Supporting Information

Does the Multiply Bound Oxo Ligand Directly Participate in the B–H bond Activation by the High-Valent Di-Oxo-Molybdenum(VI) Complex? A Density Functional Theory Study

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1. Complete refrence of 28
2. **Table S1** The calculated free energies of key intermediates and transition states at M06(BS1) and M06(BS2) are listed for MoO_2Cl_2 catalyzing the reduction of benzamide, N-(diphenylmethylene)benzenamine, and benzonitrile and sulfoxides with boranes.
3. **Figure 1a**. Calculated geometric structures along ionic outer-sphere pathway: **TS4→4→TS5→5→TS6** for MoO_2Cl_2-catalyzed hydroboration of (diphenylmethylene)benzenamine (PhCPh=NPh). **Figure 1b.** Calculated geometric structures along ionic outer-sphere pathway: **TS4→4→TS5→5→TS6** for MoO_2Cl_2-catalyzed hydroboration of benzonitrile (PhC≡N). **Figure 1c.** Calculated geometric structures along ionic outer-sphere pathway: **TS4→4→TS5→5→TS6** for MoO_2Cl_2-catalyzed hydroboration of sulfoxides (Ph_2S=O).
4. **Table S2**. The NBO charge along the ionic outer-sphere mechanistic pathway calculated for catalytic reduction of benzamide, N-(diphenylmethylene)benzenamine, and benzonitrile and sulfoxides with boranes by the high-valent di-oxo-molybdenum(VI) complex MoO_2Cl_2.
5. **Figure 2** Selected molecular orbitals (HOMO and LUMO) along the ionic outer-sphere mechanistic pathway **(TS4→ 4→ TS5→ 5)**.
6. **Figure 3a.** Calculated geometric structures along the [2+2] addition pathway: **8→TS9→9→TS10** for MoO_2Cl_2-catalyzed hydroboration of (diphenylmethylene)benzenamine (PhCPh=NPh). **Figure 3b.** Calculated geometric structures along the [2+2] addition pathway: **8→TS9→9→TS10** or MoO_2Cl_2-catalyzed hydroboration of benzonitrile (PhC≡N).
7. **Figure 4.** Calculated geometric structures with the [2+2] addition transition state (**TS11)** and the [2+2] intermediate (**11**) start with sulfoxide complex, $MoO_2Cl_2(Ph_2SO)$.

Table S3 Cartesian coordinates for all optimized structures in XYZ format.

Complete refrence of 28

Frisch, M. J. et al. *Gaussian 09*; Gaussian, Inc. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Pittsburgh PA,, 2009.

Table S1 The calculated free energies of key intermediates and transition states at M06(BS1) and M06(BS2) are listed for MoO_2Cl_2 catalyzing the reduction of benzamide, N-(diphenylmethylene)benzenamine, and benzonitrile and sulfoxides with boranes.

	PhCPh=NPh		PhC≡N	
	M06 *{6-311G(d,p) +Lan2LDZ}*	M06 *{6-311++G(2d,p) +QVZP}*	M06 *{6-311G(d,p) +Lan2LDZ}*	M06 *{6-311++G(2d,p) +QVZP}*
1	0.0	0.0	0.0	0.0
2	9.3	10.6	9.3	10.6
TS4	15.1	19.3	20.8	23.4
4	7.7	15.3	18.1	23.9
TS5	9.4	19.7	21.0	29.9
5	-0.6	11.7	4.7	28.5
TS6	6.5	17.3	21.9	30.6
6	-17.0	-12.4	-4.9	-2.9

	$PhC=ONH_2$		$PhC=ONH_2$
	M06 *{6-311G(d,p) +Lan2LDZ}*	M06 *{6-311++G(2d,p) +QVZP}*	M06 *{6-311G(d,p) +SDD}*
1	0.0	0.0	
2	8.8	10.6	
3	15.9	19.0	
TS4	17.1	17.2	
4	9.8	13.3	
TS5	11.0	15.9	
5	9.3	14.2	
TS6	18.7	22.7	
6	1.0	2.7	
TS7	27.5	27.6	26.6
7	-1.1	3.6	-1.0

	$Ph_2S=O$	
	M06 *{6-311G(d,p) +Lan2LDZ}*	M06 *{6-311++G(2d,p) +QVZP}*
1	0.0	0.0
2	9.3	10.6
TS4	15.1	21.3
4	9.6	17.0
TS5	9.1	18.3
5	0.6	11.1
TS6	23.7	38.8
6	-60.2	-50.4
TS1	17.3	24.0
1	-9.7	-0.3
11		

Figure 1a. Calculated geometric structures along ionic outer-sphere pathway: **TS4→4→TS5→5→TS6** for MoO_2Cl_2-catalyzed hydroboration of (diphenylmethylene)benzenamine (PhCPh=NPh).

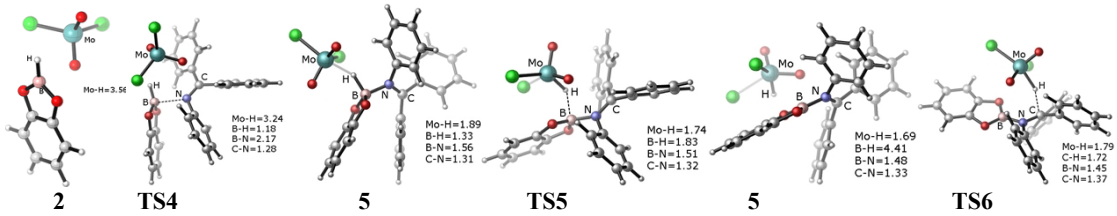


Figure 1b. Calculated geometric structures along ionic outer-sphere pathway: **TS4→4→TS5→5→TS6** for MoO_2Cl_2-catalyzed hydroboration of benzonitrile (PhC≡N)

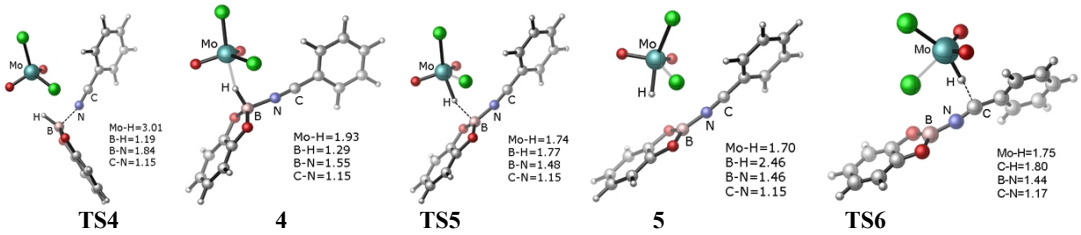


Figure 1c. Calculated geometric structures along ionic outer-sphere pathway: **TS4→4→TS5→5** for MoO_2Cl_2-catalyzed hydroboration of sulfoxides (Ph_2S=O).

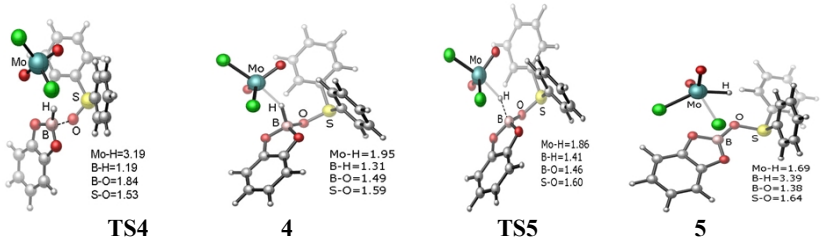


Table S2. The NBO charge along the ionic outer-sphere mechanistic pathway calculated for catalytic reduction of benzamide, N-(diphenylmethylene)benzenamine, and benzonitrile and sulfoxides with boranes by the high-valent di-oxo-molybdenum(VI) complex MoO_2Cl_2.

		3	**TS4**	**4**	**TS5**	**5**
$Ph_2S=O$	Mo	0.98	0.98	0.85	0.84	0.73
	H	-0.12	-0.15	-0.15	-0.14	-0.00
	B	0.97	0.96	1.08	1.14	1.28
	O(S=O)	-0.97	-0.92	-0.86	-0.86	-0.84
PhC≡N	Mo	0.97	0.96	0.85	0.77	0.72
	H	-0.12	-0.13	-0.13	-0.08	-0.02
	B	0.95	0.90	0.97	1.14	1.17
	N(C≡N)	-0.40	-0.40	-0.41	-0.47	-0.49
PhCPh=NPh	Mo	0.98	0.98	0.86	0.70	0.71
	H	-0.11	-0.13	-0.12	-0.02	0.03
	B	0.95	0.96	1.08	1.29	1.30
	N(C=N)	-0.51	-0.51	-0.59	-0.64	-0.65
$PhC=ONH_2$	Mo	1.03	1.03	0.91	0.83	0.80
	H	-0.12	-0.13	-0.14	-0.10	-0.02
	B	0.98	0.97	1.07	1.25	1.29
	O(C=O)	-0.67	-0.67	-0.65	-0.67	-0.67

Conclusion: our conclusion for NBO electronic charges change along the ionic outer-sphere mechanistic pathway is similar with four substrates of benzamide ($PhC=ONH_2$), N-(diphenylmethylene)benzenamine (PhCPh=NPh), benzonitrile (PhC≡N), and diphenyl sulfoxide ($Ph_2S=O$). For example, along the ionic outer-sphere mechanistic pathway, with substrate of *N-(diphenylmethylene)benzenamine*, as a consequence of the transformation from van der Waals species **3** into the ion pair **5**, natural bond order (NBO) charge analysis reveals that the migrating H atom of borane in **3** has a negative charge (-0.11 *e*). Accompanied by the B–H bond cleavage, the calculated NBO negative charge on the borane hydrogen decreases to -0.02 *e* in **TS5**, and to almost neutral in intermediate **5** (0.03 *e*). Accordingly, the NBO charge trend on the borane center is reversed and becomes positively charged, i.e., 0.96 *e*, 1.08 *e* (**TS4**, **4**) →1.29 *e*, 1.30 *e* (**TS5**, **5**) during this step. When the electron density from borane effectively drains to the molybdenum metal center, the NBO charge on the molybdenum center becomes less positively charged, going from 0.98 *e* → 0.86 *e* → 0.70 *e*→ 0.71 *e*. This trend is similar to the substrate of benzamide ($PhC=ONH_2$), as discussed in the manuscript, Page 4, paragraph 3. Also, along the ionic outer-sphere mechanistic pathway, with substrate of *benzonitrile (PhC≡N),* as a consequence of the transformation from van der Waals species **3** into the ion pair **5**, natural bond order (NBO) charge analysis reveals that the migrating H atom of borane in **3** has a negative charge (-0.12 *e*). Accompanied by the B–H bond cleavage, the calculated NBO negative charge on the borane hydrogen decreases to -0.08 *e* in **TS5**, and to almost neutral in intermediate **5** (-0.02 *e*). Accordingly, the NBO charge trend on the borane center is reversed and becomes positively charged, i.e., 0.90 *e*, 0.97 *e* (**TS4**, **4**) →1.14 *e*, 1.17 *e* (**TS5**, **5**) during this step. When the electron density from borane effectively drains to the molybdenum metal center, the NBO charge on the molybdenum center becomes less positively charged, going from 0.96 *e* → 0.85 *e* → 0.77 *e*→ 0.72 *e*.

Figure 2 Selected molecular orbitals (HOMO and LUMO) along the ionic outer-sphere mechanistic pathway **(TS4→ 4→ TS5→ 5)**.

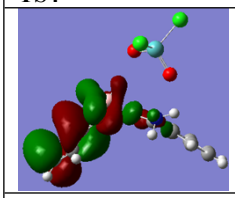
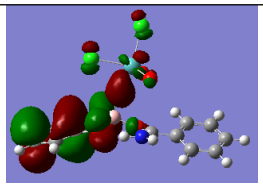
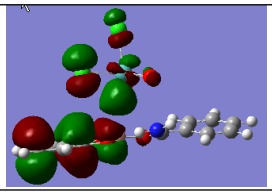
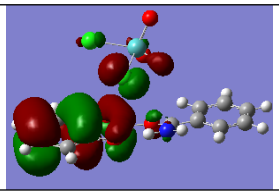
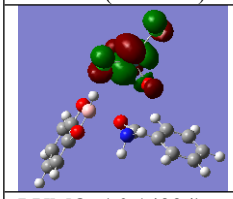
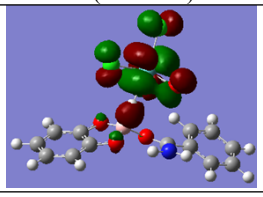
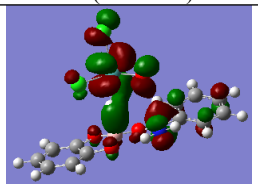
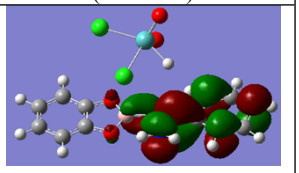
TS4	**4**	**TS5**	**5**
			
HOMO: (-0.23038)	HOMO: (-0.23089)	HOMO: (-0.25028)	HOMO: (-0.26054)
			
LUMO: (-0.14234)	LUMO: (-0.13135)	LUMO: (-0.10591)	LUMO: (-0.10011)

Figure 3a. Calculated geometric structures along the [2+2] addition pathway: **8→TS9→9→TS10** for MoO_2Cl_2-catalyzed hydroboration of (diphenylmethylene)benzenamine (PhCPh=NPh).

