.878984	0.045011	3.781008
18	6	0	4.072766	-1.283874	4.116341
19	6	0	3.033356	-2.189584	3.969136
20	6	0	1.809557	-1.770353	3.480834
21	1	0	2.521265	1.513337	3.033893
22	1	0	4.684973	0.760405	3.897203
23	1	0	5.032976	-1.615156	4.494853
24	1	0	3.176341	-3.231751	4.231375
25	1	0	1.011543	-2.494047	3.356192
26	6	0	-0.215863	1.797196	2.895332
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30	6	0	0.344125	4.126127	2.629164
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32	1	0	-1.618316	1.365092	4.476019
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35	1	0	0.883743	4.902888	2.098296

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37	6	0	1.120877	-0.366502	-3.256629
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41	6	0	1.559103	-2.756082	-3.375268
42	1	0	-1.062112	-2.504925	-4.048118
43	1	0	-0.957557	-2.542077	-2.278405
44	1	0	-1.319934	-1.015280	-3.120039
45	1	0	1.332507	-3.327488	-4.280989
46	1	0	2.584919	-2.396497	-3.427579
47	1	0	1.453433	-3.422557	-2.512841
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50	6	0	1.284861	-3.891614	0.253786
51	6	0	2.657246	-3.763802	0.112830
52	6	0	3.227814	-2.500127	0.054295
53	6	0	2.432194	-1.368048	0.155854
54	1	0	-0.592170	-2.878328	0.474933
55	1	0	0.830847	-4.876099	0.298248
56	1	0	3.282731	-4.647056	0.048604
57	1	0	4.301309	-2.391652	-0.060938
58	1	0	2.891709	-0.383632	0.133729
59	7	0	-1.198784	1.476078	-1.104422
60	6	0	-2.478749	1.130632	-1.720172
61	6	0	-3.087062	-0.057772	-1.017288
62	1	0	-3.188741	1.970486	-1.693039
63	1	0	-2.337778	0.893497	-2.786014
64	6	0	-4.319097	-0.618219	-1.703420
65	1	0	-2.327700	-0.851042	-0.949274
66	1	0	-3.334786	0.216917	0.015649
67	6	0	-4.764870	-1.879288	-1.028347
68	1	0	-5.128625	0.117882	-1.704596
69	1	0	-4.080243	-0.835249	-2.752273
70	6	0	-5.883380	-2.036444	-0.384695
71	6	0	-7.000804	-2.192801	0.258629
72	1	0	-4.061047	-2.713697	-1.056210
73	1	0	-7.085140	-1.957118	1.316493
74	1	0	-7.895628	-2.564643	-0.233365
75	16	0	-0.647641	2.917316	-1.446607
76	6	0	-1.576976	4.070684	-0.444393
77	8	0	0.723055	3.026395	-1.003757
78	8	0	-0.914912	3.301542	-2.815846
79	6	0	-2.451700	3.638765	0.539004
80	6	0	-3.134468	4.569234	1.307916
81	6	0	-2.932253	5.923701	1.103577
82	6	0	-2.049387	6.352455	0.122638
83	6	0	-1.375703	5.428296	-0.655963
84	1	0	-2.594275	2.576363	0.706833
85	1	0	-3.822056	4.230414	2.074924
86	1	0	-3.463984	6.649421	1.708556
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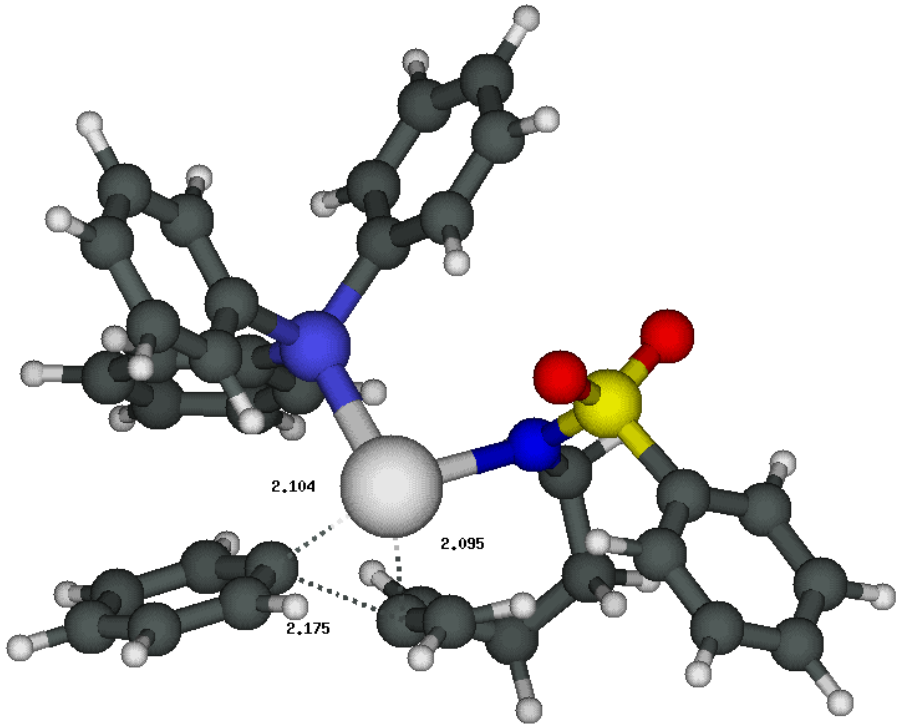
88	1	0	-0.691393	5.759356	-1.430002

27 **TS_G**



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4	6	0	-0.590019	1.382182	2.165023
5	1	0	-1.104545	-0.680988	1.735108
6	1	0	0.590235	-0.421595	2.053270
7	6	0	-2.079322	1.770145	2.317964
8	1	0	-0.148654	1.410985	3.166393
9	1	0	-0.069271	2.158255	1.597432
10	6	0	-2.861856	1.327189	1.120872
11	1	0	-2.495687	1.297304	3.210312
12	1	0	-2.145072	2.851060	2.470947
13	46	0	-1.805588	0.212821	-1.197149
14	6	0	-2.614711	1.798771	-0.093420
15	6	0	2.148911	1.616164	-0.041478
16	8	0	2.327944	-0.910599	0.336933
17	8	0	1.481329	-0.114396	-1.843906
18	1	0	-3.485370	0.441979	1.221331
19	6	0	-1.589040	2.359242	-0.820787
20	1	0	-1.792176	3.020870	-1.656993
21	1	0	-0.589518	2.402433	-0.403679
22	15	0	-2.296189	-2.105791	-1.546629
23	6	0	-3.770692	-2.610349	-0.607158
24	6	0	-2.643964	-2.527152	-3.284034
25	6	0	-1.034175	-3.346280	-1.103859
26	6	0	-3.711728	0.912210	-1.748546
27	6	0	-3.737865	1.681253	-2.911957
28	6	0	-4.909400	1.818055	-3.642581
29	6	0	-6.080725	1.228363	-3.198063
30	6	0	-6.074855	0.504164	-2.013707
31	6	0	-4.902546	0.349213	-1.295345
32	1	0	-2.834521	2.158228	-3.277757
33	1	0	-4.903174	2.395554	-4.560798
34	1	0	-6.999246	1.344075	-3.762128

35	1	0	-6.990932	0.054435	-1.644651
36	1	0	-4.924963	-0.216587	-0.369092
37	6	0	-4.957468	-3.011646	-1.206226
38	6	0	-6.077498	-3.275971	-0.431595
39	6	0	-6.020354	-3.144128	0.944542
40	6	0	-4.836755	-2.747413	1.551383
41	6	0	-3.722312	-2.477066	0.779959
42	1	0	-5.024185	-3.102524	-2.284842
43	1	0	-7.000017	-3.582309	-0.911672
44	1	0	-6.897638	-3.348944	1.547508
45	1	0	-4.784817	-2.642476	2.629077
46	1	0	-2.803248	-2.149341	1.259746
47	6	0	-2.849027	-3.847557	-3.681740
48	6	0	-3.104386	-4.143195	-5.007691
49	6	0	-3.151496	-3.126266	-5.951281
50	6	0	-2.936088	-1.814879	-5.566723
51	6	0	-2.679760	-1.516988	-4.236918
52	1	0	-2.810747	-4.648922	-2.949785
53	1	0	-3.265436	-5.172093	-5.308749
54	1	0	-3.350209	-3.361752	-6.990729
55	1	0	-2.960879	-1.018507	-6.301961
56	1	0	-2.496273	-0.491827	-3.932450
57	6	0	-1.308939	-4.495711	-0.370176
58	6	0	-0.312610	-5.431656	-0.142556
59	6	0	0.960608	-5.231204	-0.649414
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61	6	0	0.249325	-3.147850	-1.604782
62	1	0	-2.304844	-4.672747	0.020492
63	1	0	-0.536868	-6.324398	0.430378
64	1	0	1.738132	-5.965372	-0.470648
65	1	0	2.236798	-3.920049	-1.772966
66	1	0	0.481121	-2.240581	-2.155444
67	6	0	1.957315	2.660122	-0.936382
68	6	0	2.399887	3.932401	-0.615595
69	6	0	3.032893	4.164413	0.596198
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71	6	0	2.795885	1.843464	1.164849
72	1	0	1.464329	2.470999	-1.883655
73	1	0	2.253750	4.746038	-1.317202
74	1	0	3.377666	5.161505	0.845697
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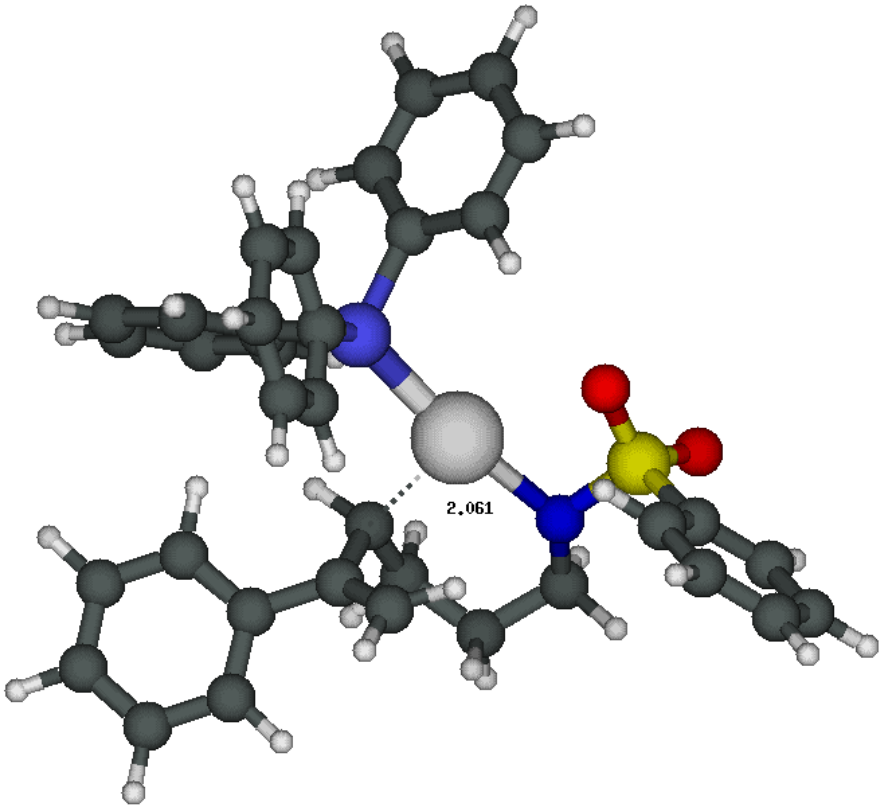
28 Int. G