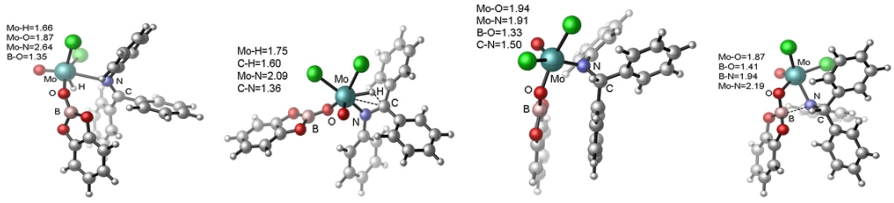


Figure 3b Calculated geometric structures along the [2+2] addition pathway: **8→TS9→9→TS10** for MoO_2Cl_2-catalyzed hydroboration of benzonitrile (PhC≡N)

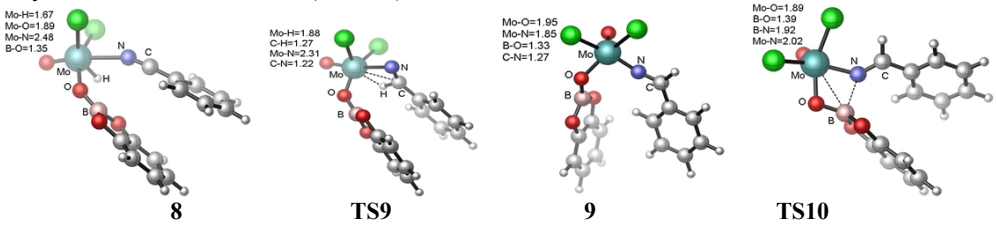


Figure 4 Calculated geometric structures with the [2+2] addition transition state (**TS11)** and the [2+2] intermediate (**INT11**) start with sulfoxide complex, $MoO_2Cl_2(Ph_2SO)$.

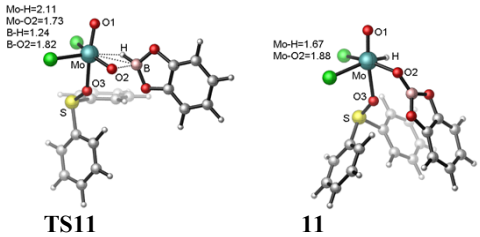


Table S3 Cartesian coordinates for all optimized structures in XYZ format.

1 (MoO_2Cl_2)

Mo	0.096913	-0.396874	0.240281
O	-0.067752	0.711872	1.469659
O	1.652949	-0.225419	-0.322890
Cl	-1.358231	0.106173	-1.419921
Cl	-0.169882	-2.484229	1.076028

2

Cl	-3.801342	0.178321	-0.646172
Mo	-1.760454	0.950074	-0.037721
H	1.540327	2.085669	0.236600
B	1.948821	0.998352	0.049148
O	2.556396	0.591698	-1.116638
C	2.845986	-0.732790	-0.922271
C	2.430197	-1.105235	0.348589
C	2.598615	-2.384124	0.828338
C	3.209311	-3.293542	-0.033498
C	3.625259	-2.921210	-1.308996
C	3.450480	-1.621382	-1.782263
O	1.872959	-0.020496	0.973122
O	-0.581316	0.081652	-0.832533
O	-1.582349	2.527607	-0.536357
Cl	-1.374888	0.814094	2.184003
H	2.273201	-2.662916	1.824527
H	3.364380	-4.314830	0.299529
H	4.097250	-3.657949	-1.951139
H	3.772165	-1.319484	-2.772924

3 (PhCPh=NPh)

Mo	2.664906	-1.272534	-0.649756
Cl	4.781247	-1.709886	-1.331108
O	2.645208	-1.121471	1.004110
O	2.177943	0.197288	-1.264945
Cl	1.266172	-2.928992	-1.309963
H	0.107495	-2.303627	1.544143
B	-1.043395	-2.117228	1.393940
O	-1.760169	-2.548858	0.297252
O	-1.869833	-1.559979	2.353383
C	-3.050796	-2.165664	0.541688
C	-3.118144	-1.563013	1.791257
C	-4.296920	-1.066874	2.299484
H	-4.339076	-0.597884	3.276722
C	-4.157023	-2.298160	-0.264778
C	-5.357095	-1.794666	0.236310
C	-5.425890	-1.192307	1.488990
N	-0.652113	0.434335	0.207139
C	0.013169	1.489293	0.499601
C	0.973303	1.439509	1.625146
C	-1.655274	0.463476	-0.780748
C	-1.491559	-0.280101	-1.947559
C	-0.100641	2.782983	-0.230874
C	0.096396	2.846220	-1.609325
C	-0.411561	3.948222	0.468925
C	-0.552168	5.152953	-0.204222
C	-0.353555	5.209313	-1.577213
C	-0.021012	4.056342	-2.276324
C	-2.847261	1.157097	-0.573495
C	-3.846182	1.124505	-1.534959
C	-3.668302	0.409073	-2.712272
C	-2.485460	-0.293374	-2.912643
C	2.168486	2.158452	1.560852
C	3.088992	2.079950	2.594569
C	2.811223	1.308252	3.715541
C	1.615595	0.605711	3.794787
C	0.704770	0.662387	2.752160
H	0.145443	4.098237	-3.348449
H	0.353017	1.945581	-2.158688
H	-0.555456	3.906391	1.545829
H	-0.810862	6.051958	0.347128
H	-0.454349	6.154288	-2.102735
H	-4.089436	-2.761460	-1.243429
H	-6.255817	-1.872039	-0.367695
H	-6.377831	-0.812043	1.846139
H	-2.984279	1.716395	0.349077
H	-4.771581	1.666932	-1.361922
H	-4.449351	0.392173	-3.466337
H	-2.336456	-0.860993	-3.826887
H	-0.567148	-0.833012	-2.087368
H	-0.233441	0.118844	2.810003
H	1.391188	0.011398	4.675516
H	3.526584	1.258862	4.531328
H	4.022831	2.630314	2.529571
H	2.384363	2.769519	0.688548

TS4 (PhCPh=NPh)

Mo	2.684359	-1.412396	-0.559405
Cl	4.717128	-1.692968	-1.518815
O	2.868537	-1.358477	1.091605
O	2.064040	0.066376	-1.013215
Cl	1.251020	-3.059095	-1.148813
H	0.175067	-1.550259	1.482009
B	-0.976858	-1.424167	1.251135
O	-1.612314	-2.162626	0.242797
O	-1.912797	-1.076442	2.247100
C	-2.944318	-2.067885	0.512800
C	-3.126156	-1.410994	1.726597
C	-4.380764	-1.166144	2.236887
H	-4.512947	-0.650778	3.182641
C	-4.007914	-2.502114	-0.244181
C	-5.286381	-2.254832	0.262270
C	-5.468460	-1.601699	1.475290
N	-0.810237	0.489113	0.244410
C	-0.048414	1.490274	0.503964
C	0.877825	1.451649	1.658703
C	-1.772271	0.566324	-0.796382
C	-1.589996	-0.168745	-1.963758
C	-0.037998	2.746433	-0.296354
C	0.201033	2.740530	-1.670026
C	-0.272952	3.958002	0.352798
C	-0.302840	5.143209	-0.366615
C	-0.065741	5.131489	-1.734416
C	0.195697	3.930697	-2.381522
C	-2.943844	1.293537	-0.608265
C	-3.917120	1.303699	-1.596617
C	-3.728260	0.589683	-2.772508
C	-2.561847	-0.144809	-2.951731
C	2.162508	1.986028	1.524919

C	3.049053	1.954601	2.588707
C	2.652686	1.420727	3.808629
C	1.369446	0.913094	3.957742
C	0.486497	0.921125	2.888034
H	0.395796	3.919510	-3.448521
H	0.409248	1.805031	-2.179089
H	-0.446139	3.967839	1.425864
H	-0.503901	6.079374	0.145118
H	-0.078334	6.060453	-2.296373
H	-3.852741	-3.002158	-1.194872
H	-6.153133	-2.577366	-0.306411
H	-6.475392	-1.423548	1.840181
H	-3.085528	1.841391	0.320276
H	-4.829251	1.873039	-1.444171
H	-4.490410	0.600208	-3.545637
H	-2.408927	-0.708783	-3.867258
H	-0.681228	-0.752290	-2.087911
H	-0.519259	0.533436	3.009858
H	1.050607	0.510512	4.914241
H	3.343687	1.408119	4.646237
H	4.050256	2.356989	2.469019
H	2.470375	2.418080	0.576869

4 (PhCPh=NPh)

Mo	3.011229	-0.644643	-0.294705
O	3.048982	-1.415650	1.192795
Cl	4.878927	-1.547870	-1.369341
Cl	1.686852	-1.258042	-2.204450
O	3.405043	0.966575	-0.083163
H	1.222944	-0.270920	0.171046
B	0.236530	0.595040	0.378263
N	-0.966496	-0.405587	0.379730
C	-0.794670	-1.602432	1.173978
C	-2.133336	-0.148236	-0.168390
C	-3.074644	-1.220919	-0.496953
O	0.241351	1.547167	-0.678479
O	0.462529	1.264687	1.621511
C	0.710404	2.555728	1.283688
C	0.576863	2.724819	-0.096469
C	0.745704	3.952739	-0.695264
C	1.048531	5.029077	0.141016
C	1.174678	4.863010	1.516009
C	1.006016	3.613077	2.115073
C	-1.441270	-1.632543	2.403714
C	-1.272199	-2.727245	3.237397
C	-0.457881	-3.780848	2.844765
C	0.184655	-3.739944	1.614836
C	0.022355	-2.648362	0.775199
C	-4.427656	-1.083713	-0.173949
C	-5.318310	-2.095887	-0.487950
C	-4.876189	-3.225466	-1.164664
C	-3.538815	-3.349348	-1.523427
C	-2.635421	-2.360352	-1.179933
C	-2.554429	1.231889	-0.410556
C	-3.130964	1.606827	-1.626758
C	-3.542861	2.913590	-1.816049
C	-3.436087	3.837264	-0.780813
C	-2.908097	3.456937	0.445514
C	-2.453079	2.162147	0.628800
H	1.101880	3.472364	3.186678
H	-3.199857	-4.220210	-2.074874
H	-1.594712	-2.445778	-1.476692
H	-4.770072	-0.195769	0.349398
H	-6.363311	-2.000459	-0.211811
H	-5.579455	-4.011018	-1.423035
H	0.638204	4.070723	-1.768579
H	1.187807	6.014176	-0.293337
H	1.411564	5.720751	2.137842
H	-2.065486	-0.793324	2.700673
H	-1.775426	-2.752579	4.198658
H	-0.323002	-4.636104	3.499242
H	0.818512	-4.563562	1.302177
H	0.499233	-2.627535	-0.199045
H	-2.031513	1.859790	1.583733
H	-2.836449	4.173289	1.258160
H	-3.773012	4.858284	-0.931316
H	-3.957407	3.215117	-2.772512
H	-3.220499	0.879089	-2.427951

TS5 (PhCPh=NPh)