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4	6	0	-1.413798	-0.022059	1.881788
5	1	0	0.538473	-0.906123	1.893870
6	1	0	0.539837	0.854262	1.757027
7	6	0	-2.243271	-1.198987	1.396451
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9	1	0	-1.880681	0.917380	1.566781
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11	1	0	-1.699773	-2.135509	1.573877
12	1	0	-3.148566	-1.256214	2.020568
13	46	0	-1.130859	-1.270720	-1.327172
14	6	0	-3.638254	-0.022376	-0.331421
15	6	0	1.774268	1.630207	-1.066847
16	8	0	2.577722	-0.601165	-0.048647
17	8	0	1.179453	-0.683425	-2.093481
18	1	0	-3.284419	-2.116276	-0.202992
19	6	0	-3.219746	1.171395	-0.750265
20	1	0	-3.916584	1.985990	-0.918944
21	1	0	-2.173696	1.361946	-0.965140
22	15	0	-2.196706	-2.631195	-2.842808
23	6	0	-3.397118	-3.836929	-2.199916
24	6	0	-3.045537	-1.824658	-4.237076
25	6	0	-0.923993	-3.644962	-3.666480
26	6	0	-5.078130	-0.240088	-0.040754
27	6	0	-5.793046	0.683867	0.719500
28	6	0	-7.140890	0.499557	0.978801
29	6	0	-7.801580	-0.612039	0.481491
30	6	0	-7.101804	-1.540939	-0.272544
31	6	0	-5.752349	-1.361848	-0.522457
32	1	0	-5.277581	1.549491	1.122710

33	1	0	-7.676281	1.226660	1.579358
34	1	0	-8.856449	-0.757004	0.685210
35	1	0	-7.609448	-2.412954	-0.670844
36	1	0	-5.220750	-2.094555	-1.122512
37	6	0	-4.617694	-4.090442	-2.815027
38	6	0	-5.509469	-4.990770	-2.252141
39	6	0	-5.188350	-5.645186	-1.075532
40	6	0	-3.967952	-5.405129	-0.460687
41	6	0	-3.079631	-4.503265	-1.017046
42	1	0	-4.887455	-3.576809	-3.731295
43	1	0	-6.461042	-5.177040	-2.736976
44	1	0	-5.889207	-6.344710	-0.634382
45	1	0	-3.710896	-5.917605	0.459218
46	1	0	-2.128778	-4.305678	-0.527580
47	6	0	-3.159600	-2.444643	-5.479338
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51	6	0	-3.622469	-0.574406	-4.043619
52	1	0	-2.716206	-3.422114	-5.642636
53	1	0	-3.925994	-2.310215	-7.472642
54	1	0	-4.951041	-0.088719	-7.116004
55	1	0	-4.754859	1.021063	-4.915361
56	1	0	-3.528484	-0.080657	-3.080691
57	6	0	-0.956288	-5.033473	-3.710212
58	6	0	0.049523	-5.733398	-4.359219
59	6	0	1.088267	-5.054025	-4.971614
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61	6	0	0.126785	-2.967250	-4.282702
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63	1	0	0.015296	-6.816624	-4.388424
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65	1	0	1.934786	-3.130814	-5.414265
66	1	0	0.162035	-1.882253	-4.249884
67	6	0	1.026107	2.311148	-2.019143
68	6	0	1.230709	3.665107	-2.205947
69	6	0	2.171686	4.339197	-1.439537
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71	6	0	2.714708	2.297357	-0.298938
72	1	0	0.293384	1.776464	-2.614481
73	1	0	0.655300	4.198691	-2.953730
74	1	0	2.329320	5.401329	-1.588441
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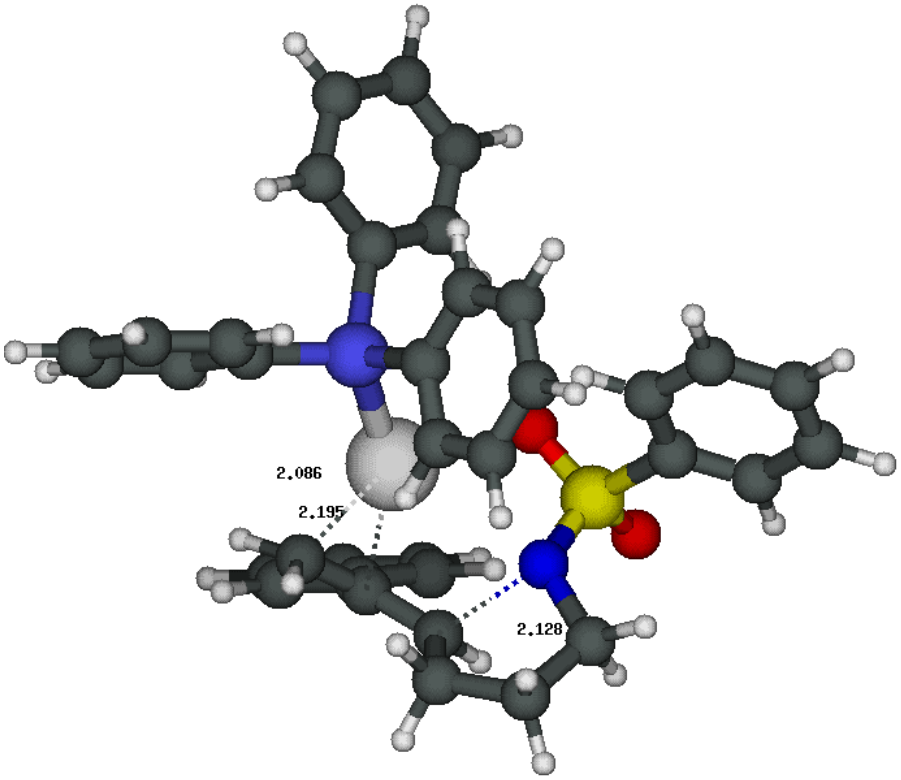
76	1	0	3.294023	1.751561	0.436173

29 **TS_H**



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4	6	0	-1.437435	-0.253010	1.826492
5	1	0	0.639071	-0.870508	1.871110
6	1	0	0.409734	0.879967	1.866857
7	6	0	-2.128766	-1.101584	0.756025
8	1	0	-1.514601	-0.708078	2.815511
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13	46	0	-1.038766	-0.545232	-2.625531
14	6	0	-1.525597	-2.314339	-1.421191
15	6	0	2.102832	1.605641	-0.357311
16	8	0	2.444630	-0.956924	-0.148744
17	8	0	1.256976	-0.095028	-2.125202
18	1	0	-0.389552	-2.347095	0.374541
19	6	0	-2.639108	-1.792511	-2.143119
20	1	0	-3.018539	-2.348850	-2.994004
21	1	0	-3.402291	-1.212190	-1.633250
22	15	0	-1.711606	1.189628	-3.961450
23	6	0	-1.720811	2.707643	-2.947141
24	6	0	-0.668500	1.630647	-5.389605
25	6	0	-3.392030	1.109182	-4.661029
26	6	0	-0.764370	-3.477471	-1.951184
27	6	0	0.596640	-3.647278	-1.684864
28	6	0	1.288801	-4.741887	-2.171760
29	6	0	0.643915	-5.697997	-2.940607
30	6	0	-0.705702	-5.545435	-3.211079
31	6	0	-1.399893	-4.452370	-2.721103
32	1	0	1.135127	-2.904047	-1.104800

33	1	0	2.346482	-4.842983	-1.953745
34	1	0	1.187930	-6.554219	-3.322721
35	1	0	-1.229578	-6.288604	-3.802372
36	1	0	-2.461297	-4.367056	-2.926263
37	6	0	-1.177185	3.916806	-3.366283
38	6	0	-1.178615	5.014895	-2.518620
39	6	0	-1.727092	4.917103	-1.251098
40	6	0	-2.279300	3.716457	-0.828028
41	6	0	-2.269963	2.618261	-1.668386
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43	1	0	-0.747757	5.951775	-2.853898
44	1	0	-1.723085	5.776096	-0.589632
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47	6	0	-1.174775	2.145875	-6.577729
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51	6	0	0.707998	1.469017	-5.247971
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53	1	0	-0.719589	2.892632	-8.532523
54	1	0	1.721429	2.613413	-8.264856
55	1	0	2.633924	1.702037	-6.153602
56	1	0	1.106728	1.057362	-4.323756
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58	6	0	-5.542583	2.047570	-5.199403
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64	1	0	-6.887220	0.775417	-6.281089
65	1	0	-5.295918	-1.117523	-6.368339
66	1	0	-3.073596	-0.910473	-5.315918
67	6	0	1.568541	2.682546	-1.052602
68	6	0	2.023628	3.959554	-0.780131
69	6	0	2.997431	4.159817	0.188126
70	6	0	3.517702	3.082253	0.884812
71	6	0	3.070984	1.798159	0.614558
72	1	0	0.804764	2.519529	-1.807624
73	1	0	1.615811	4.802032	-1.327932
74	1	0	3.351395	5.162499	0.399008
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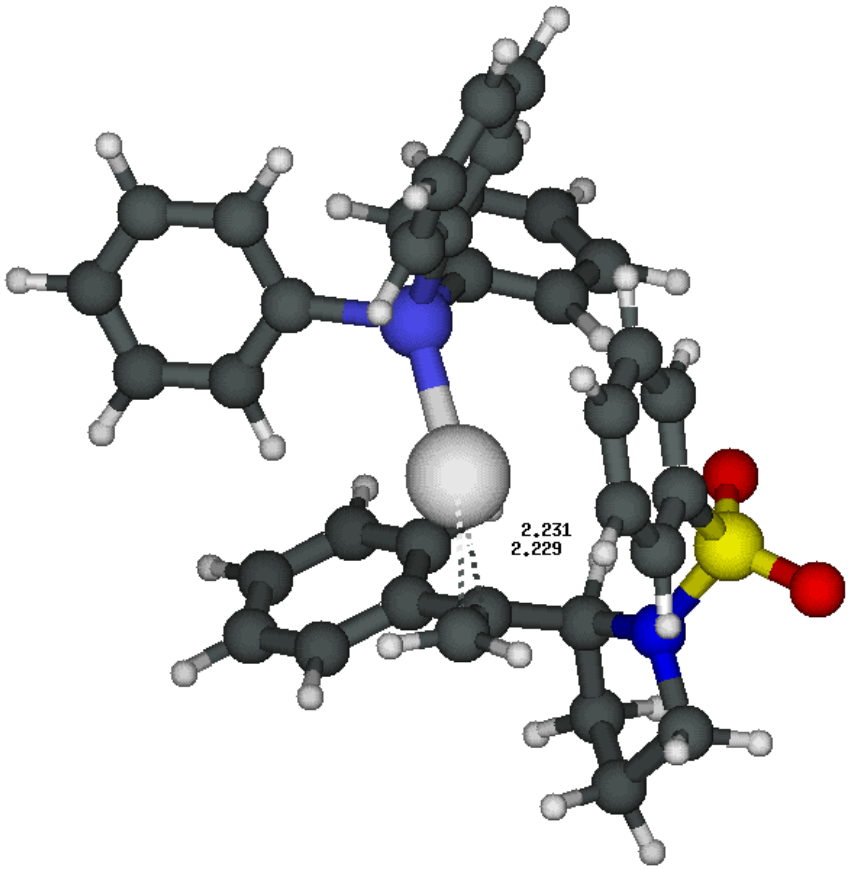
76	1	0	3.475274	0.945897	1.147873

30 Int. H



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4	6	0	-1.651294	-1.218561	1.590750
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6	1	0	0.299268	-0.258174	1.856710
7	6	0	-2.224068	-1.710767	0.274445
8	1	0	-1.833743	-1.902626	2.419458
9	1	0	-2.087381	-0.251461	1.854341
10	6	0	-1.460388	-0.879543	-0.761292
11	1	0	-1.982611	-2.766736	0.124566
12	1	0	-3.305277	-1.592445	0.197460
13	46	0	-1.116816	1.708167	-2.522468
14	6	0	-2.120735	0.474604	-0.957379
15	6	0	1.872010	0.550107	-1.399551
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17	8	0	0.932386	-1.713946	-2.236920
18	1	0	-1.393082	-1.401609	-1.716485
19	6	0	-1.628866	1.604854	-0.355707
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21	1	0	-0.735133	1.557400	0.256245
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23	6	0	-2.428869	3.166394	-5.374835
24	6	0	0.406833	2.868335	-5.568004
25	6	0	-1.306512	0.555319	-5.736344
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27	6	0	-3.759467	-0.428737	-2.635211
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30	6	0	-5.732059	1.292156	-1.750899
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35	1	0	-6.504805	1.960840	-1.387611
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39	6	0	-4.627453	4.660923	-6.204669
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41	6	0	-3.610857	3.154912	-4.638878
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43	1	0	-3.386622	5.287517	-7.838735
44	1	0	-5.481181	5.246393	-6.526953
45	1	0	-5.621876	3.871641	-4.472532
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48	6	0	2.240903	2.939945	-7.127267
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51	6	0	0.854656	4.067645	-5.016057
52	1	0	0.777635	1.376978	-7.073235
53	1	0	2.783526	2.492785	-7.952668
54	1	0	3.553879	4.627971	-6.974216
55	1	0	2.305533	5.639091	-5.089157
56	1	0	0.320889	4.501373	-4.173382
57	6	0	-2.172473	0.440090	-6.818017
58	6	0	-2.331557	-0.778535	-7.461285
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62	1	0	-2.736184	1.300602	-7.162757
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66	1	0	0.058943	-0.497313	-4.453650
67	6	0	2.229654	0.851762	-2.703229
68	6	0	2.779222	2.092899	-2.984855
69	6	0	2.948479	3.023233	-1.974452
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71	6	0	2.061870	1.468083	-0.375923
72	1	0	2.085011	0.121383	-3.490393
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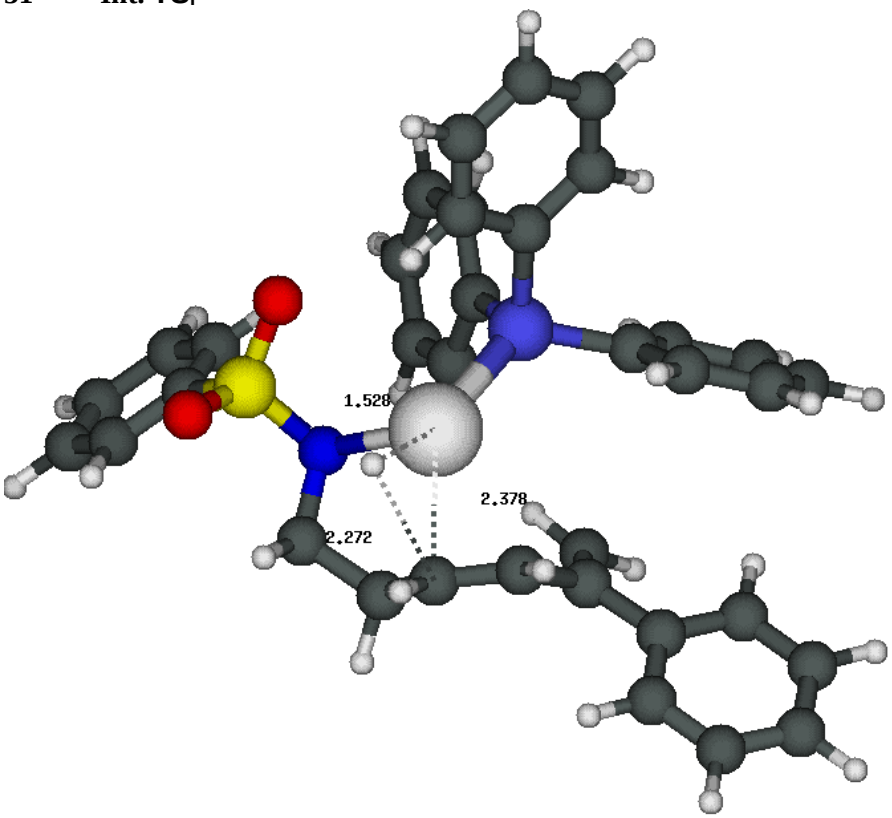
31 Int. TS_I



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4	6	0	-1.384143	-0.311611	1.944646
5	1	0	0.720492	-0.726274	1.852819
6	1	0	0.309172	0.992824	1.773411
7	6	0	-1.826734	-1.690703	1.577270
8	1	0	-1.341599	-0.245084	3.038653
9	1	0	-2.087684	0.447604	1.599126
10	6	0	-3.033831	-2.127566	1.111435
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12	1	0	-1.146352	-2.472504	1.908782
13	46	0	-1.294563	-1.587571	-0.737642
14	6	0	-4.301320	-1.382055	1.001415
15	6	0	2.005803	1.669145	-0.472249
16	8	0	2.463273	-0.840336	-0.018700
17	8	0	1.353929	-0.221344	-2.125875
18	1	0	-3.146101	-3.208377	1.066194
19	6	0	-4.422126	-0.147381	0.509200
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21	1	0	-3.579686	0.373878	0.074448
22	15	0	-2.478382	-0.542067	-2.646992
23	6	0	-4.298030	-0.593485	-2.773340
24	6	0	-2.050958	1.193728	-3.014189
25	6	0	-1.959098	-1.471506	-4.129839
26	6	0	-5.493639	-2.099457	1.517321
27	6	0	-5.093793	0.520318	-3.004341
28	6	0	-6.475387	0.393738	-3.055522
29	6	0	-7.068783	-0.845315	-2.891421
30	6	0	-6.278586	-1.964018	-2.663556
31	6	0	-4.904639	-1.836177	-2.593781
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33	1	0	-7.087412	1.270772	-3.233983
34	1	0	-8.147588	-0.942577	-2.936959
35	1	0	-6.738023	-2.936783	-2.527215
36	1	0	-4.289675	-2.711409	-2.395701
37	6	0	-1.632318	1.623339	-4.268906
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39	6	0	-1.430084	3.875983	-3.456363
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41	6	0	-2.140556	2.123748	-1.979419
42	1	0	-1.544705	0.917220	-5.087536
43	1	0	-0.991043	3.276709	-5.468416
44	1	0	-1.187589	4.918600	-3.628904
45	1	0	-1.922321	4.168440	-1.386819
46	1	0	-2.443557	1.803833	-0.986758
47	6	0	-2.732196	-1.530999	-5.286941
48	6	0	-2.291709	-2.247044	-6.386187
49	6	0	-1.075460	-2.911576	-6.341551
50	6	0	-0.298641	-2.855521	-5.196496
51	6	0	-0.737891	-2.139158	-4.094761
52	1	0	-3.684119	-1.011032	-5.332007
53	1	0	-2.900512	-2.285891	-7.282457
54	1	0	-0.733866	-3.474970	-7.202621
55	1	0	0.652740	-3.373882	-5.157795
56	1	0	-0.122890	-2.082966	-3.199869
57	6	0	1.487136	2.648238	-1.308870
58	6	0	1.842268	3.970447	-1.115651
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63	1	0	1.441837	4.735570	-1.771882
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66	1	0	3.268154	1.231150	1.200486
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68	6	0	-7.864331	-2.570115	1.433115
69	6	0	-7.750893	-3.417217	2.524441
70	6	0	-6.510838	-3.609306	3.110675
71	6	0	-5.394570	-2.961987	2.609068
72	1	0	-6.848061	-1.277217	0.066673
73	1	0	-8.828092	-2.420581	0.958938
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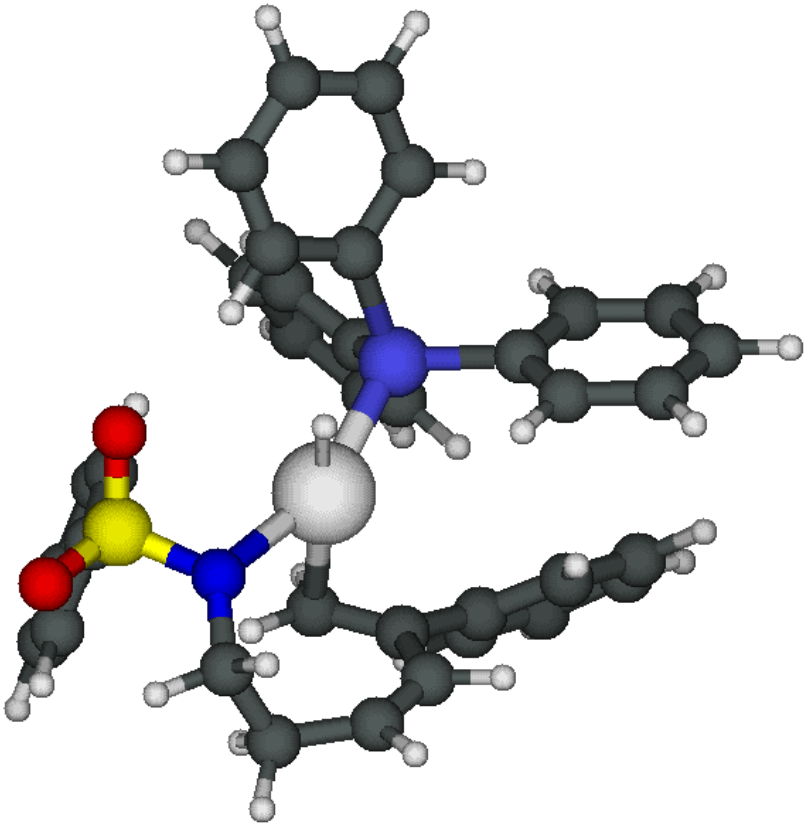
32 Int. I