Mo	-1.419214	-1.341339	-1.325707
Cl	-2.949590	-0.536852	-2.952060
O	-1.245415	-3.000378	-1.447972
O	0.014545	-0.669505	-1.941880
Cl	-3.342378	-1.229721	0.271636
H	-0.801442	-0.920418	0.239992
B	-0.426636	0.817092	0.680882
O	-1.231758	1.422083	-0.282062
O	-0.959592	0.958941	1.945222
C	-2.329829	1.873566	0.411742
C	-2.168707	1.583806	1.757248
C	-3.130032	1.887627	2.690535
H	-3.000354	1.645344	3.739449
C	-3.459490	2.481883	-0.078949
C	-4.443014	2.798238	0.857197
C	-4.282314	2.508311	2.208726
N	1.064774	0.706440	0.456748
C	1.833561	-0.351490	0.628634
C	1.352423	-1.540985	1.319249
C	1.654676	1.979816	0.064806
C	1.382237	2.535420	-1.176126
C	3.200229	-0.383093	0.099552
C	3.460998	-0.048265	-1.232814
C	4.242046	-0.799226	0.932123
C	5.540485	-0.822023	0.451600
C	5.797412	-0.478824	-0.869177
C	4.756163	-0.110928	-1.713842
C	2.479140	2.618579	0.980660
C	3.068833	3.823692	0.630652
C	2.824095	4.381087	-0.616921
C	1.979348	3.740010	-1.514079
C	1.612535	-2.792216	0.744319
C	1.102055	-3.936828	1.326601
C	0.377171	-3.850156	2.509537
C	0.166466	-2.618130	3.116125
C	0.639519	-1.462432	2.521304
H	4.955224	0.126798	-2.753610
H	2.642070	0.214671	-1.893843
H	4.032531	-1.074724	1.961758
H	6.353387	-1.117520	1.106666
H	6.814384	-0.509370	-1.247590
H	-3.579024	2.687564	-1.137096
H	-5.357029	3.276591	0.520454
H	-5.073037	2.766447	2.905738

H	2.659229	2.166590	1.952323
H	3.720539	4.327126	1.337320
H	3.289533	5.322884	-0.889891
H	1.785540	4.177083	-2.488255
H	0.732622	2.017849	-1.873111
H	0.477548	-0.502303	2.996551
H	-0.374113	-2.557492	4.054709
H	-0.018075	-4.751581	2.967337
H	1.266080	-4.900329	0.855884
H	2.166359	-2.851532	-0.188211

5 (**PhCPh=NPh**)

Mo	-1.262887	-1.695339	-1.691949
Cl	-2.002212	0.519042	-2.374376
O	-1.112818	-2.691392	-3.030934
O	0.299049	-1.286255	-1.157222
Cl	-3.640168	-1.942178	-0.973903
H	-1.332470	-2.858702	-0.463173
B	-0.311723	1.265428	0.710458
O	-1.313945	0.338954	0.831510
O	-0.751526	2.555948	0.804430
C	-2.443727	1.094728	1.066909
C	-2.102597	2.438269	1.039897
C	-3.027766	3.436287	1.236927
H	-2.748305	4.483381	1.207089
C	-3.728346	0.669836	1.309394
C	-4.676169	1.670623	1.515163
C	-4.335843	3.020197	1.477391
N	1.116525	0.970095	0.482816
C	1.711519	-0.112471	0.973852
C	1.073798	-0.804381	2.086488
C	1.825376	1.922867	-0.347802
C	1.371771	2.169786	-1.634609
C	2.995631	-0.595511	0.487490
C	3.321498	-0.603942	-0.876982
C	3.919758	-1.086130	1.419816
C	5.158592	-1.538698	1.000431
C	5.471160	-1.542519	-0.351615
C	4.546841	-1.088516	-1.288024
C	2.929042	2.581297	0.172881
C	3.611454	3.483817	-0.627904
C	3.181662	3.728038	-1.925804
C	2.060864	3.077204	-2.424791
C	0.981910	-2.199818	2.075878
C	0.322136	-2.850297	3.102909
C	-0.208295	-2.122346	4.161418
C	-0.085644	-0.738035	4.196799
C	0.542390	-0.076391	3.158434
H	4.784665	-1.117840	-2.346058
H	2.594619	-0.278469	-1.611046
H	3.674919	-1.081484	2.477223
H	5.877912	-1.896026	1.729516
H	6.437960	-1.909274	-0.682321
H	-3.981489	-0.383811	1.316523
H	-5.706428	1.387832	1.705214
H	-5.106071	3.767549	1.638091
H	3.249211	2.380841	1.191306
H	4.479716	4.001388	-0.233129
H	3.719541	4.434566	-2.549903
H	1.721641	3.270346	-3.437137
H	0.503427	1.638375	-2.020785
H	0.657249	1.004720	3.195287
H	-0.479298	-0.175868	5.036843
H	-0.716379	-2.638718	4.969723
H	0.219536	-3.929868	3.078794
H	1.386533	-2.760610	1.239005

TS6 (**PhCPh=NPh**)

Mo	-1.091215	-1.156387	-1.647385
O	-0.318280	-2.031099	-2.840944
Cl	-3.413662	-1.030599	-2.135003
Cl	-1.676389	-2.818739	0.036791
O	-0.656533	0.474049	-1.859775
H	0.240704	-1.115314	-0.445716
B	-0.500783	1.308002	0.717069
N	0.891989	0.955064	0.552942
C	1.809226	2.006535	0.174958
C	1.337356	-0.341421	0.625240
C	2.591969	-0.670867	-0.086241
O	-1.532375	0.391846	0.790745
O	-0.941600	2.605892	0.778851
C	-2.310031	2.503213	0.855086
C	-2.671338	1.164756	0.865038
C	-3.980660	0.754883	0.941023
C	-4.937611	1.767113	1.004358
C	-4.577633	3.111545	0.994790
C	-3.243710	3.510926	0.920874
C	2.907705	2.241663	0.991342
C	3.820582	3.224123	0.639719
C	3.623750	3.976057	-0.511042
C	2.509348	3.748228	-1.307985
C	1.597096	2.759933	-0.970244
C	3.663093	-1.224546	0.617688
C	4.882828	-1.423751	-0.012092
C	5.037165	-1.090203	-1.348584
C	3.966973	-0.558002	-2.062672
C	2.755109	-0.343746	-1.436752
C	0.938481	-1.169629	1.764645
C	1.043412	-2.564516	1.688755
C	0.742857	-3.346040	2.787793
C	0.323874	-2.748807	3.970337
C	0.219742	-1.365329	4.058043
C	0.524602	-0.577465	2.963252
H	-2.952284	4.555251	0.912495
H	4.080468	-0.313467	-3.113667
H	1.922063	0.069865	-1.997403
H	3.554550	-1.462326	1.671127
H	5.714723	-1.838027	0.548034
H	5.991297	-1.248538	-1.841531
H	-4.244829	-0.296793	0.941029
H	-5.987244	1.497529	1.059484
H	-5.352666	3.869655	1.043637
H	3.044665	1.648636	1.892358
H	4.684944	3.405939	1.270509
H	4.339430	4.744477	-0.786077
H	2.352875	4.335208	-2.207435
H	0.739775	2.550343	-1.602432
H	0.486591	0.504266	3.053254
H	-0.087797	-0.899256	4.988271
H	0.081169	-3.364214	4.831130
H	0.816630	-4.426173	2.717738
H	1.342017	-3.028941	0.754055

6 (**PhCPh=NPh**)

C	-4.000178	1.615822	-0.478757
C	-3.223703	0.730503	0.267927
C	-3.833403	-0.016749	1.274386
C	-5.190193	0.127140	1.528344
C	-5.953790	1.025161	0.796181
C	-5.350491	1.771871	-0.206934
N	-1.840724	0.595157	-0.034401
B	-1.001258	1.720945	-0.128452
O	0.336102	1.647570	-0.520792
C	0.799831	2.931890	-0.442184
C	-0.228214	3.767296	-0.021953
C	-0.044156	5.120554	0.141683
C	1.232016	5.617303	-0.131499
C	2.260575	4.781750	-0.550067
C	2.060808	3.409425	-0.714090
O	-1.361874	3.029950	0.176628
C	-1.228670	-0.737251	-0.232259
C	-0.477873	-1.253003	0.980624
C	-0.539745	-0.639183	2.224625
C	0.202017	-1.126966	3.296490
C	1.023693	-2.230940	3.136788
C	1.102455	-2.847992	1.893417
C	0.360532	-2.361633	0.826247
O	1.834211	-0.902698	-1.536546
Mo	3.180779	-0.749388	-0.571418
Cl	2.772472	0.420853	1.322825
O	4.250809	0.172082	-1.454739
Cl	4.170646	-2.776421	-0.293653
H	0.416605	-2.860561	-0.139819
H	1.741488	-3.715278	1.753971
H	1.603658	-2.609308	3.972986
H	0.137486	-0.631343	4.260781
H	-1.162434	0.240562	2.363243
H	-0.461433	-0.583485	-1.004974
H	-0.853595	5.763906	0.469375
H	1.422055	6.679392	-0.013722
H	3.240687	5.200781	-0.753938
H	2.860402	2.753002	-1.042382
C	-2.222941	-1.709168	-0.839050
H	-3.248883	-0.714826	1.864453
H	-5.650578	-0.465583	2.313330
H	-7.013743	1.138142	1.001995
H	-5.937742	2.469536	-0.796719
H	-3.536098	2.177890	-1.284064
C	-2.669655	-1.453938	-2.135029
C	-3.608405	-2.275274	-2.737535
C	-4.112563	-3.373428	-2.050492
C	-3.668952	-3.639818	-0.763965
C	-2.729467	-2.811865	-0.160673
H	-2.277363	-0.590821	-2.669672
H	-3.945424	-2.061702	-3.747549
H	-4.847794	-4.020385	-2.519617
H	-4.057855	-4.496007	-0.220716
H	-2.394966	-3.030040	0.849973

3 (**PhC≡N**)

Mo	-0.672268	0.661045	1.379670
O	0.077501	-0.157823	2.618118
O	0.474636	1.696348	0.761067
Cl	-1.294596	-0.785307	-0.249018
Cl	-2.383601	1.894028	2.207707
H	1.577964	-1.736570	0.826018
B	1.651540	-2.884566	0.579834
N	-0.475827	-3.536635	2.226029
C	-1.361740	-2.901085	2.605055
C	-2.451997	-2.100795	3.057384
C	-2.355047	-1.415658	4.272559
C	-3.413355	-0.630451	4.695353
C	-4.560973	-0.528865	3.917850
C	-4.657901	-1.212680	2.712262
C	-3.606235	-1.999675	2.275171
O	0.991606	-3.492735	-0.467600
C	1.371982	-4.804368	-0.408350
C	0.978456	-5.855202	-1.205772
C	1.541065	-7.098944	-0.919857
C	2.454012	-7.262002	0.117886
C	2.845970	-6.189171	0.918325
C	2.282401	-4.967267	0.628072
O	2.488009	-3.760991	1.237438
H	-3.343279	-0.094667	5.636221
H	-1.452966	-1.504622	4.869282
H	-3.669446	-2.542091	1.337132
H	-5.556461	-1.132640	2.109540
H	-5.387054	0.089589	4.254998
H	0.266615	-5.716479	-2.012368
H	1.259180	-7.957683	-1.520951
H	2.871134	-8.245368	0.310794
H	3.556893	-6.305188	1.729218

TS4 (**PhC≡N**)

Mo	0.438876	0.502290	1.044017
Cl	1.113868	1.170085	3.100817
Cl	2.206477	-0.275187	-0.138708
O	-0.256077	1.805462	0.274457
O	-0.748069	-0.653575	1.192057
H	-0.587258	-0.180965	-1.702912
B	-0.115345	-0.166991	-2.799167
N	0.739993	1.458673	-2.721088
C	1.121101	2.505722	-2.436756
C	1.602513	3.790152	-2.075489
C	1.413425	4.867644	-2.944757
C	1.885446	6.115742	-2.580941
C	2.537984	6.286518	-1.366030
C	2.724792	5.211826	-0.504510
C	2.259512	3.957183	-0.852459
O	0.926391	-1.083218	-3.118167
C	0.850079	-1.239231	-4.463683
C	1.706463	-1.921660	-5.298083
C	1.386157	-1.950869	-6.658919
C	0.248627	-1.319529	-7.143494
C	-0.618047	-0.631258	-6.288495
C	-0.293941	-0.604139	-4.950574
O	-0.973937	-0.029271	-3.925959
H	1.744355	6.959355	-3.247986
H	0.901183	4.715520	-3.888791
H	2.400835	3.109208	-0.189056
H	3.235905	5.352759	0.441701
H	2.905320	7.268857	-1.086345
H	2.590728	-2.415302	-4.907550
H	2.041394	-2.477568	-7.346199
H	0.024555	-1.359425	-8.205199
H	-1.512796	-0.139478	-6.656744

4 (**PhC≡N**)

C	-1.909359	-2.136627	-6.954220
C	-0.516344	-2.056868	-7.063511
C	0.101963	-1.410955	-8.142279
C	-0.693412	-0.842340	-9.117793
C	-2.078200	-0.918271	-9.016275
C	-2.684163	-1.560260	-7.941499
C	0.304706	-2.636534	-6.080467
N	1.010222	-3.100447	-5.302963
B	2.079686	-3.658057	-4.324974
O	2.126475	-5.080550	-4.310546
C	2.196712	-5.412032	-2.995069
C	2.350598	-6.661234	-2.437424
C	2.380442	-6.734221	-1.043000
C	2.262387	-5.594048	-0.257500
C	2.108723	-4.329939	-0.831296
C	2.077416	-4.267255	-2.206015
O	1.930871	-3.171441	-2.995350
O	3.211702	-0.863671	-5.479732
Mo	4.336534	-2.047872	-5.852213
Cl	5.682654	-1.058409	-7.461783
Cl	3.775930	-3.800213	-7.345754
O	5.354232	-2.279944	-4.545071
H	-3.765345	-1.610807	-7.875706
H	-2.359315	-2.643144	-6.107550
H	1.185117	-1.364574	-8.197579
H	-0.233629	-0.337714	-9.960242
H	-2.695680	-0.468880	-9.787456
H	3.166112	-3.203967	-4.851302
H	2.444176	-7.544340	-3.060656
H	2.501034	-7.702148	-0.566574
H	2.292630	-5.683655	0.823909
H	2.017827	-3.432647	-0.228199

TS5 (PhC≡N)

Mo	0.408220	-0.558873	0.438042
O	0.486350	-0.567821	2.120558
O	1.952813	-0.593303	-0.216678
Cl	-1.552636	-1.289037	-0.854376
Cl	-0.437605	1.630942	-0.030429
H	0.327917	-2.298015	0.483652
B	-0.057700	-3.860905	1.231009
N	-1.161996	-3.300398	2.034200
C	-1.944942	-2.706077	2.633277
C	-2.889758	-1.934832	3.314045
C	-3.252120	-2.259875	4.629204
C	-4.167835	-1.456607	5.275989
C	-4.708343	-0.352119	4.624224
C	-4.343804	-0.035465	3.319688
C	-3.430793	-0.822032	2.648390
O	-0.301969	-4.553429	0.071281
C	0.899458	-5.163868	-0.190806
C	1.254871	-5.919026	-1.284424
C	2.548013	-6.437577	-1.281728
C	3.427534	-6.200274	-0.228493
C	3.057216	-5.431759	0.873265
C	1.778052	-4.925495	0.860026
O	1.154130	-4.153920	1.809730
H	-4.462140	-1.687166	6.293659
H	-2.812279	-3.122603	5.116530
H	-3.126665	-0.592676	1.630560
H	-4.771837	0.829821	2.826423
H	-5.426007	0.274412	5.144021
H	0.561696	-6.095109	-2.099203
H	2.876929	-7.038331	-2.123521
H	4.427522	-6.619992	-0.266620
H	3.733923	-5.237111	1.697566

5

Mo	-0.179059	0.601729	-0.545965
Cl	0.332346	1.540631	1.623952
Cl	2.303417	0.308838	-0.582739
O	-0.933303	1.877856	-1.350980
O	-1.269523	-0.637210	-0.222357
H	0.314976	-0.108068	-2.012567
B	1.141925	0.909394	-4.098196
N	1.536815	2.141613	-3.429514
C	1.770829	3.078128	-2.799102
C	2.044232	4.190857	-2.006958
C	1.843569	5.480901	-2.525007
C	2.096617	6.562080	-1.708461
C	2.533468	6.361182	-0.401701
C	2.726108	5.080449	0.105884
C	2.487290	3.979438	-0.689770
O	1.966335	-0.163956	-4.201509
C	1.201162	-1.090092	-4.876202
C	1.526173	-2.380185	-5.224836
C	0.545281	-3.092517	-5.910192
C	-0.689342	-2.525960	-6.220380
C	-1.006000	-1.218145	-5.861334
C	-0.028821	-0.525587	-5.185344
O	-0.064162	0.767344	-4.708098
H	1.951096	7.567650	-2.086463
H	1.498074	5.609716	-3.544396
H	2.619105	2.966799	-0.317217
H	3.060399	4.940501	1.127709
H	2.724783	7.220329	0.233292
H	2.488636	-2.810944	-4.974019
H	0.748892	-4.116123	-6.206863
H	-1.426155	-3.118700	-6.752359
H	-1.964650	-0.768624	-6.093320

TS6 (PhC≡N)

Mo	0.580198	-1.161197	-1.451178
Cl	-1.702301	-0.393238	-0.953970
Cl	0.285652	0.102392	-3.454735
O	1.945307	-0.493895	-0.732384
O	0.925805	-2.713789	-1.990488
H	0.090916	-1.820971	0.097389
B	-2.859348	-1.387518	1.527018
N	-1.663124	-2.189449	1.629576
C	-0.620279	-2.697563	1.499475
C	0.400210	-3.641540	1.776110
C	1.749996	-3.422092	1.487004
C	2.675410	-4.382444	1.843743
C	2.259760	-5.555535	2.463719
C	0.915905	-5.775094	2.744627
C	-0.024136	-4.821026	2.410751
O	-2.974190	-0.158369	2.110470
C	-4.262623	0.220566	1.813736
C	-4.902636	1.398260	2.121592
C	-6.223969	1.509828	1.693093
C	-6.854206	0.483360	0.994523
C	-6.194591	-0.705699	0.689294
C	-4.891093	-0.803145	1.116755

O	-4.011596	-1.849240	0.958498
H	3.725888	-4.220136	1.630391
H	2.061223	-2.504779	1.000091
H	-1.076769	-4.970257	2.626705
H	0.600163	-6.693762	3.226632
H	2.993036	-6.310047	2.729960
H	-4.400309	2.191457	2.663536
H	-6.772436	2.421002	1.908522
H	-7.883615	0.611421	0.676135
H	-6.674018	-1.510292	0.143375

6 (PhC≡N)

Mo	0.185668	0.342277	-0.067988
Cl	0.828793	0.111776	2.084316
Cl	0.147545	2.506545	-0.722694
O	1.229643	-0.516855	-1.037334
O	-1.317880	-0.338330	-0.302600
H	-1.269532	-3.275798	0.242563
B	-2.734099	-1.642657	1.658103
N	-1.607438	-2.390561	2.099217
C	-0.992291	-3.176690	1.308162
C	0.145591	-4.000116	1.707454
C	0.745977	-4.831333	0.761329
C	1.827144	-5.624337	1.113424
C	2.313710	-5.586107	2.413344
C	1.722587	-4.755029	3.362205
C	0.644121	-3.964164	3.013089
O	-3.050459	-0.384852	2.157170
C	-4.172058	-0.002851	1.480060
C	-4.874431	1.177353	1.571750
C	-5.997273	1.301701	0.752858
C	-6.383229	0.280867	-0.109990
C	-5.663969	-0.911653	-0.194399
C	-4.556976	-1.022241	0.615702
O	-3.679157	-2.061733	0.727926
H	2.291620	-6.271435	0.376172
H	0.354181	-4.850370	-0.253059
H	0.170227	-3.305815	3.735729
H	2.110846	-4.728479	4.375660
H	3.160876	-6.205735	2.691998
H	-4.565203	1.966760	2.248390
H	-6.580676	2.216223	0.790524
H	-7.261374	0.413982	-0.733941
H	-5.954252	-1.713134	-0.865175

3 (PhC=ONH$_2$)

Mo	-1.361874	0.989491	0.494637
Cl	-3.441791	1.811592	0.840793
Cl	0.067796	1.509621	2.168036
O	-1.434500	-0.663431	0.326026
O	-0.742048	1.586236	-0.930078
H	1.002809	-0.616504	-1.217942
B	1.465817	-0.733090	-2.290467
O	-0.732385	-0.663782	-3.279814
C	-1.326242	0.391999	-3.480921
C	-2.773828	0.534945	-3.135611
C	-3.375801	-0.513395	-2.440110
C	-4.708827	-0.437555	-2.066848
C	-5.456690	0.688179	-2.388496
C	-4.867316	1.735135	-3.086500
C	-3.532369	1.661760	-3.456125
O	1.815196	-1.946478	-2.858593
C	2.417742	-1.627256	-4.040256
C	2.893459	-2.464642	-5.024148
C	3.474444	-1.855926	-6.138011
C	3.569092	-0.471700	-6.244349
C	3.086224	0.368038	-5.239142
C	2.515829	-0.245395	-4.147079
O	1.969063	0.331502	-3.033228
N	-0.711232	1.457465	-4.037578
H	-5.166079	-1.259317	-1.524049
H	-2.778456	-1.386342	-2.197255
H	-3.103930	2.490155	-4.013503
H	-5.450175	2.613474	-3.346405
H	-6.501839	0.749289	-2.099613
H	2.815248	-3.543076	-4.936225
H	3.859872	-2.478799	-6.939346
H	4.026755	-0.034003	-7.126028
H	3.157890	1.448785	-5.308894
H	-1.121315	2.378646	-3.998827
H	0.299374	1.417225	-4.088718

TS4 (PhC=ONH$_2$)

Mo	-0.570130	-0.233588	0.995876
Cl	-1.867492	-0.031586	2.833760
Cl	1.589778	-0.659078	1.506694
O	-1.180398	-1.444927	0.032524
O	-0.679563	1.166576	0.103135
H	1.441707	0.015698	-1.642461
B	1.232847	0.389648	-2.738728
O	-0.402786	-1.107606	-3.096714
C	-1.601129	-0.948221	-2.856519
N	-2.116426	0.249576	-2.525456
C	-2.549103	-2.095002	-2.937929
C	-2.033460	-3.380857	-2.787486
C	-2.872415	-4.481748	-2.849482
C	-4.232822	-4.307257	-3.075681
C	-4.750658	-3.029308	-3.241007
C	-3.913454	-1.925020	-3.168471
O	0.479695	1.533918	-3.023480
C	0.623560	1.716602	-4.371435
C	0.006420	2.638934	-5.184945
C	0.348539	2.607592	-6.538722
C	1.269650	1.688483	-7.030454
C	1.889041	0.758039	-6.193332
C	1.541275	0.793960	-4.861830
O	1.989741	0.010821	-3.839727
H	-2.465495	-5.480133	-2.721004
H	-0.968742	-3.501769	-2.614556
H	-4.329940	-0.933158	-3.321642
H	-5.810422	-2.891407	-3.432804
H	-4.890194	-5.170089	-3.129339
H	2.606575	0.036831	-6.570330
H	1.512332	1.690963	-8.088652
H	-0.115097	3.315290	-7.219071
H	-0.708410	3.353529	-4.789933
H	-1.480318	1.032371	-2.421644
H	-3.054215	0.341499	-2.164069

4 (PhC=ONH$_2$)

C	-6.344198	3.462657	2.067782
C	-6.499272	2.076364	2.160647
C	-6.716906	1.388947	0.988038
C	-6.779184	2.048408	-0.239033

C	-6.629686	3.411368	-0.342769
C	-6.408156	4.116758	0.843941
O	-6.891925	0.053618	0.817228
B	-7.171881	-0.124764	-0.565974
O	-6.426381	-1.255114	-1.159913
C	-6.385426	-1.528025	-2.413486
N	-6.717047	-0.641278	-3.319980
O	-6.993727	1.143064	-1.234546
C	-5.955928	-2.874369	-2.786409
C	-6.097906	-3.901851	-1.851052
C	-5.725478	-5.192088	-2.186299
C	-5.199048	-5.458545	-3.444054
C	-5.042982	-4.435032	-4.371998
C	-5.422553	-3.144417	-4.048914
Mo	-9.838106	-1.709852	-0.546986
Cl	-10.679795	0.369656	0.159451
O	-8.821698	-2.577552	0.457554
Cl	-11.903892	-2.710742	-0.257856
O	-9.457019	-2.073187	-2.141694
H	-8.415694	-0.447227	-0.751281
H	-5.846607	-5.992733	-1.464228
H	-6.511642	-3.685118	-0.871650
H	-5.268441	-2.348057	-4.771130
H	-4.617215	-4.643780	-5.347872
H	-4.903054	-6.470533	-3.702851
H	-6.452741	1.558340	3.112987
H	-6.173085	4.037363	2.972925
H	-6.286648	5.194880	0.804798
H	-6.684019	3.911666	-1.304199
H	-6.766001	-0.889920	-4.300143
H	-6.933287	0.316658	-3.050468