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5	1	0	-0.429139	-0.869784	1.804958
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12	46	0	-1.647374	0.288361	-1.417275
13	6	0	-2.805986	2.419623	-0.184064
14	6	0	1.609568	1.651595	-1.443628
15	8	0	2.530059	-0.233368	0.076052
16	8	0	1.345517	-0.845256	-1.989309
17	1	0	-4.061141	1.297521	1.148607
18	6	0	-1.614771	2.715643	-0.760467
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20	1	0	-0.661008	2.445425	-0.332480
21	15	0	-2.794759	0.135393	-3.371779
22	6	0	-4.593415	-0.086251	-3.254934
23	6	0	-2.499817	1.626087	-4.378030
24	6	0	-2.248713	-1.209713	-4.480507
25	6	0	-4.037439	3.046111	-0.730129
26	6	0	-4.020358	4.385373	-1.118156
27	6	0	-5.148972	4.986314	-1.647209
28	6	0	-6.317257	4.257682	-1.804139
29	6	0	-6.353301	2.930109	-1.407310
30	6	0	-5.228449	2.334632	-0.863515

31	1	0	-3.112236	4.964845	-0.991737
32	1	0	-5.115769	6.030979	-1.935456
33	1	0	-7.200548	4.726054	-2.223138
34	1	0	-7.261949	2.349223	-1.523238
35	1	0	-5.274295	1.291704	-0.570806
36	6	0	-5.493253	0.459070	-4.165631
37	6	0	-6.850848	0.223911	-4.026906
38	6	0	-7.318804	-0.563787	-2.986997
39	6	0	-6.426963	-1.118973	-2.082969
40	6	0	-5.070587	-0.876541	-2.213060
41	1	0	-5.136903	1.072101	-4.986603
42	1	0	-7.545956	0.657100	-4.737055
43	1	0	-8.382381	-0.744801	-2.880421
44	1	0	-6.788845	-1.735399	-1.268105
45	1	0	-4.372250	-1.292090	-1.491514
46	6	0	-1.534247	1.627873	-5.381656
47	6	0	-1.237034	2.795647	-6.065897
48	6	0	-1.894623	3.973610	-5.753613
49	6	0	-2.853621	3.981357	-4.752110
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53	1	0	-1.661760	4.885884	-6.290867
54	1	0	-3.375869	4.898804	-4.503214
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56	6	0	-3.050419	-1.610525	-5.545841
57	6	0	-2.605213	-2.575984	-6.431620
58	6	0	-1.349999	-3.141342	-6.269977
59	6	0	-0.542723	-2.738309	-5.219903
60	6	0	-0.989032	-1.778316	-4.325198
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63	1	0	-1.001971	-3.897916	-6.964121
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65	1	0	-0.348491	-1.466158	-3.503955
66	6	0	1.186697	1.971577	-2.724982
67	6	0	1.238176	3.287508	-3.157214
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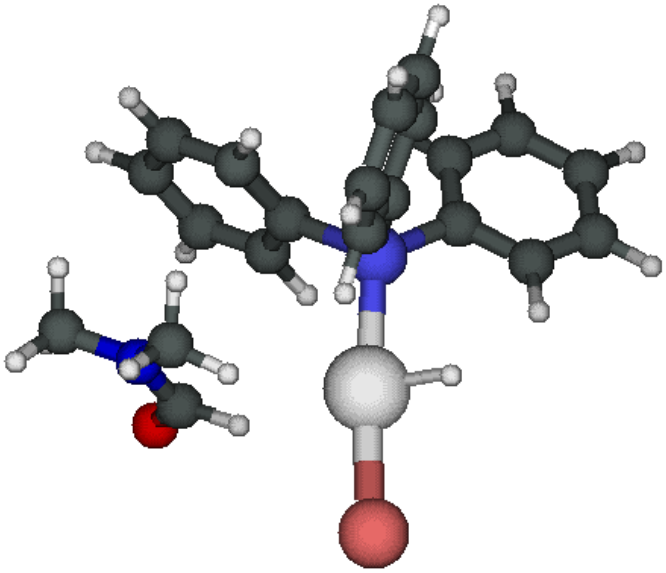
69	6	0	2.142417	3.954250	-1.035427
70	6	0	2.091373	2.641394	-0.598437
71	1	0	0.816469	1.189686	-3.380277
72	1	0	0.907002	3.536300	-4.160099
73	1	0	1.751558	5.308111	-2.653483
74	1	0	2.521833	4.726921	-0.376298
75	1	0	2.423692	2.381030	0.401008
76	1	0	-1.547893	-1.208674	-1.733311

33 [H-Pd^0-Br (DMF)(PPh$_3$)] V



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4	6	0	-1.668452	0.080452	-0.648469
5	6	0	-2.559907	-0.940437	-0.322619
6	6	0	-3.867437	-0.893274	-0.767372
7	6	0	-4.302533	0.182212	-1.527782
8	6	0	-3.426843	1.208579	-1.839608
9	6	0	-2.111775	1.160795	-1.403100
10	1	0	-2.223806	-1.778545	0.282348
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12	1	0	-5.329514	0.221992	-1.872760
13	1	0	-3.765345	2.052713	-2.429692
14	1	0	-1.433909	1.968690	-1.657417
15	6	0	0.919065	1.367732	-0.705907
16	6	0	1.343471	1.381725	-2.031512
17	6	0	1.974577	2.500459	-2.546039
18	6	0	2.182593	3.612332	-1.744147
19	6	0	1.762247	3.604747	-0.424540
20	6	0	1.135567	2.484143	0.094531
21	1	0	1.179439	0.517407	-2.667173
22	1	0	2.306242	2.504225	-3.577969
23	1	0	2.678887	4.486614	-2.149826
24	1	0	1.928533	4.470631	0.205892
25	1	0	0.814521	2.466637	1.132521
26	6	0	0.724906	-1.511654	-0.821901
27	6	0	0.213736	-1.991920	-2.024951
28	6	0	0.802412	-3.078927	-2.648057
29	6	0	1.906492	-3.692945	-2.079776
30	6	0	2.422177	-3.219037	-0.884382
31	6	0	1.831481	-2.137061	-0.255480
32	1	0	-0.646686	-1.515330	-2.482623
33	1	0	0.395455	-3.446591	-3.583045
34	1	0	2.363956	-4.546125	-2.567626
35	1	0	3.282867	-3.699149	-0.433185
36	1	0	2.229275	-1.778309	0.688750
37	1	0	1.495289	-0.192242	2.048208
38	6	0	-3.324929	0.435289	2.563451

39	8	0	-4.194896	-0.392685	2.721368
40	7	0	-3.465366	1.661611	2.034222
41	6	0	-2.379906	2.605774	1.964210
42	6	0	-4.751815	2.131780	1.577892
43	1	0	-1.469167	2.170851	2.385641
44	1	0	-2.181837	2.891591	0.925526
45	1	0	-2.623922	3.510649	2.529313
46	1	0	-5.464192	1.309055	1.584050
47	1	0	-5.122278	2.931798	2.226641
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49	1	0	-2.271099	0.243418	2.882754

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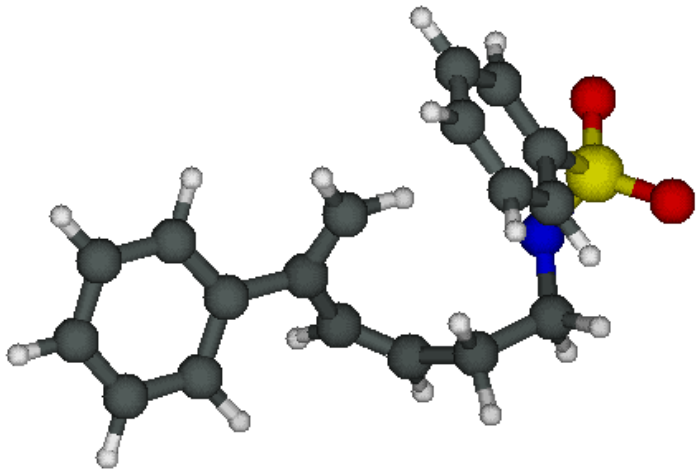
34 **P_H**



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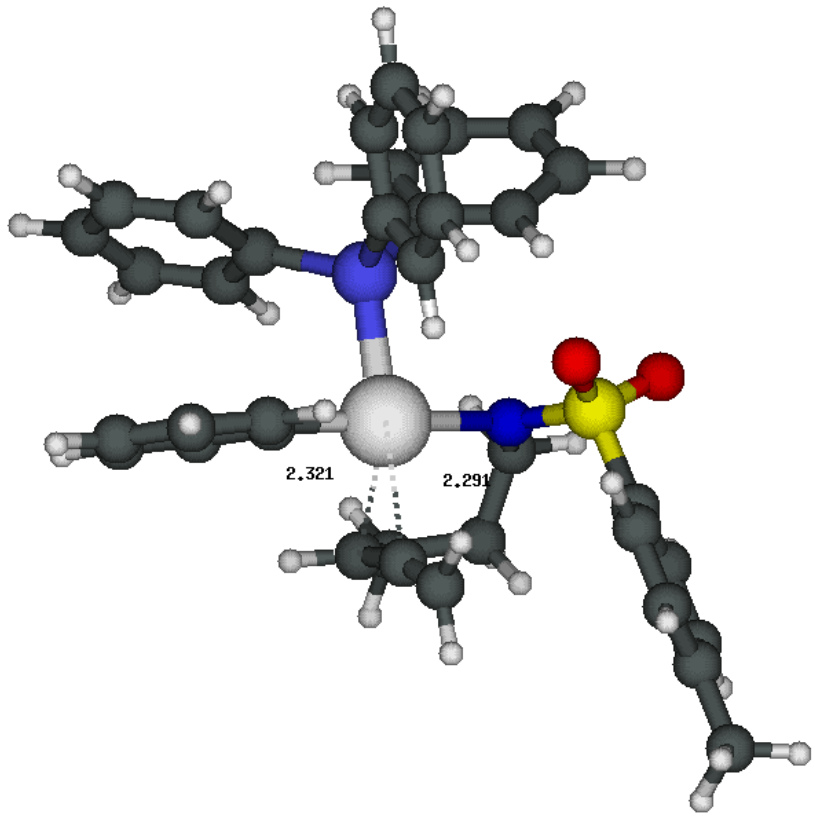
5	1	0	-0.501052	-0.757766	1.954607
6	1	0	1.078681	-0.003177	1.926917
7	6	0	-2.025399	1.454149	1.759612
8	1	0	-0.438226	1.370146	3.134806
9	1	0	-0.031529	2.239210	1.653297
10	6	0	-2.702269	2.380808	1.081799
11	1	0	-2.612457	0.648465	2.201957
12	6	0	-2.163657	3.556647	0.379249
13	1	0	-3.787801	2.292229	1.060153
14	6	0	-1.125508	3.458042	-0.455172
15	1	0	-0.707828	4.324809	-0.956950
16	1	0	-0.666155	2.496502	-0.661149
17	6	0	-2.849923	4.845139	0.621967
18	6	0	-2.898698	5.841914	-0.353495
19	6	0	-3.526994	7.048779	-0.107251
20	6	0	-4.128599	7.287168	1.119458
21	6	0	-4.098400	6.304380	2.094451
22	6	0	-3.470704	5.095365	1.845452
23	1	0	-2.454548	5.659234	-1.326128
24	1	0	-3.557670	7.805943	-0.883010
25	1	0	-4.624980	8.231922	1.310293
26	1	0	-4.566541	6.478268	3.057047
27	1	0	-3.446744	4.335820	2.620036
28	6	0	1.967416	1.595587	-0.892749
29	8	0	2.463501	-0.741869	0.045967

30	8	0	1.162657	-0.565177	-2.034652
31	6	0	1.756248	2.271663	-2.085478
32	6	0	2.131953	3.600424	-2.210261
33	6	0	2.713409	4.263201	-1.141400
34	6	0	2.928485	3.587790	0.051459
35	6	0	2.561806	2.258193	0.174842
36	1	0	1.296707	1.747059	-2.915329
37	1	0	1.968658	4.120480	-3.148072
38	1	0	3.006316	5.302586	-1.238522
39	1	0	3.392990	4.098250	0.888120
40	1	0	2.744382	1.727139	1.102936

Pictures and Cartesian coordinates of excited state optimized structures M06/def2-SVP.

35 Tosyl Int. E

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Excited State   1:      Singlet-?Sym    2.8730 eV  431.55 nm  f=0.0132
     163 -> 166       -0.02987
     165 -> 166        0.70572
Total Energy, E(TD-HF/TD-DFT) =  -2504.65745989
 Excited State   2:      Singlet-?Sym    3.3436 eV  370.81 nm  f=0.0003
 Excited State   3:      Singlet-?Sym    3.5150 eV  352.73 nm  f=0.0916
 Excited State   4:      Singlet-?Sym    3.5308 eV  351.15 nm  f=0.0152
 Excited State   5:      Singlet-?Sym    3.6428 eV  340.35 nm  f=0.0207
 Excited State   6:      Singlet-?Sym    3.7473 eV  330.86 nm  f=0.0014
 Excited State   7:      Singlet-?Sym    3.7903 eV  327.11 nm  f=0.0045
 Excited State   8:      Singlet-?Sym    3.7922 eV  326.95 nm  f=0.0031
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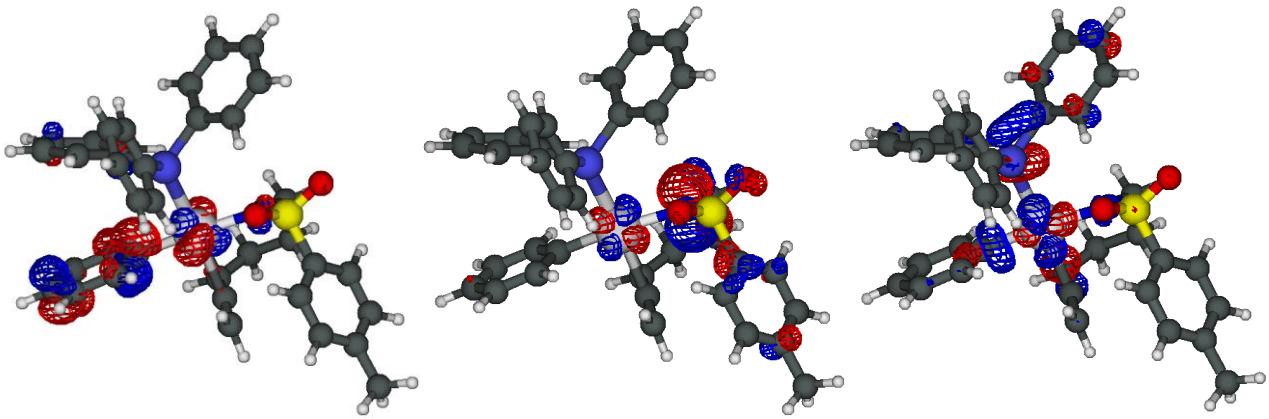
Molecular Orbitals involved in the first electronic transition:

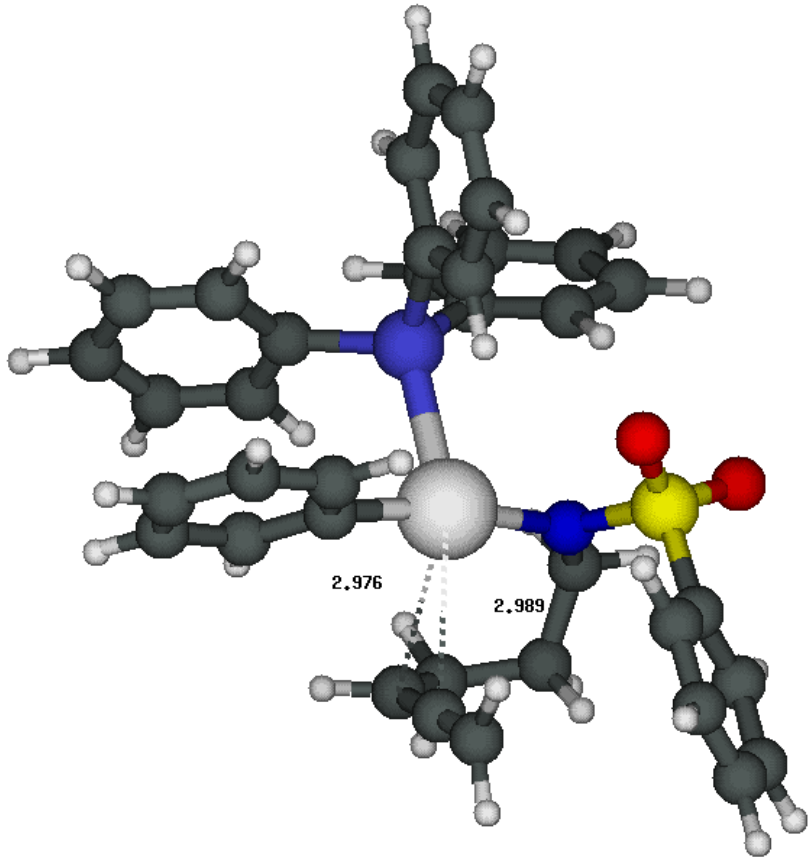


MO 163 **MO 165 (HOMO)** **MO 166 (LUMO)**

1	7	0	-0.007088	-0.003153	-0.004520
2	6	0	-0.000275	0.006427	1.447094
3	16	0	1.355344	-0.000361	-0.788544
4	6	0	-0.457960	1.320638	2.058914
5	1	0	-0.674571	-0.792743	1.797559
6	1	0	0.994670	-0.248940	1.828759
7	6	0	-1.922220	1.642024	1.844287
8	1	0	-0.283570	1.269095	3.138414
9	1	0	0.162649	2.140991	1.682062
10	6	0	-2.361238	2.068199	0.476125
11	1	0	-2.540078	0.785455	2.146153
12	1	0	-2.221586	2.459113	2.513374
13	46	0	-1.946400	0.268671	-0.930324
14	6	0	-1.638647	2.507665	-0.554914
15	6	0	2.030158	1.652189	-0.853145
16	8	0	2.374402	-0.762111	-0.096524
17	8	0	1.084774	-0.351053	-2.165603
18	1	0	-3.437794	2.206110	0.378577
19	6	0	-1.032246	3.178546	-1.489252
20	1	0	-0.842470	4.243286	-1.371074
21	1	0	-0.689212	2.714198	-2.408665
22	15	0	-2.309583	-1.979394	-1.490542
23	6	0	-4.047406	-2.423985	-1.199272
24	6	0	-1.931193	-2.398294	-3.215910
25	6	0	-1.338454	-3.228585	-0.572185
26	6	0	-3.733144	0.645035	-1.814192
27	6	0	-4.930605	0.658842	-1.104276
28	6	0	-6.129292	0.972414	-1.728515
29	6	0	-6.152696	1.283413	-3.079906
30	6	0	-4.965867	1.292346	-3.793535
31	6	0	-3.765766	0.979863	-3.164257
32	1	0	-4.941739	0.408988	-0.046698
33	1	0	-7.050046	0.970745	-1.153435
34	1	0	-7.089329	1.522738	-3.571163
35	1	0	-4.966958	1.543769	-4.849300
36	1	0	-2.850802	0.997964	-3.749200
37	6	0	-4.932543	-2.714534	-2.230068
38	6	0	-6.274847	-2.930511	-1.958048
39	6	0	-6.742876	-2.865061	-0.656995
40	6	0	-5.867572	-2.566006	0.376224
41	6	0	-4.532294	-2.332266	0.104729
42	1	0	-4.583982	-2.762022	-3.255719
43	1	0	-6.956330	-3.151642	-2.771649
44	1	0	-7.792102	-3.038846	-0.447017
45	1	0	-6.229159	-2.499255	1.395959
46	1	0	-3.861306	-2.053783	0.914153
47	6	0	-2.139647	-3.689922	-3.697336
48	6	0	-1.814806	-4.004682	-5.003365
49	6	0	-1.268324	-3.037274	-5.834949
50	6	0	-1.038831	-1.759223	-5.356245
51	6	0	-1.366690	-1.440353	-4.047711
52	1	0	-2.555908	-4.452824	-3.045865
53	1	0	-1.982906	-5.009484	-5.373691
54	1	0	-1.012112	-3.286878	-6.858447
55	1	0	-0.596410	-1.007449	-5.999742
56	1	0	-1.155225	-0.451470	-3.653732
57	6	0	-1.901176	-4.184779	0.266944
58	6	0	-1.096840	-5.112532	0.910479

59	6	0	0.273737	-5.098392	0.721324
60	6	0	0.840197	-4.156299	-0.123443
61	6	0	0.041885	-3.228226	-0.766487
62	1	0	-2.972423	-4.225779	0.418988
63	1	0	-1.550873	-5.852963	1.559337
64	1	0	0.900822	-5.824482	1.226265
65	1	0	1.912357	-4.141569	-0.283961
66	1	0	0.495514	-2.496428	-1.427125
67	6	0	2.068775	2.355102	-2.043892
68	6	0	2.574697	3.646254	-2.073073
69	6	0	3.046150	4.258373	-0.920075
70	6	0	3.011462	3.532416	0.270267
71	6	0	2.518873	2.243291	0.306699
72	1	0	1.700255	1.889522	-2.950195
73	1	0	2.602480	4.190064	-3.012469
74	6	0	3.598380	5.644811	-0.942448
75	1	0	3.388644	3.989972	1.180275
76	1	0	2.518856	1.691344	1.240623
77	1	0	3.456457	6.116859	-1.915736
78	1	0	3.122595	6.272572	-0.184722
79	1	0	4.670123	5.643492	-0.723573