TS5 (PhC=ONH$_2$)

Mo	0.110826	-0.020192	-0.373869
Cl	0.558421	0.161856	1.952926
Cl	2.511345	0.201746	-0.625140
O	-0.653890	-1.507523	-0.531722
O	-1.001967	1.219604	-0.645801
H	0.486061	-0.002861	-2.077731
B	0.114497	-0.429566	-3.744503
O	-1.268834	-0.190222	-3.684865
C	-1.851662	0.966316	-3.553878
C	-3.274261	0.939098	-3.258411
C	-3.812146	-0.191295	-2.636873
C	-5.158693	-0.221016	-2.321579
C	-5.970871	0.860771	-2.639079
C	-5.440291	1.980452	-3.270584
C	-4.093201	2.026148	-3.577506
O	0.586637	-1.722103	-3.767260
C	1.902061	-1.584458	-4.133218
C	2.878451	-2.550946	-4.189197
C	4.148589	-2.128658	-4.582711
C	4.408731	-0.799355	-4.901323
C	3.409859	0.173016	-4.841727
C	2.165313	-0.257700	-4.451461
O	1.012234	0.480074	-4.293602
N	-1.186198	2.079346	-3.681852
H	-5.576393	-1.089886	-1.824266
H	-3.170219	-1.028117	-2.382975
H	-3.689399	2.892061	-4.093821
H	-6.081734	2.816138	-3.529271
H	-7.028454	0.831100	-2.395594
H	2.668132	-3.582971	-3.930762
H	4.952534	-2.855813	-4.636205
H	5.411062	-0.508705	-5.199191
H	3.603681	1.212953	-5.080327
H	-1.625923	2.968143	-3.469177
H	-0.194389	2.085413	-3.912119

5 (PhC=ONH$_2$)

C	0.218858	1.123349	0.039536
C	0.377751	0.733873	1.346865
C	1.319192	1.310998	2.187666
C	2.151932	2.319473	1.765678
C	2.002707	2.727565	0.440391
C	1.061555	2.143482	-0.402312
O	1.248781	0.721104	3.429293
B	0.207944	-0.150735	3.314992
O	-0.314928	-0.235470	2.049186
O	-0.146652	-0.977849	4.369084
C	-1.264303	-1.633233	4.541406
N	-2.204360	-1.594348	3.642406
C	-1.378619	-2.380244	5.781192
C	-0.480026	-2.107054	6.818416
C	-0.579296	-2.798023	8.012121
C	-1.561565	-3.766592	8.174448
C	-2.450088	-4.049520	7.142258
C	-2.364619	-3.359785	5.948355
Cl	-1.783770	1.831254	4.047268
Mo	-0.763760	2.335842	6.279405
Cl	0.144262	4.172004	5.035635
O	-1.782046	3.017496	7.429276
O	0.627017	1.732250	7.020581
H	-1.483732	0.789750	6.303475
H	0.110704	-2.578245	8.819613
H	0.281902	-1.346663	6.691639
H	-3.053204	-3.609599	5.146819
H	-3.207521	-4.815482	7.268965
H	-1.634650	-4.309597	9.111655
H	2.872818	2.775815	2.435033
H	2.633761	3.524549	0.060540
H	0.974433	2.492255	-1.426278
H	-0.522241	0.666476	-0.606810
H	-2.095929	-1.071251	2.775817
H	-3.104896	-2.028828	3.810014

TS6 (PhC=ONH$_2$)

C	0.336381	1.455269	-0.694249
C	1.061413	1.666507	0.454524
C	2.150357	2.527235	0.487874
C	2.575974	3.220128	-0.619083
C	1.848245	3.013549	-1.791649
C	0.755681	2.152676	-1.827624
O	0.872640	1.115682	1.699366
B	1.894642	1.631682	2.450501
O	2.671643	2.539444	1.765077
O	2.047637	1.312583	3.771957
C	3.036677	1.722275	4.574679
N	3.449784	2.986022	4.475215
C	3.112884	1.021008	5.870220
C	2.163702	0.051435	6.187780
C	2.232303	-0.602702	7.408267
C	3.248650	-0.303547	8.304538
C	4.208091	0.649355	7.978812

C	4.145438	1.307433	6.764354
Cl	3.830452	-0.561943	1.782946
Mo	5.678872	0.293179	3.062945
Cl	7.074689	-0.542765	1.359039
O	6.123264	-0.519582	4.459281
O	6.131841	1.910719	3.186859
H	4.166975	0.841779	3.877507
H	1.487525	-1.351399	7.658071
H	1.370252	-0.183176	5.487400
H	4.926390	2.017600	6.505389
H	5.014839	0.870402	8.669932
H	3.302036	-0.820606	9.257622
H	-0.511481	0.779443	-0.714533
H	0.216579	2.016102	-2.759622
H	2.145201	3.535924	-2.695355
H	3.431192	3.885654	-0.580398
H	3.460390	3.443727	3.568999
H	4.109657	3.342440	5.155744

6 ($PhC{=}ONH_2$)

C	0.336713	1.748893	1.369239
C	0.365354	0.375623	1.135620
C	1.507165	-0.205924	0.598554
C	2.616082	0.575408	0.294763
C	2.584131	1.942974	0.529330
C	1.441714	2.528995	1.065107
C	-0.805148	-0.479115	1.531558
N	-2.042523	0.021392	1.005786
O	-0.875286	-0.443182	2.970679
B	-1.191523	-1.517555	3.686731
O	-1.807653	-2.672670	3.229068
C	-1.900929	-3.486801	4.327082
C	-2.438130	-4.749537	4.411001
C	-2.417478	-5.354757	5.668844
C	-1.883363	-4.706292	6.776518
C	-1.341596	-3.422992	6.678396
C	-1.363115	-2.839733	5.433058
O	-0.899262	-1.601298	5.054398
Cl	1.715077	-2.674980	3.593244
Mo	2.124326	-1.017021	5.109487
O	1.503090	0.437245	4.608407
Cl	1.588560	-1.386094	7.282744
O	3.774713	-0.812509	5.076326
H	3.506011	0.114036	-0.123094
H	1.531459	-1.279508	0.423978
H	-0.550258	2.198975	1.806823
H	1.417321	3.598465	1.252995
H	3.450899	2.554878	0.297065
H	-0.932432	-2.908140	7.540572
H	-1.888369	-5.203993	7.741030
H	-2.831633	-6.351656	5.782094
H	-2.857562	-5.244300	3.541646
H	-2.764014	-0.694696	1.016695
H	-1.927662	0.338025	0.047705
H	-0.598593	-1.523675	1.245877

3 ($Ph_2S{=}O$)

C	-0.621286	3.250386	1.249845
C	-0.101930	2.091141	1.809984
C	-0.924727	1.136071	2.385238
C	-2.299155	1.338501	2.382381
C	-2.834799	2.484479	1.809614
C	-1.996193	3.438129	1.244889
S	1.691647	1.798606	1.934002
C	2.188060	2.400662	0.305507
C	2.078048	1.583198	-0.809613
C	2.506076	2.072320	-2.034699
C	3.033327	3.355442	-2.133254
C	3.146644	4.156633	-1.005434
C	2.732658	3.674623	0.229677
O	1.861312	0.296740	1.959741
B	1.116108	-1.814567	1.039225
O	2.035050	-2.482609	1.827999
C	3.167269	-2.549625	1.070397
C	2.913259	-2.011394	-0.185626
C	3.880918	-1.941179	-1.161185
C	5.139038	-2.447458	-0.830367
C	5.392437	-2.993712	0.423399
C	4.402624	-3.054970	1.405661
O	1.610244	-1.602757	-0.240960
O	-0.833151	0.441581	-0.579881
Mo	-2.182931	-0.455496	-0.943265
Cl	-1.645211	-1.896555	-2.609262
O	-2.543865	-1.334739	0.422594
Cl	-3.914199	0.935398	-1.424287
H	-0.010778	-1.651258	1.330535
H	2.426669	1.448899	-2.920485
H	1.665055	0.583905	-0.715215
H	2.833528	4.284158	1.124667
H	3.569867	5.153207	-1.082564
H	3.365412	3.730062	-3.096779
H	3.668906	-1.512564	-2.135514
H	5.934970	-2.412709	-1.567662
H	6.382840	-3.378193	0.646356
H	4.592554	-3.474626	2.387804
H	0.029315	3.996315	0.801747
H	-2.413413	4.334476	0.796253
H	-3.909844	2.637595	1.805099
H	-2.952336	0.595878	2.830831
H	-0.494026	0.233718	2.808783

TS4 ($Ph_2S{=}O$)

Mo	-0.108557	0.265374	0.013694
Cl	-0.203908	0.316933	2.268976
Cl	2.044818	0.372798	-0.670963
O	-0.964115	1.514585	-0.670777
O	-0.790607	-1.144866	-0.555409
B	-3.886834	1.742720	1.378170
O	-5.187984	0.504903	0.955566
S	-4.976470	-0.977139	0.649087
C	-3.708219	-1.540846	1.827677
C	-3.881435	-1.096203	3.133319
C	-3.019605	-1.552948	4.117215
C	-2.006332	-2.448237	3.800302
C	-1.847455	-2.883324	2.493244
C	-2.704110	-2.436234	1.495590
O	-4.114215	2.739274	0.397244
C	-4.895852	3.667034	1.010760
C	-5.035020	3.344150	2.360072
C	-5.766942	4.133625	3.216623
C	-6.368443	5.273981	2.678688
C	-6.229960	5.594349	1.335598
C	-5.483567	4.788173	0.472770
O	-4.349113	2.203073	2.633983

C	-4.105211	-1.090907	-0.922515
C	-3.605414	0.046169	-1.536765
C	-2.983978	-0.091976	-2.771089
C	-2.881701	-1.337026	-3.374211
C	-3.419763	-2.460504	-2.759516
C	-4.051071	-2.338957	-1.531989
H	-2.909704	1.065495	1.308310
H	-2.580538	0.788780	-3.260595
H	-3.711497	1.023899	-1.075964
H	-4.500120	-3.206379	-1.053322
H	-3.360351	-3.430140	-3.242809
H	-2.393369	-1.432349	-4.338770
H	-5.365712	5.027268	-0.578629
H	-6.709590	6.486730	0.945896
H	-6.955036	5.919247	3.325107
H	-5.866372	3.872348	4.264711
H	-2.554127	-2.757599	0.470652
H	-1.045453	-3.569109	2.238307
H	-1.331088	-2.799297	4.574056
H	-3.136621	-1.197632	5.135676
H	-4.649904	-0.365022	3.366112

4 (Ph_2S=O)

C	-5.522554	-0.932606	5.304587
C	-5.107436	0.229858	4.663152
C	-3.800082	0.698677	4.750959
C	-2.895385	-0.019476	5.511441
C	-3.297228	-1.177901	6.168344
C	-4.601983	-1.638990	6.061845
S	-6.414621	1.129090	3.859132
O	-6.872845	2.308086	4.825478
B	-6.105567	2.900031	5.961208
O	-6.873622	3.952664	6.547401
C	-6.976906	3.641721	7.863317
C	-6.310100	2.444096	8.126696
C	-6.256760	1.910458	9.393570
C	-6.907165	2.615407	10.411407
C	-7.570458	3.806436	10.149897
C	-7.614264	4.344608	8.859508
O	-5.765707	1.955016	6.985243
C	-5.587792	1.991265	2.518395
C	-5.927562	3.313408	2.281381
C	-5.361037	3.953111	1.188191
C	-4.497675	3.266608	0.347187
C	-4.196961	1.931323	0.586127
C	-4.747566	1.274665	1.675225
O	-5.194831	5.560841	4.428462
Mo	-3.810548	4.847314	5.040033
Cl	-2.300783	6.613460	5.117135
O	-3.170982	3.823382	3.877545
Cl	-3.382753	4.324525	7.301335
H	-5.001048	3.357330	5.424534
H	-5.598791	4.994954	0.999284
H	-6.603478	3.843196	2.943754
H	-4.509984	0.231978	1.865398
H	-3.525971	1.394754	-0.076475
H	-4.057054	3.773270	-0.505414
H	-8.125745	5.277565	8.645579
H	-8.064118	4.334299	10.960226
H	-6.888170	2.223109	11.423657
H	-5.730891	0.980442	9.584952
H	-3.488424	1.599905	4.233300
H	-1.871258	0.328624	5.595157
H	-2.580032	-1.729990	6.767564
H	-4.905586	-2.547358	6.570751
H	-6.550485	-1.273559	5.221933

TS5 (Ph_2S=O)