36 Int. ^{1}E*



1	7	0	0.106899	0.011156	-0.135703
2	6	0	0.211149	-0.120661	1.307451
3	16	0	1.525375	0.146161	-0.991577
4	6	0	-0.250681	1.085395	2.124275
5	1	0	-0.407194	-0.993765	1.602915
6	1	0	1.250318	-0.371341	1.584374
7	6	0	-1.754116	1.300355	2.167433
8	1	0	0.101777	0.908608	3.154379
9	1	0	0.269576	1.997855	1.777959
10	6	0	-2.378623	2.070558	1.041289
11	1	0	-2.267964	0.324087	2.253662
12	1	0	-2.019574	1.834602	3.100142
13	46	0	-1.643622	0.234474	-1.182759
14	6	0	-1.790476	2.885453	0.191115
15	6	0	1.946796	1.877852	-0.992068
16	8	0	2.594959	-0.575275	-0.291863
17	8	0	1.223490	-0.229393	-2.376808
18	1	0	-3.476299	2.006728	0.973790
19	6	0	-1.265452	3.731015	-0.658310
20	1	0	-1.133059	4.792238	-0.405794
21	1	0	-0.945549	3.413774	-1.660711
22	15	0	-2.155394	-2.236656	-1.580460
23	6	0	-3.931770	-2.511643	-1.277206
24	6	0	-1.826492	-2.866913	-3.266236
25	6	0	-1.235443	-3.415959	-0.524299
26	6	0	-3.323039	0.836057	-2.236067
27	6	0	-4.590832	0.910439	-1.622978
28	6	0	-5.749128	1.168675	-2.356257
29	6	0	-5.671900	1.368967	-3.736094
30	6	0	-4.429464	1.319583	-4.369813

31	6	0	-3.275674	1.059843	-3.627698
32	1	0	-4.686131	0.744501	-0.540859
33	1	0	-6.720627	1.208306	-1.850714
34	1	0	-6.579039	1.566859	-4.316177
35	1	0	-4.360203	1.482353	-5.451003
36	1	0	-2.313678	1.022412	-4.156673
37	6	0	-4.840578	-2.720871	-2.321269
38	6	0	-6.211012	-2.751853	-2.062657
39	6	0	-6.686169	-2.579082	-0.764589
40	6	0	-5.786357	-2.357881	0.279369
41	6	0	-4.419502	-2.308620	0.023554
42	1	0	-4.483019	-2.850653	-3.348523
43	1	0	-6.912089	-2.914370	-2.886834
44	1	0	-7.761352	-2.608510	-0.564731
45	1	0	-6.153199	-2.210078	1.299425
46	1	0	-3.721753	-2.096003	0.843704
47	6	0	-2.065834	-4.208591	-3.596130
48	6	0	-1.788361	-4.671090	-4.878545
49	6	0	-1.263984	-3.801249	-5.837046
50	6	0	-1.013694	-2.470868	-5.511117
51	6	0	-1.292856	-2.002750	-4.226451
52	1	0	-2.474533	-4.893985	-2.844040
53	1	0	-1.978759	-5.717980	-5.133065
54	1	0	-1.044394	-4.168128	-6.844227
55	1	0	-0.593992	-1.791100	-6.258429
56	1	0	-1.079752	-0.962252	-3.956369
57	6	0	-1.827296	-4.374932	0.305398
58	6	0	-1.030548	-5.195893	1.103391
59	6	0	0.356913	-5.066632	1.082413
60	6	0	0.952786	-4.117368	0.251021
61	6	0	0.162928	-3.295669	-0.546909
62	1	0	-2.915687	-4.491774	0.329337
63	1	0	-1.502158	-5.945342	1.746253
64	1	0	0.977140	-5.708836	1.714779
65	1	0	2.041412	-4.008051	0.227661
66	1	0	0.636077	-2.547708	-1.193801
67	6	0	1.654238	2.654121	-2.111521
68	6	0	1.966951	4.012141	-2.091007
69	6	0	2.550535	4.577934	-0.959103
70	6	0	2.840642	3.788042	0.155021
71	6	0	2.548076	2.427898	0.142030
72	1	0	1.190141	2.194843	-2.989200
73	1	0	1.748477	4.631766	-2.965413
74	1	0	2.788864	5.645391	-0.945074
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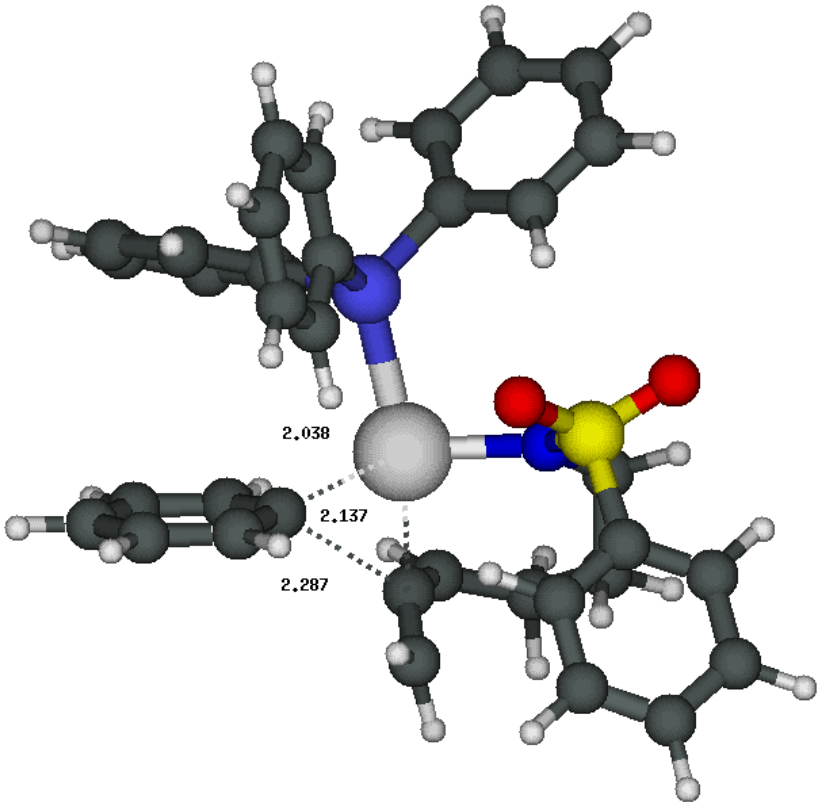
76	1	0	2.791398	1.796326	1.001899

37 **^{1}TS*$_G$**



1	7	0	0.016822	-0.004190	-0.053744
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3	16	0	1.498529	0.033368	-0.767183
4	6	0	-0.259579	1.251914	2.139242
5	1	0	-0.764595	-0.796985	1.701716
6	1	0	0.971297	-0.482843	1.748069
7	6	0	-1.740928	1.583568	2.278356
8	1	0	0.170001	1.171256	3.152563
9	1	0	0.283616	2.076223	1.641978
10	6	0	-2.492521	1.723668	0.996550
11	1	0	-2.226986	0.811747	2.901952
12	1	0	-1.832390	2.527993	2.859013
13	46	0	-1.693351	0.503599	-1.195531
14	6	0	-1.941741	2.337972	-0.127983
15	6	0	2.256027	1.596807	-0.358595
16	8	0	2.348890	-1.014743	-0.183297
17	8	0	1.281971	0.015292	-2.219098
18	1	0	-3.521897	1.347234	0.956516
19	6	0	-1.285609	3.480536	-0.379742
20	1	0	-0.772168	3.670633	-1.328373
21	1	0	-1.298553	4.299708	0.354130
22	15	0	-1.893041	-1.563819	-2.555350
23	6	0	-3.698149	-1.790111	-2.775176
24	6	0	-1.231804	-1.504869	-4.260248
25	6	0	-1.261936	-3.164607	-1.919811
26	6	0	-3.044670	1.768311	-2.048333
27	6	0	-2.704517	2.467888	-3.216640
28	6	0	-3.697233	2.835510	-4.121072
29	6	0	-5.040630	2.562922	-3.842711
30	6	0	-5.386061	1.923022	-2.653802
31	6	0	-4.394187	1.540933	-1.746363

32	1	0	-1.656264	2.711218	-3.430279
33	1	0	-3.423136	3.347566	-5.049279
34	1	0	-5.818934	2.866953	-4.549099
35	1	0	-6.437228	1.720662	-2.422124
36	1	0	-4.683076	1.033609	-0.817767
37	6	0	-4.334668	-1.625803	-4.010393
38	6	0	-5.726585	-1.684084	-4.096026
39	6	0	-6.492601	-1.912310	-2.955653
40	6	0	-5.865094	-2.066113	-1.718038
41	6	0	-4.478998	-1.990016	-1.625775
42	1	0	-3.747546	-1.447164	-4.917570
43	1	0	-6.213220	-1.552968	-5.067230
44	1	0	-7.583075	-1.963277	-3.027765
45	1	0	-6.461091	-2.236055	-0.816426
46	1	0	-3.993864	-2.081298	-0.645523
47	6	0	-1.240261	-2.641703	-5.079303
48	6	0	-0.771762	-2.563568	-6.387682
49	6	0	-0.291087	-1.351525	-6.886037
50	6	0	-0.274366	-0.219964	-6.073513
51	6	0	-0.739723	-0.296203	-4.760909
52	1	0	-1.624862	-3.593390	-4.693892
53	1	0	-0.781845	-3.453643	-7.023866
54	1	0	0.077362	-1.291875	-7.914619
55	1	0	0.110500	0.728348	-6.460146
56	1	0	-0.706159	0.582661	-4.108430
57	6	0	-2.063492	-4.284435	-1.672646
58	6	0	-1.496955	-5.451634	-1.160329
59	6	0	-0.131314	-5.511297	-0.890622
60	6	0	0.673645	-4.400116	-1.142890
61	6	0	0.114012	-3.233048	-1.654171
62	1	0	-3.137339	-4.256069	-1.883913
63	1	0	-2.132149	-6.322782	-0.973287
64	1	0	0.308245	-6.427340	-0.484769
65	1	0	1.747707	-4.437468	-0.935967
66	1	0	0.755021	-2.368128	-1.856937
67	6	0	1.940933	2.720533	-1.121462
68	6	0	2.455566	3.958405	-0.745590
69	6	0	3.277325	4.062243	0.376982
70	6	0	3.601303	2.927476	1.120579
71	6	0	3.092182	1.683824	0.754390
72	1	0	1.298552	2.621702	-2.002148
73	1	0	2.214715	4.848324	-1.334527
74	1	0	3.676571	5.037458	0.670568
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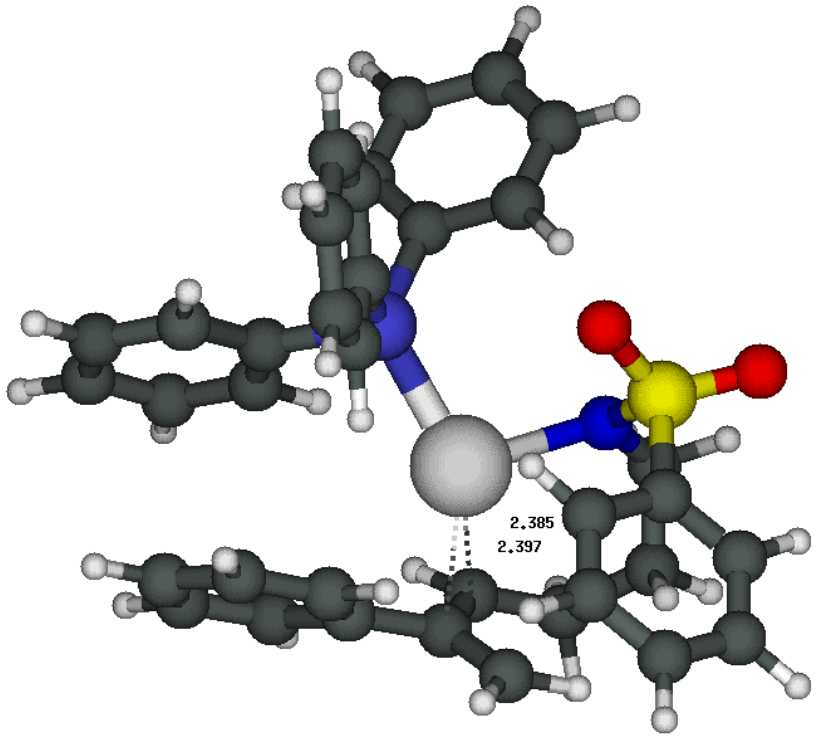
76	1	0	3.340417	0.783556	1.323607

38 Int. ^{1}G*



1	7	0	0.075343	-0.020852	-0.021577
2	6	0	0.041696	-0.033291	1.435041
3	16	0	1.476645	-0.007862	-0.791260
4	6	0	-0.150786	1.322972	2.110340
5	1	0	-0.793136	-0.696740	1.747052
6	1	0	0.963204	-0.513920	1.816278
7	6	0	-1.593349	1.860862	2.178423
8	1	0	0.206203	1.245927	3.153917
9	1	0	0.519334	2.050266	1.618212
10	6	0	-2.372541	2.103808	0.913586
11	1	0	-2.185108	1.173439	2.808952
12	1	0	-1.543948	2.817717	2.741850
13	46	0	-1.589920	0.989222	-1.044367
14	6	0	-2.053838	3.115271	-0.038804
15	6	0	1.959552	1.714582	-0.991017
16	8	0	2.570228	-0.645817	-0.030773
17	8	0	1.227635	-0.491469	-2.165233
18	1	0	-3.370339	1.659100	0.853644
19	6	0	-0.898350	3.888668	0.001827
20	1	0	-0.710207	4.665527	-0.745655
21	1	0	-0.171824	3.786967	0.811962
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23	6	0	-4.236309	-0.391590	-2.692250
24	6	0	-1.735534	-0.581599	-4.130831
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26	6	0	-2.999806	3.293497	-1.186759
27	6	0	-2.508602	3.590276	-2.471430
28	6	0	-3.375402	3.730317	-3.554788
29	6	0	-4.750098	3.599834	-3.374874
30	6	0	-5.252950	3.334630	-2.099939
31	6	0	-4.390124	3.180883	-1.019667
32	1	0	-1.428235	3.697631	-2.624100
33	1	0	-2.968792	3.943210	-4.548429
34	1	0	-5.431560	3.711977	-4.223730

35	1	0	-6.333070	3.246675	-1.945389
36	1	0	-4.799792	2.977926	-0.025018
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39	6	0	-6.992828	0.031240	-2.909421
40	6	0	-6.409992	-0.140718	-1.651917
41	6	0	-5.037915	-0.337464	-1.543047
42	1	0	-4.212970	-0.253503	-4.857030
43	1	0	-6.650520	0.135326	-5.039420
44	1	0	-8.071136	0.194070	-2.995849
45	1	0	-7.028531	-0.112873	-0.750026
46	1	0	-4.580011	-0.462450	-0.553900
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51	6	0	-1.362542	0.677788	-4.617273
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53	1	0	-1.041055	-2.459175	-6.880415
54	1	0	-0.389189	-0.220346	-7.751419
55	1	0	-0.598899	1.792603	-6.297633
56	1	0	-1.453179	1.562149	-3.972748
57	6	0	-3.424610	-3.292085	-1.966196
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59	6	0	-2.004508	-5.096250	-1.210128
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61	6	0	-1.065441	-2.899282	-1.566311
62	1	0	-4.413326	-2.938948	-2.275606
63	1	0	-4.119267	-5.300801	-1.610236
64	1	0	-1.879108	-6.142937	-0.917739
65	1	0	0.078046	-4.599908	-0.904022
66	1	0	-0.204384	-2.215586	-1.570135
67	6	0	1.462982	2.452123	-2.067488
68	6	0	1.792558	3.802002	-2.182233
69	6	0	2.611243	4.407288	-1.228307
70	6	0	3.107545	3.661250	-0.158964
71	6	0	2.784009	2.310913	-0.037197
72	1	0	0.833883	1.962855	-2.820054
73	1	0	1.412827	4.383797	-3.027966
74	1	0	2.869997	5.466106	-1.322755
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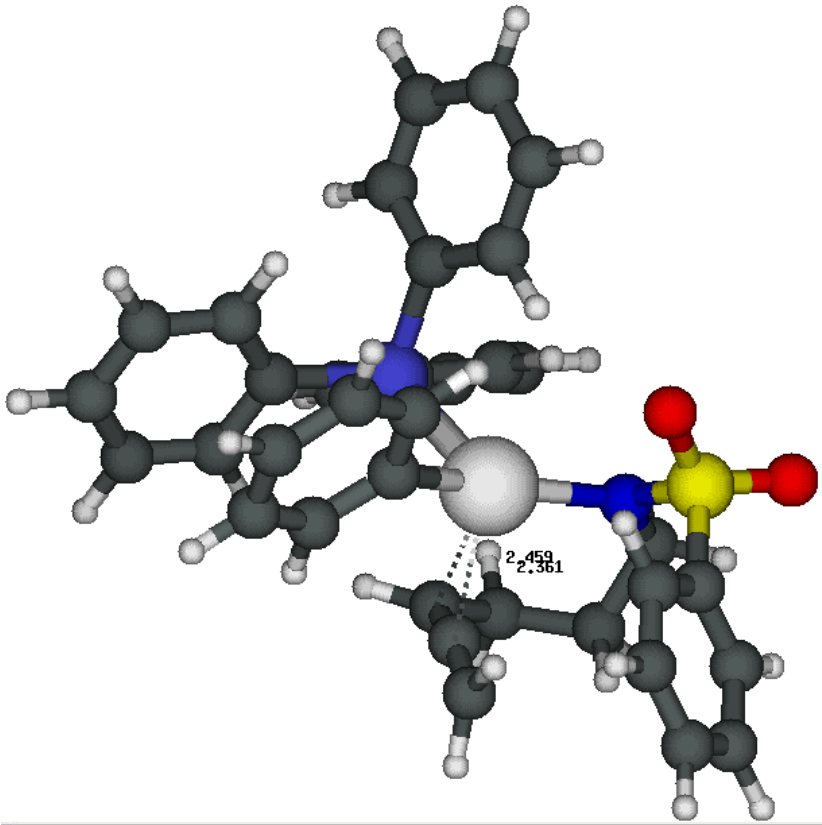
76	1	0	3.177904	1.710949	0.788850

39 Int. ^{3}E*



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9	1	0	-0.076025	1.609828	1.781336
10	6	0	-2.486370	0.776328	0.758444
11	1	0	-1.866197	-0.896594	1.936624
12	1	0	-2.233795	0.572805	2.819796
13	46	0	-1.466040	0.130255	-1.348183
14	6	0	-2.103861	1.855962	0.046122
15	6	0	1.690371	2.032231	-1.343799
16	8	0	2.930566	-0.196225	-0.734559
17	8	0	1.292999	-0.189285	-2.655125
18	1	0	-3.522296	0.425428	0.635759
19	6	0	-1.833076	3.088917	-0.308151
20	1	0	-2.116730	3.916730	0.357612
21	1	0	-1.344259	3.348576	-1.254919
22	15	0	-3.073027	-1.680566	-1.657386
23	6	0	-4.756299	-1.247052	-2.193986
24	6	0	-2.401084	-2.834445	-2.913123
25	6	0	-3.220787	-2.777891	-0.197050
26	6	0	-2.453221	1.020279	-3.023659
27	6	0	-3.629266	1.776089	-2.947637
28	6	0	-4.208286	2.325500	-4.094505
29	6	0	-3.623270	2.118943	-5.344724
30	6	0	-2.452190	1.368044	-5.436099
31	6	0	-1.873337	0.822323	-4.284418