Mo	-0.009144	-0.142161	0.119642
Cl	0.181217	-0.217813	2.506839
O	1.422745	-0.086702	-0.750576
O	-1.212806	-0.773290	-0.862407
Cl	-0.660785	2.110294	0.321657
H	0.391964	-1.914113	0.524695
B	0.075748	-3.249622	0.855584
O	0.525589	-4.008602	-0.305320
S	2.016213	-4.204621	-0.853343
C	2.118105	-2.974640	-2.154974
C	0.945828	-2.509619	-2.728288
C	1.042205	-1.636658	-3.802351
C	2.285377	-1.265597	-4.293078
C	3.447134	-1.767053	-3.718936
C	3.374229	-2.637440	-2.643211
C	3.147439	-3.619259	0.383251
C	3.672028	-4.618116	1.198310
C	4.464342	-4.248919	2.272441
C	4.710991	-2.905018	2.518083
C	4.191446	-1.920209	1.684186
C	3.402196	-2.268529	0.603167
O	-1.325780	-3.327550	1.033588
C	-1.503630	-3.485411	2.373144
C	-0.267074	-3.586439	3.007621
C	-0.161298	-3.738382	4.370084
C	-1.354458	-3.792950	5.095374
C	-2.587539	-3.692209	4.463945
C	-2.683564	-3.533764	3.078735
O	0.731844	-3.500000	2.088449
H	0.135176	-1.245241	-4.251164
H	-0.023124	-2.800222	-2.337685
H	4.280892	-3.030148	-2.192510
H	4.418325	-1.478361	-4.106753
H	2.351732	-0.581514	-5.132827
H	-3.641280	-3.446434	2.576417
H	-3.496835	-3.733421	5.055570
H	-1.313898	-3.911950	6.173751
H	0.808619	-3.806644	4.852106
H	3.001854	-1.505407	-0.056277
H	4.397362	-0.873325	1.880059
H	5.323385	-2.618743	3.367287
H	4.883323	-5.010780	2.920790
H	3.455776	-5.664420	1.003168

5 (Ph_2S=O)

C	5.104442	-1.264796	-3.623261
C	4.007956	-0.702679	-2.982516
C	4.094413	-0.064297	-1.752569
C	5.338442	-0.002937	-1.144939
C	6.449386	-0.570601	-1.757153
C	6.335361	-1.200127	-2.989013
S	2.463021	-0.856965	-3.849663
C	1.675784	-2.275914	-3.155633
C	1.858986	-2.671828	-1.833328
C	1.167251	-3.781185	-1.384749
C	0.314882	-4.469598	-2.242958

C	0.145835	-4.062924	-3.558742
C	0.827786	-2.953427	-4.029554
O	1.696963	0.416839	-3.167264
B	0.529460	0.908669	-3.713506
O	-0.054795	0.425830	-4.854262
C	-1.134702	1.266027	-5.039907
C	-1.139177	2.230325	-4.040633
C	-2.098419	3.211615	-3.980540
C	-3.073423	3.185493	-4.977652
C	-3.069864	2.217659	-5.976314
C	-2.087984	1.227682	-6.027710
O	-0.066700	2.026244	-3.200312
Cl	-1.308769	-0.677009	-1.928579
Mo	-0.370709	0.723262	-0.047772
Cl	-2.345930	2.033800	-0.512792
O	-0.606318	0.016603	1.458841
O	0.819421	1.916846	0.064242
H	0.785643	-0.388451	-0.594713
H	5.436792	0.494911	-0.186179
H	3.222665	0.383687	-1.287308
H	5.006937	-1.738228	-4.596349
H	7.208072	-1.630540	-3.467956
H	7.417426	-0.513737	-1.269969
H	-2.093853	3.958892	-3.195222
H	-3.854699	3.938679	-4.969690
H	-3.848274	2.228580	-6.732350
H	-2.073690	0.467277	-6.800621
H	2.533471	-2.140061	-1.170880
H	1.291832	-4.111062	-0.359112
H	-0.221348	-5.339695	-1.878260
H	-0.518803	-4.606540	-4.220985
H	0.704603	-2.622512	-5.056443

TS6 (Ph_2S=O)

C	-3.393473	-0.619589	-1.178540
C	-4.186956	0.346002	-1.795723
C	-5.505821	0.118672	-2.184518
C	-6.042838	-1.131581	-1.933487
C	-5.273194	-2.109870	-1.313633
C	-3.959093	-1.859269	-0.936871
S	-3.478855	1.938775	-2.070216
C	-3.449923	3.367918	-1.003465
C	-3.082424	3.179953	0.318939
C	-3.029398	4.305166	1.127619
C	-3.292321	5.560942	0.597584
C	-3.654670	5.708045	-0.735767
C	-3.765065	4.598100	-1.557950
O	-2.798010	2.237014	-3.522056
B	-1.548265	1.716486	-3.829808
O	-0.840686	2.203554	-4.893202
C	0.255620	1.376091	-4.961488
C	0.152688	0.389677	-3.989608
C	1.102132	-0.590733	-3.833083
C	2.192759	-0.536199	-4.701395
C	2.305215	0.459806	-5.665393
C	1.328469	1.444272	-5.817401
O	-1.014391	0.579621	-3.277533
Mo	0.635774	1.549492	-0.357297
O	0.711834	-0.135289	-0.462242
O	0.636084	2.017787	1.256793
Cl	2.759455	2.164997	-1.325710
Cl	-0.158323	3.411987	-1.865815
H	-1.043959	1.471044	-0.545400
H	-3.369631	-2.631024	-0.453961
H	-2.368004	-0.398503	-0.900199
H	-6.086745	0.898972	-2.662855
H	-7.067211	-1.341525	-2.221339
H	-5.706944	-3.085814	-1.120080
H	1.008346	-1.352341	-3.067424
H	2.973830	-1.284432	-4.614313
H	3.173749	0.474878	-6.315997
H	1.406437	2.224756	-6.565979
H	-2.828054	2.198242	0.704499
H	-2.744600	4.195634	2.168567
H	-3.215558	6.437596	1.232439
H	-3.867439	6.691714	-1.140599
H	-4.060603	4.693372	-2.596798

6 (Ph_2S=O)

C	0.057888	1.122719	0.817583
C	-0.004862	1.484321	2.158711
C	0.761752	0.809768	3.105997
C	1.599601	-0.218572	2.704793
C	1.662121	-0.585897	1.365456
C	0.889930	0.081021	0.426025
S	-1.103052	2.796829	2.689595
C	0.056360	4.088395	3.134018
C	1.306866	4.216317	2.535542
C	2.148124	5.249378	2.923699
C	1.741308	6.169466	3.881158
C	0.484592	6.049525	4.458796
C	-0.355163	5.005566	4.096567
O	-2.831658	2.839757	-0.094835
B	-3.410540	3.788851	-0.823032
O	-4.405834	3.522608	-1.742587
C	-4.817948	4.739751	-2.205555
C	-4.081787	5.751042	-1.605508
C	-4.325052	7.080748	-1.850968
C	-5.338046	7.367789	-2.767290
C	-6.060128	6.356563	-3.389097
C	-5.815529	5.011784	-3.111978
O	-3.147725	5.174426	-0.760705
O	-0.501696	4.585808	0.041313
Mo	-0.826501	6.221156	-0.005658
Cl	-2.271112	6.860889	1.655200
O	0.595770	6.930431	0.481841
Cl	-0.973391	6.937115	-2.179772
H	0.936469	-0.202529	-0.620920
H	-0.537212	1.649269	0.077830
H	0.702233	1.095711	4.152435
H	2.200286	-0.741774	3.442521
H	2.314266	-1.396730	1.055460
H	-3.769145	7.870840	-1.359161
H	-5.562623	8.404759	-2.994535
H	-6.838111	6.616787	-4.099486
H	-6.382261	4.213521	-3.578349
H	1.626991	3.509588	1.775427
H	3.126516	5.340800	2.461433
H	2.402793	6.978040	4.176223
H	0.157411	6.762225	5.210013
H	-1.330276	4.901675	4.565895
H	-2.211479	3.133592	0.594204

TS7

Cl	-0.639166	-1.683695	-0.251597
Mo	1.531563	-1.105437	-0.095116
O	2.009854	-1.397388	1.547281
B	3.701806	-1.033677	1.243512
O	4.021575	0.108449	1.984648
C	4.825004	-0.356268	2.983988
C	5.073847	-1.715062	2.793112
C	5.867922	-2.436393	3.655857
C	6.415213	-1.739474	4.733090
C	6.169993	-0.381512	4.921246
C	5.363749	0.340819	4.041811
O	1.558208	0.528051	-0.366372
Cl	2.265258	-2.359462	-1.861600
O	4.440766	-2.144516	1.663374
H	3.566718	-0.889501	0.008264
H	6.055088	-3.493497	3.500699
H	7.046646	-2.269325	5.439463
H	6.614778	0.127775	5.770450
H	5.166750	1.398724	4.178416

Im7

Cl	-4.259038	-2.387358	-0.633056
Mo	-3.035453	-0.448763	-1.008479
H	-4.473282	-0.226061	-1.808539
O	-3.193346	0.212788	0.491060
Cl	-1.095574	-1.616953	-1.479767
O	-2.681649	1.099536	-2.032790
B	-3.042957	1.775430	-3.147539
O	-2.526893	3.007882	-3.481795
O	-3.959385	1.318785	-4.072326
C	-4.020015	2.310723	-5.015536
C	-3.144162	3.331077	-4.660623
C	-2.986586	4.459409	-5.432033
C	-3.758979	4.529334	-6.590019
C	-4.638544	3.508792	-6.943276
C	-4.788554	2.369244	-6.154987
H	-5.468880	1.567893	-6.420968
H	-5.221415	3.601020	-7.853921
H	-3.672023	5.400955	-7.230539
H	-2.299974	5.248503	-5.146722

Im8 (PhCPh=NPh)

C	-2.731757	-0.473375	-1.919603
C	-2.974671	-1.723770	-1.364357
C	-4.249264	-2.170043	-1.103345
C	-5.288959	-1.297049	-1.421801
C	-5.044407	-0.043476	-1.976114
C	-3.747601	0.397088	-2.240109
O	-1.782570	-2.350837	-1.118772
B	-0.822790	-1.442483	-1.511641
O	-1.376297	-0.285194	-2.027283
O	0.506522	-1.661841	-1.410646
Mo	2.039131	-1.728278	-0.333031
O	2.513993	-3.300698	-0.504027
N	0.881317	0.550598	0.345101
C	-0.219813	0.782384	0.971760
C	-0.935946	-0.272031	1.726390
C	-0.269992	-1.090801	2.641166
C	-0.967520	-2.059147	3.347750
C	-2.330829	-2.224024	3.143605
C	-3.004363	-1.397566	2.253481
C	-2.316608	-0.411666	1.563627
Cl	3.148088	-1.407357	1.777668
Cl	3.738228	-0.401288	-1.233429
H	-3.545914	1.372686	-2.669787
H	-5.880830	0.607384	-2.209177
H	-6.312701	-1.603585	-1.232747
H	-4.426464	-3.144767	-0.661904
H	-2.854457	0.245607	0.883318
H	-4.073315	-1.512796	2.102062
H	-2.873406	-2.987822	3.692209
H	-0.442610	-2.683562	4.063828
H	0.789936	-0.942922	2.822580
C	1.554161	1.668593	-0.240075
C	-0.888312	2.114098	0.993759
H	0.949125	-1.962085	0.892920
C	2.370171	2.457130	0.561304
C	3.086948	3.501946	-0.004989
C	2.988072	3.762001	-1.364662
C	2.167556	2.970580	-2.159624
C	1.455482	1.919818	-1.603514
H	2.445005	2.238141	1.623426
H	3.726084	4.115370	0.622924
H	3.549579	4.579496	-1.806092
H	2.084369	3.170387	-3.223754
H	0.822205	1.288735	-2.221822
C	-1.047195	2.776039	2.209281
C	-1.686729	4.005687	2.251639
C	-2.205910	4.560249	1.089013
C	-2.076433	3.887544	-0.118872
C	-1.410391	2.672176	-0.171753
H	-0.658489	2.327739	3.120464
H	-1.790216	4.527453	3.197953
H	-2.718730	5.516474	1.125772
H	-2.493271	4.312032	-1.027229
H	-1.309350	2.143130	-1.115099

TS9 (PhCPh=NPh)

Mo	-0.060266	-1.010319	-0.601210
Cl	1.349299	-2.839282	-1.646495
Cl	-1.706949	-2.767480	-0.743303
O	-0.324802	-0.203197	-2.009739
O	-1.395194	-0.298787	0.666556
N	0.961425	0.453431	0.476648
H	1.678268	-0.964643	-0.825988
C	2.252529	0.143824	0.176098
C	2.883550	-0.961074	0.927077
C	3.979309	-1.655543	0.401146
C	4.515196	-2.726455	1.092185
C	3.961613	-3.117408	2.306245
C	2.869103	-2.437240	2.831061
C	2.321829	-1.368688	2.142173
B	-2.704657	-0.158043	0.481829
O	-3.286219	0.342318	-0.687120
C	-4.626768	0.366414	-0.439099
C	-4.863697	-0.093329	0.853125
C	-6.135068	-0.170666	1.372573
C	-7.180719	0.231103	0.538753
C	-6.943333	0.687868	-0.752505
C	-5.648672	0.764201	-1.269181
O	-3.677806	-0.418527	1.444784
C	0.577997	1.767660	0.818412
C	1.295795	2.400868	1.835201
C	0.980702	3.698349	2.205234

C	-0.055010	4.373133	1.574137
C	-0.770561	3.740479	0.565063
C	-0.461045	2.445288	0.182967
C	3.082861	1.086544	-0.594916
C	4.390966	1.378857	-0.197217
C	5.127989	2.330442	-0.882309
C	4.577812	2.979178	-1.979081
C	3.281202	2.685974	-2.387641
C	2.532847	1.753511	-1.694816
H	-6.310017	-0.529380	2.381353
H	-8.200017	0.184172	0.909074
H	-7.780130	0.990108	-1.374410
H	-5.450463	1.117792	-2.275540
H	1.521908	1.522687	-2.016419
H	2.854157	3.187394	-3.249880
H	5.161124	3.718096	-2.519736
H	6.135539	2.567941	-0.556781
H	4.817179	0.888388	0.672003
H	2.097374	1.863768	2.337192
H	1.545875	4.180851	2.996793
H	-0.304902	5.388168	1.866294
H	-1.578377	4.262694	0.061570
H	-1.021484	1.970072	-0.615260
H	4.384559	-1.371521	-0.565468
H	5.356734	-3.270584	0.676558
H	4.382011	-3.961390	2.844201
H	2.442564	-2.742844	3.780865
H	1.466250	-0.831402	2.541346

Im9 (PhCPh=NPh)

C	4.001498	1.504646	-0.210276
C	3.482034	1.324507	1.067071
C	4.274501	0.978361	2.136905
C	5.637114	0.818932	1.878150
C	6.158667	1.003416	0.601716
C	5.343207	1.354005	-0.475195
O	2.128214	1.512554	1.030030
B	1.832379	1.763051	-0.312078
O	2.991094	1.801840	-1.076812
O	0.605578	1.964092	-0.790367
Mo	-1.242801	1.635660	-0.300535
O	-1.442475	2.432280	1.119710
N	-0.952949	-0.191360	0.192264
C	-0.721140	-1.092908	-0.985709
C	0.765974	-1.236205	-1.239268
C	1.691650	-1.486695	-0.227152
C	3.036376	-1.648608	-0.536070
C	3.466222	-1.566882	-1.853237
C	2.548635	-1.315810	-2.864092
C	1.207922	-1.142884	-2.557063
Cl	-3.568753	1.009808	-0.669180
Cl	-1.682457	3.156298	-2.084420
H	5.738057	1.490705	-1.476338
H	7.223377	0.871536	0.437138
H	6.301474	0.545682	2.691758
H	3.856830	0.835549	3.128012
H	0.490904	-0.933937	-3.347686
H	2.878179	-1.242131	-3.895847
H	4.519240	-1.688229	-2.089301
H	3.751726	-1.838696	0.259401
H	1.370742	-1.560570	0.808253
C	-1.136160	-0.680101	1.514736
H	-1.129274	-0.535788	-1.845650
C	-1.480385	-2.396551	-0.942118
C	-0.258580	-0.256455	2.514810
C	-0.431691	-0.703971	3.812895
C	-1.488811	-1.548977	4.126235
C	-2.379873	-1.940310	3.136166
C	-2.212957	-1.514531	1.828361
H	0.566799	0.399601	2.254846
H	0.263579	-0.387751	4.583845
H	-1.624398	-1.894690	5.146096
H	-3.223755	-2.577045	3.381443
H	-2.931604	-1.795786	1.068130
C	-2.732025	-2.462473	-1.551068
C	-3.477288	-3.630876	-1.500314
C	-2.973653	-4.746090	-0.844256
C	-1.718007	-4.692910	-0.253100
C	-0.971373	-3.525264	-0.304753
H	-3.128851	-1.586330	-2.057306
H	-4.451676	-3.670437	-1.977233
H	-3.555580	-5.661831	-0.802890
H	-1.315492	-5.567076	0.249190
H	0.009545	-3.494142	0.160993

TS10 (PhCPh=NPh)

Mo	-0.443892	0.191812	0.798868
Cl	-2.112216	0.553753	2.359667
Cl	1.300895	0.220282	2.261109
O	-0.766536	-1.407117	0.547005
O	0.548465	0.607970	-0.735106
N	-1.712912	1.317237	-0.588194
B	-0.339079	0.720435	-1.825641
C	-1.422757	2.807085	-0.514534
C	-1.261793	3.307021	0.911684
C	0.027330	3.262246	1.444986
C	0.278804	3.625457	2.764996
C	-0.758490	4.066440	3.565682
C	-2.040797	4.162677	3.031885
C	-2.291091	3.788697	1.723829
O	-0.781729	-0.461551	-2.470958
C	-1.035491	-0.097759	-3.754720
C	-0.620217	1.217478	-3.958776
C	-0.759538	1.840961	-5.177526
C	-1.339763	1.093712	-6.204567
C	-1.760079	-0.216032	-5.999201
C	-1.615828	-0.839650	-4.758318
O	-0.116250	1.720333	-2.800395
C	-3.074208	0.870470	-0.594104
C	-3.349301	-0.453221	-0.959205
C	-4.646891	-0.932898	-0.970083
C	-5.708777	-0.113261	-0.610864
C	-5.448850	1.197041	-0.242858
C	-4.150997	1.683894	-0.231703
C	-2.238587	3.686297	-1.448778
C	-2.841838	3.204591	-2.610103
C	-3.469102	4.066379	-3.497693
C	-3.502634	5.431146	-3.248693
C	-2.893942	5.924896	-2.105083
C	-2.267104	5.061481	-1.216785
H	-0.442934	2.868984	-5.320926
H	-1.467481	1.548384	-7.181970
H	-2.211466	-0.766355	-6.818754
H	-1.940287	-1.860795	-4.586655

H	-1.784768	5.471079	-0.334183
H	-2.901007	6.990966	-1.898000
H	-3.995364	6.104408	-3.943575
H	-3.931131	3.660089	-4.393092
H	-2.842772	2.143990	-2.837757
H	-0.410786	2.884302	-0.926994
H	-2.541250	-1.119088	-1.232983
H	-4.826067	-1.963666	-1.260305
H	-6.725405	-0.493142	-0.616589
H	-6.262267	1.858086	0.040156
H	-3.993569	2.717140	0.037617
H	0.863943	2.986493	0.804999
H	1.291379	3.570601	3.153266
H	-0.572898	4.355306	4.595428
H	-2.856041	4.532645	3.646307
H	-3.300487	3.890598	1.341543

Im8 (PhC≡N)

C	0.682081	4.215110	0.451732
C	0.025142	4.065111	1.666860
C	-1.003639	4.893265	2.049895
C	-1.359568	5.896865	1.148515
C	-0.705225	6.044834	-0.070674
C	0.339782	5.199615	-0.445729
O	0.584580	3.019699	2.356582
B	1.597127	2.563838	1.534995
O	1.669428	3.268410	0.350811
O	2.447274	1.558942	1.845486
Mo	3.436773	0.826566	3.276524
O	3.227447	-0.783476	2.968298
N	3.352272	3.236172	3.872023
C	2.909628	4.298176	3.931443
C	2.314572	5.586602	3.944599
C	1.586315	6.008941	5.059476
C	0.956094	7.240148	5.022941
C	1.047074	8.036799	3.887570
C	1.771150	7.611847	2.779788
C	2.409095	6.384587	2.800179
Cl	3.916086	0.588565	5.559134
Cl	5.632034	1.476465	2.790741
H	0.858037	5.307866	-1.392106
H	-1.013417	6.834841	-0.747932
H	-2.167108	6.574927	1.405519
H	-1.503833	4.768665	3.004190
H	2.975975	6.033956	1.942956
H	1.835203	8.237163	1.895573
H	0.547404	9.000191	3.865559
H	0.389327	7.580150	5.883102
H	1.520002	5.371266	5.934533
H	2.029288	1.202840	4.089065

TS9 (PhC≡N)

Mo	-0.162972	0.148135	-0.700367
O	-0.399983	0.834678	0.806048
Cl	1.982872	-0.465583	-0.149212
Cl	0.237337	2.239071	-1.689837
H	-1.230953	0.137643	-2.244782
N	0.599202	-0.825363	-2.654586
C	-0.513602	-0.531786	-3.049385
O	-1.214005	-1.401548	-0.411867
B	-1.829119	-2.327644	-1.192631
O	-1.240710	-3.506145	-1.592206
C	-2.146628	-4.064972	-2.458119
C	-3.260710	-3.239845	-2.551241
C	-4.323351	-3.534331	-3.372781
C	-4.224961	-4.712873	-4.112321
C	-3.109154	-5.539740	-4.018980
C	-2.038410	-5.230369	-3.180624
O	-3.082439	-2.148291	-1.737895
C	-1.407364	-0.762138	-4.181891
C	-2.581151	-0.027693	-4.330432
C	-3.418483	-0.289120	-5.401136
C	-3.092611	-1.293639	-6.304532
C	-1.927830	-2.036429	-6.145417
C	-1.077393	-1.774641	-5.085908
H	-1.162474	-5.864877	-3.103300
H	-3.069056	-6.447665	-4.612142
H	-5.038352	-4.989425	-4.775405
H	-5.186195	-2.880536	-3.438338
H	-0.165099	-2.345580	-4.939939
H	-1.683662	-2.824743	-6.850068
H	-3.755320	-1.503560	-7.138379
H	-4.329928	0.285442	-5.528542
H	-2.830253	0.745857	-3.606899

Im9 (PhC≡N)

C	3.451099	-0.852974	0.423752
C	2.161066	-1.321908	0.648121
C	1.136175	-1.095376	-0.241473
C	1.458627	-0.377020	-1.394331
C	2.750238	0.086989	-1.622216
C	3.779669	-0.144046	-0.708923
O	2.120989	-1.967479	1.854230
B	3.417660	-1.869235	2.363326
O	4.249369	-1.195513	1.476942
O	3.803740	-2.338652	3.548641
Mo	3.006813	-2.299111	5.326223
O	1.816213	-3.432143	5.309460
N	2.042554	-0.738025	5.079749
C	1.704670	0.460779	5.342032
C	1.411796	1.483575	4.377768
C	1.375050	1.193535	3.005807
C	1.163355	2.207633	2.097873
C	0.986972	3.514486	2.552675
C	1.009270	3.807601	3.911633
C	1.217448	2.794773	4.829448
Cl	3.018311	-1.649171	7.689455
Cl	4.934424	-3.552224	5.957841
H	4.789129	0.215735	-0.875815
H	2.964902	0.640695	-2.530660
H	0.683465	-0.178045	-2.127436
H	0.132670	-1.461190	-0.052223
H	1.246880	3.004224	5.894782
H	0.865222	4.827677	4.250561
H	0.825138	4.313190	1.835440
H	1.133123	1.987528	1.035026
H	1.488917	0.164812	2.678770
H	1.646043	0.725751	6.411708

TS10 (PhC≡N)

Mo	0.223558	-0.195927	0.014949
Cl	-0.252614	0.492697	2.218810
Cl	2.483081	-0.299258	0.458208
O	-0.346746	-1.742122	0.108133