32	1	0	-4.119652	1.944305	-1.979383
33	1	0	-5.129378	2.913815	-4.010750
34	1	0	-4.078913	2.543699	-6.245005
35	1	0	-1.980728	1.202754	-6.411406
36	1	0	-0.950111	0.235302	-4.383426
37	6	0	-5.129554	-1.319062	-3.542459
38	6	0	-6.369671	-0.835234	-3.954185
39	6	0	-7.245955	-0.270154	-3.029533
40	6	0	-6.877275	-0.185781	-1.687070
41	6	0	-5.637705	-0.663929	-1.271015
42	1	0	-4.445710	-1.745171	-4.284122
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44	1	0	-8.218847	0.108997	-3.355868
45	1	0	-7.558361	0.260242	-0.956445
46	1	0	-5.355143	-0.576401	-0.215915
47	6	0	-3.136554	-3.965127	-3.296897
48	6	0	-2.597090	-4.875249	-4.200024
49	6	0	-1.316607	-4.670783	-4.717300
50	6	0	-0.575898	-3.558981	-4.325333
51	6	0	-1.113243	-2.639084	-3.423115
52	1	0	-4.137577	-4.136659	-2.883950
53	1	0	-3.176879	-5.753696	-4.498463
54	1	0	-0.893077	-5.388835	-5.425905
55	1	0	0.432398	-3.402659	-4.720019
56	1	0	-0.511667	-1.775098	-3.108394
57	6	0	-4.422265	-3.298887	0.295113
58	6	0	-4.411867	-4.145129	1.403814
59	6	0	-3.209586	-4.480899	2.023092
60	6	0	-2.007395	-3.972812	1.529316
61	6	0	-2.012965	-3.122400	0.428028
62	1	0	-5.373386	-3.057674	-0.190037
63	1	0	-5.355463	-4.549437	1.782208
64	1	0	-3.208169	-5.144166	2.893103
65	1	0	-1.059093	-4.235844	2.007796
66	1	0	-1.067405	-2.717073	0.043788
67	6	0	1.105294	2.709541	-2.412903
68	6	0	1.090329	4.103820	-2.411257
69	6	0	1.645801	4.809485	-1.344941
70	6	0	2.232752	4.122384	-0.281491
71	6	0	2.264625	2.729871	-0.279874
72	1	0	0.666403	2.143928	-3.240582
73	1	0	0.638157	4.641299	-3.250204
74	1	0	1.628681	5.903366	-1.344784
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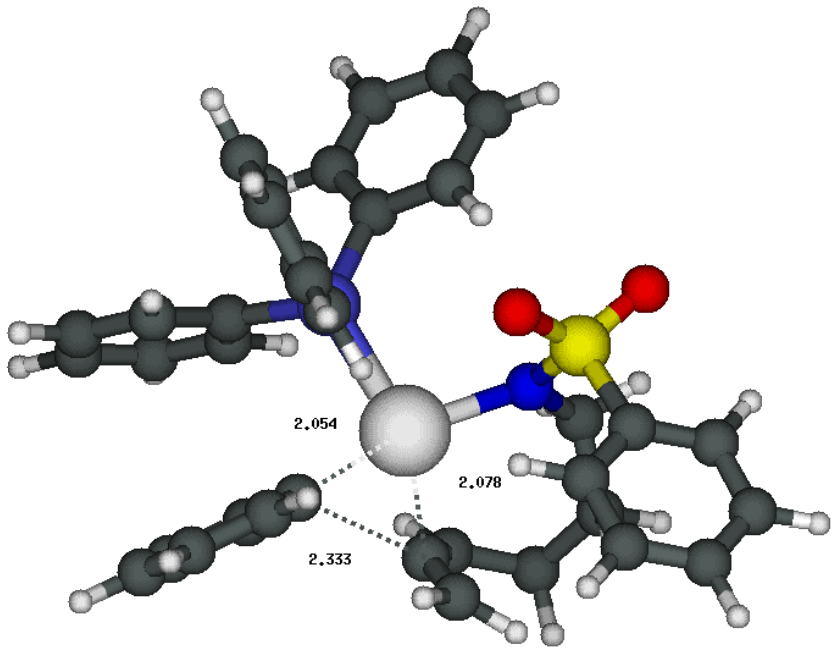
40 **$^{3}TS^{*}_{G}$**



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4	6	0	-0.120133	1.492943	2.103817
5	1	0	-0.801668	-0.552023	1.901457
6	1	0	0.946710	-0.378865	1.904791
7	6	0	-1.561142	1.979602	2.322584
8	1	0	0.389983	1.523386	3.082869
9	1	0	0.423176	2.210737	1.462672
10	6	0	-2.430148	1.790512	1.118689
11	1	0	-2.010774	1.433670	3.168950
12	1	0	-1.536067	3.047913	2.611422
13	46	0	-1.730839	0.588651	-1.070238
14	6	0	-2.135545	2.382045	-0.101587
15	6	0	2.174654	1.596143	-0.510316
16	8	0	2.391833	-0.957865	-0.014623
17	8	0	1.218715	-0.227416	-2.117604
18	1	0	-3.231703	1.040111	1.165425
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21	1	0	-0.782914	4.026350	0.205558
22	15	0	-2.177906	-1.391737	-2.330056
23	6	0	-3.983503	-1.644984	-2.493796
24	6	0	-1.537504	-1.321187	-4.042646
25	6	0	-1.536794	-3.008204	-1.722867
26	6	0	-3.377486	1.515085	-1.876248
27	6	0	-3.229318	2.243664	-3.068089
28	6	0	-4.342034	2.754931	-3.737179
29	6	0	-5.623268	2.568871	-3.216665
30	6	0	-5.781934	1.872893	-2.017370
31	6	0	-4.670381	1.351832	-1.355609
32	1	0	-2.230505	2.412136	-3.489664
33	1	0	-4.204724	3.305825	-4.673592
34	1	0	-6.495412	2.972387	-3.740287
35	1	0	-6.781590	1.729697	-1.592812
36	1	0	-4.819266	0.804595	-0.416865

37	6	0	-4.658848	-1.498869	-3.709236
38	6	0	-6.048917	-1.612591	-3.757294
39	6	0	-6.772605	-1.881661	-2.598256
40	6	0	-6.105738	-2.018602	-1.380121
41	6	0	-4.721974	-1.884316	-1.325563
42	1	0	-4.104971	-1.287111	-4.629760
43	1	0	-6.567109	-1.493237	-4.713489
44	1	0	-7.861514	-1.978655	-2.641197
45	1	0	-6.668771	-2.218741	-0.463679
46	1	0	-4.207127	-1.958360	-0.359221
47	6	0	-1.655680	-2.425574	-4.897536
48	6	0	-1.171797	-2.354207	-6.200480
49	6	0	-0.562120	-1.183954	-6.655779
50	6	0	-0.430562	-0.088486	-5.805519
51	6	0	-0.913377	-0.157375	-4.499107
52	1	0	-2.134301	-3.346364	-4.543830
53	1	0	-1.268751	-3.217715	-6.865148
54	1	0	-0.180809	-1.130239	-7.679961
55	1	0	0.058679	0.824554	-6.157287
56	1	0	-0.786233	0.687418	-3.813372
57	6	0	-2.353608	-4.110436	-1.444306
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60	6	0	0.405106	-4.319841	-1.102882
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62	1	0	-3.436784	-4.053323	-1.585459
63	1	0	-2.441329	-6.159095	-0.781006
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65	1	0	1.489244	-4.392820	-0.971345
66	1	0	0.501372	-2.278922	-1.795673
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68	6	0	2.203386	3.918021	-1.142926
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70	6	0	3.590124	3.137312	0.677892
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73	1	0	1.852069	4.731178	-1.785699
74	1	0	3.505989	5.192265	0.017685
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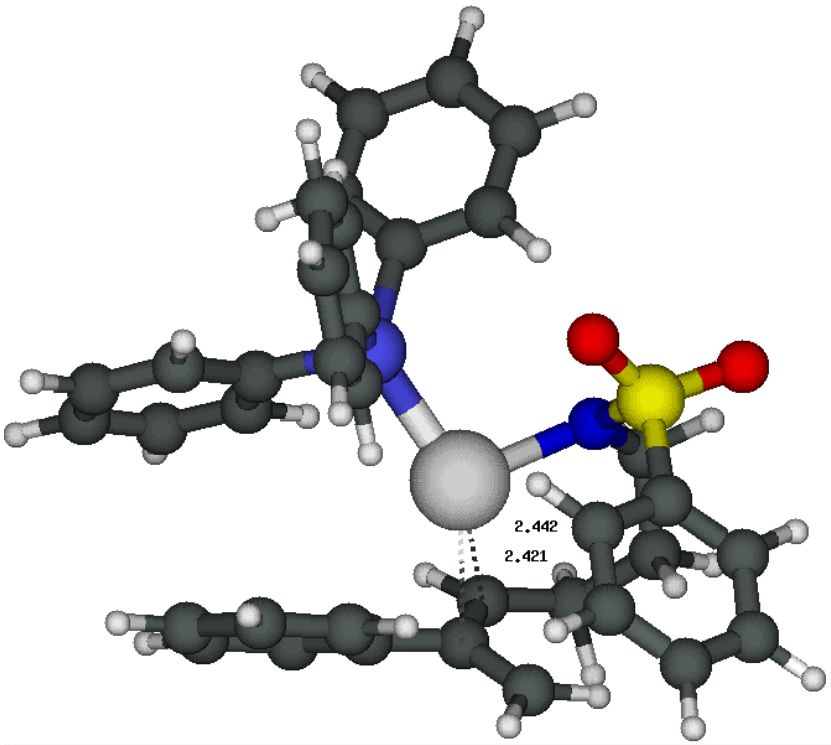
41 Int. ^{3}G*



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5	1	0	0.953448	-1.000574	3.591223
6	1	0	2.665052	-0.573083	3.598338
7	6	0	-0.151296	1.433616	3.984165
8	1	0	1.744164	1.106292	4.896563
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13	46	0	-0.083837	0.417357	0.744477
14	6	0	-0.864027	2.484438	1.734546
15	6	0	3.301601	1.672934	0.689120
16	8	0	4.215559	-0.505434	1.816182
17	8	0	2.937970	-0.686117	-0.345702
18	1	0	-1.873545	0.859606	2.710829
19	6	0	0.124001	3.477203	1.762104
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23	6	0	-2.407919	-1.412198	-0.924387
24	6	0	0.095518	-1.296154	-2.358454
25	6	0	-0.208932	-3.104415	-0.121827
26	6	0	-1.839117	2.467759	0.599432
27	6	0	-1.419702	2.794978	-0.704385
28	6	0	-2.309847	2.745330	-1.775056
29	6	0	-3.640520	2.387980	-1.565054
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31	6	0	-3.186908	2.122899	0.795489
32	1	0	-0.375735	3.077278	-0.880856
33	1	0	-1.956930	2.987251	-2.782417

34	1	0	-4.341231	2.351665	-2.404826
35	1	0	-5.124326	1.826528	-0.096469
36	1	0	-3.546426	1.892806	1.803664
37	6	0	-3.006092	-1.371093	-2.188586
38	6	0	-4.397078	-1.378730	-2.304948
39	6	0	-5.197606	-1.437079	-1.166806
40	6	0	-4.606518	-1.475140	0.097680
41	6	0	-3.221134	-1.449913	0.218712
42	1	0	-2.389215	-1.338308	-3.093055
43	1	0	-4.855796	-1.345944	-3.297801
44	1	0	-6.287380	-1.449718	-1.263037
45	1	0	-5.230623	-1.516965	0.995417
46	1	0	-2.758848	-1.471988	1.214208
47	6	0	0.375545	-2.431452	-3.125916
48	6	0	0.848408	-2.291891	-4.430268
49	6	0	1.039150	-1.023404	-4.975760
50	6	0	0.760698	0.111633	-4.214164
51	6	0	0.296749	-0.024550	-2.908403
52	1	0	0.221003	-3.433044	-2.709464
53	1	0	1.067961	-3.183523	-5.025156
54	1	0	1.410783	-0.918304	-5.999421
55	1	0	0.912832	1.109120	-4.637109
56	1	0	0.087532	0.865203	-2.301470
57	6	0	-1.155654	-4.135706	-0.148253
58	6	0	-0.800170	-5.422445	0.254439
59	6	0	0.499072	-5.690042	0.680951
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64	1	0	0.774856	-6.700736	0.996699
65	1	0	2.469671	-4.873772	1.031303
66	1	0	1.842808	-2.573725	0.311914
67	6	0	2.746835	2.258700	-0.449222
68	6	0	2.875716	3.632958	-0.643501
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71	6	0	3.987382	2.444379	1.626890
72	1	0	2.227835	1.634955	-1.184689
73	1	0	2.449231	4.097227	-1.538262
74	1	0	3.651001	5.491916	0.139261
75	1	0	4.647014	4.428341	2.158656
76	1	0	4.431475	1.962959	2.503701