O	0.463905	0.161108	-1.825923
N	-1.356077	0.937505	-0.548234
B	-0.610955	0.903300	-2.313802
C	-2.187923	1.673438	0.079065
C	-3.362314	2.308365	-0.487908
C	-3.985730	1.812700	-1.637643
C	-5.099207	2.453960	-2.146040
C	-5.592164	3.593303	-1.516488
C	-4.991616	4.078338	-0.360887
C	-3.889484	3.427090	0.164906
O	-1.500358	0.297797	-3.237129
C	-1.969661	1.308144	-4.004854
C	-1.344838	2.506484	-3.642836
C	-1.659825	3.700174	-4.257077
C	-2.625440	3.654150	-5.260342
C	-3.243705	2.457700	-5.623509
C	-2.927684	1.255983	-4.993902
O	-0.458534	2.274770	-2.648559
H	-1.174930	4.625828	-3.966589
H	-2.900750	4.570732	-5.772319
H	-3.987540	2.462573	-6.414093
H	-3.405504	0.320037	-5.263725
H	-3.415001	3.786033	1.074273
H	-5.390279	4.958521	0.132691
H	-6.462982	4.098449	-1.923059
H	-5.589061	2.066763	-3.033869
H	-3.610215	0.903463	-2.095335
H	-2.024193	1.868775	1.151075

Im8 (PhC=ONH$_2$)

Mo	-0.322345	-0.285957	-0.239964
Cl	-1.483366	-1.053366	1.696693
Cl	1.524943	-0.665775	1.273841
O	-0.765369	-1.592135	-1.147881
O	-1.294406	1.351143	-0.025589
H	1.219244	-0.264548	-0.835087
O	-0.104132	0.829595	-2.118918
C	0.138831	0.509869	-3.312595
N	0.580329	-0.685873	-3.659494
C	-0.103683	1.527737	-4.352483
C	0.001176	2.876553	-4.009623
C	-0.256161	3.851588	-4.958474
C	-0.641227	3.487357	-6.243148
C	-0.763617	2.145851	-6.582412
C	-0.491326	1.164650	-5.642391
B	-1.891013	2.179667	-0.898581
O	-1.657172	3.548214	-0.943166
C	-2.434321	4.007427	-1.970656
C	-3.140917	2.944708	-2.524021
C	-3.978239	3.110697	-3.602767
C	-4.094077	4.406728	-4.109895
C	-3.397108	5.471590	-3.548031
C	-2.545275	5.289259	-2.456610
O	-2.838910	1.798731	-1.843486
H	-1.992791	6.111897	-2.014888
H	-3.515746	6.466470	-3.966089
H	-4.745245	4.585145	-4.960029
H	-4.520511	2.275113	-4.032460
H	0.692447	-1.422156	-2.973041
H	0.846113	-0.892272	-4.613736
H	-0.619069	0.118873	-5.906825
H	-1.080417	1.861936	-7.580799
H	-0.852873	4.253904	-6.982442
H	-0.162515	4.900090	-4.693705
H	0.300154	3.155291	-3.003754

TS9 (PhC=ONH$_2$)

Mo	-1.314682	-0.760708	-0.653516
Cl	-3.089159	-0.364380	0.848642
Cl	-0.108686	-1.185381	1.338660
O	-0.276360	0.412494	-1.179699
O	-0.577740	-2.457962	-1.196454
H	-2.509051	0.475582	-1.337747
O	-2.409531	-1.292419	-2.259720
C	-2.956439	-0.095983	-2.483508
B	-0.255920	-2.899670	-2.418704
O	0.254226	-2.102410	-3.441743
C	0.490904	-2.961416	-4.478433
C	0.134739	-4.250274	-4.095523
C	0.265571	-5.324283	-4.944730
C	0.775106	-5.056498	-6.216645
C	1.132966	-3.767623	-6.598675
C	0.996526	-2.685463	-5.727358
N	-2.466208	0.577308	-3.557546
C	-4.409803	0.086618	-2.173691
C	-5.216703	-1.032957	-2.001954
C	-6.567331	-0.864880	-1.736149
C	-7.103391	0.411413	-1.624622
C	-6.290099	1.528238	-1.779797
C	-4.941651	1.368229	-2.052875
O	-0.333199	-4.229154	-2.811404
H	-0.014878	-6.326272	-4.637805
H	0.895446	-5.874197	-6.920517
H	1.528881	-3.597023	-7.594983
H	1.276720	-1.677713	-6.015227
H	-1.497927	0.434460	-3.821882
H	-2.896028	1.445965	-3.847403
H	-4.297245	2.239244	-2.147809
H	-6.706805	2.525216	-1.678743
H	-8.160014	0.537785	-1.408880
H	-7.203362	-1.735572	-1.612879
H	-4.787706	-2.026267	-2.083949

Im9 (PhC=ONH$_2$)

C	-3.434554	4.317794	-6.930792
C	-2.458969	3.712311	-6.136962
C	-2.701407	3.498470	-4.785305
C	-3.904456	3.908336	-4.221284
C	-4.867030	4.525318	-5.007877
C	-4.631703	4.728512	-6.363812
C	-1.165046	3.271828	-6.755824
H	-0.543500	2.735987	-6.021650
Mo	-2.216901	0.526651	-7.747990
Cl	-3.348811	-1.319091	-6.821839
O	-3.958845	1.204720	-8.117140
B	-5.089074	1.567270	-7.490086
O	-5.379125	1.293088	-6.161678
C	-6.602514	1.862547	-5.944351
C	-7.049191	2.451286	-7.122195
C	-8.241875	3.134221	-7.188513
C	-8.988874	3.198386	-6.011229
C	-8.546046	2.599215	-4.835053
C	-7.332238	1.913099	-4.779327
O	-6.121695	2.256217	-8.107583

Cl	-0.534531	-0.024123	-6.198291
O	-1.500615	2.204052	-7.722836
O	-1.694082	-0.091667	-9.179902
H	-6.972002	1.453191	-3.865083
H	-9.156269	2.668344	-3.939888
H	-9.938408	3.724488	-6.016207
H	-8.579420	3.596140	-8.110148
H	-1.945041	3.011951	-4.173312
H	-4.089916	3.740105	-3.164643
H	-5.810398	4.840321	-4.570009
H	-5.390161	5.199240	-6.982928
H	-3.254654	4.463218	-7.993981
N	-0.463084	4.281852	-7.422278
H	-0.863795	5.208347	-7.376461
H	0.539843	4.275610	-7.302464

TS10 (PhC=ONH$_2$)

Mo	0.052534	0.524531	-0.108160
Cl	-0.353978	0.090069	2.107089
Cl	1.606364	2.120783	0.362921
O	-1.250204	1.384262	-0.632810
O	0.978191	-0.145199	-1.566249
O	-0.497433	-1.382424	-0.417748
B	0.901036	-1.565007	-1.564954
O	0.540807	-2.228150	-2.747152
C	1.206763	-3.415444	-2.711337
C	2.022196	-3.462612	-1.580265
C	2.825841	-4.546762	-1.309315
C	2.786723	-5.602627	-2.222227
C	1.976400	-5.554488	-3.352447
C	1.162376	-4.451026	-3.616379
O	1.885750	-2.310112	-0.873548
C	-1.354287	-2.320207	0.326226
N	-2.649244	-1.805405	0.562256
C	-1.405870	-3.604668	-0.454542
C	-2.087532	-3.675690	-1.667866
C	-2.177348	-4.879888	-2.347059
C	-1.585585	-6.024056	-1.821229
C	-0.896452	-5.956334	-0.619385
C	-0.801667	-4.746145	0.057630
H	-0.850274	-2.488963	1.285887
H	3.457687	-4.573845	-0.427552
H	3.406185	-6.476891	-2.046167
H	1.974290	-6.392043	-4.043390
H	0.524446	-4.404553	-4.493080
H	-0.259109	-4.686518	0.998534
H	-0.424656	-6.844386	-0.209262
H	-1.657299	-6.967184	-2.355298
H	-2.707648	-4.928177	-3.293790
H	-2.541177	-2.783628	-2.093576
H	-3.171449	-1.609396	-0.286230
H	-2.674611	-1.003954	1.182454

TS11 (Ph2S=O)

Mo	-0.679525	-0.860114	-0.246592
Cl	-1.251416	-1.145776	2.103061
Cl	1.005322	0.643672	0.024968
O	-1.976982	0.163483	-0.467854
O	0.698503	-2.481762	0.281277
O	-0.566669	-1.601820	-1.809574
H	-1.986117	-2.510930	-0.268801
B	-1.836835	-2.857176	-1.447843
O	-1.233745	-4.094832	-1.700846
C	-1.775861	-4.491323	-2.889966
C	-1.468281	-5.602526	-3.640731
C	-2.193078	-5.783635	-4.819092
C	-3.177898	-4.882155	-5.209520
C	-3.483886	-3.759762	-4.439603
C	-2.762648	-3.588130	-3.279515
O	-2.873345	-2.598537	-2.347899
S	1.406813	-2.942268	1.578083
C	2.681440	-4.030666	0.921484
C	2.640347	-4.418698	-0.407136
C	3.639734	-5.262131	-0.872603
C	4.644330	-5.696303	-0.017609
C	4.664209	-5.291363	1.311392
C	3.677576	-4.444191	1.793063
C	0.318505	-4.180870	2.290382
C	-0.468371	-4.967820	1.463263
C	-1.293943	-5.911114	2.054361
C	-1.313123	-6.057646	3.437461
C	-0.515468	-5.258490	4.244150
C	0.306831	-4.297521	3.670423
H	-4.251179	-3.051678	-4.733544
H	-3.722754	-5.053389	-6.132484
H	-1.981312	-6.645862	-5.443442
H	-0.699432	-6.300149	-3.326246
H	-0.444475	-4.838356	0.384110
H	-1.926134	-6.536329	1.431886
H	-1.962803	-6.800250	3.889989
H	-0.542183	-5.369974	5.323098
H	0.918227	-3.645226	4.288670
H	3.685354	-4.114579	2.829323
H	5.454099	-5.629306	1.974246
H	5.423142	-6.353347	-0.391916
H	3.632748	-5.578404	-1.910853
H	1.846543	-4.058115	-1.054516

Im11 (Ph2S=O)

C	-5.835985	1.628956	1.940757
C	-4.672524	2.356181	2.037071
C	-3.863237	2.311238	3.167420
C	-4.197408	1.562160	4.270424
C	-5.382618	0.829594	4.190901
C	-6.179576	0.855554	3.051180
O	-2.768051	3.108234	2.973453
B	-2.916937	3.588646	1.687480
O	-4.115130	3.202079	1.114654
O	-2.029118	4.420166	1.071372
Mo	-0.401803	3.982533	0.237589
O	-1.497451	2.008219	0.520940
S	-1.148828	0.537605	0.197492
C	-1.588797	-0.327681	1.710677
C	-2.818021	-0.936551	1.926343
C	-3.044848	-1.555841	3.147467
C	-2.068515	-1.541041	4.134452
C	-0.853299	-0.904839	3.913644
C	-0.604128	-0.297812	2.693111
O	0.399929	5.429059	0.266059
Cl	-0.597972	3.423317	-2.045786
Cl	1.594940	2.595066	0.157640
C	-2.451693	-0.006769	-0.903418
C	-3.562342	0.793016	-1.114435
C	-4.562191	0.319049	-1.953514

C	-4.437660	-0.925128	-2.557217
C	-3.308876	-1.706495	-2.337797
C	-2.297546	-1.246153	-1.509012
H	0.070146	3.487645	1.756243
H	-3.564829	1.541658	5.151559
H	-5.684613	0.221246	5.037908
H	-7.092455	0.269033	3.024246
H	-6.453401	1.666232	1.048982
H	-3.589545	-0.939779	1.161676
H	-3.996726	-2.045063	3.328550
H	-2.256019	-2.030113	5.085423
H	-0.093111	-0.891165	4.687724
H	0.349865	0.188454	2.502388
H	-1.409741	-1.847521	-1.329019
H	-3.212363	-2.674691	-2.818121
H	-5.224473	-1.288895	-3.210571
H	-5.442306	0.928172	-2.134562
H	-3.641166	1.762173	-0.629885

TS12 (**Ph2S=O**)

Mo	0.579184	-0.527816	-0.564378
Cl	-0.777230	1.529511	-0.405864
Cl	0.866217	-0.183046	1.790009
O	1.987129	-0.002915	-1.208530
O	0.773640	-2.542897	-0.191722
O	-0.224889	-1.492247	-2.291838
H	-0.435909	-0.126511	-1.832717
B	-1.107168	-2.483134	-2.174746
O	-1.196700	-3.560065	-3.055498
C	-2.240638	-4.311573	-2.597929
C	-2.749637	-5.481437	-3.112115
C	-3.838236	-6.043020	-2.440338
C	-4.378612	-5.444271	-1.308412
C	-3.854379	-4.256023	-0.795090
C	-2.783260	-3.712878	-1.464199
O	-2.092892	-2.568233	-1.186478
S	0.878824	-3.354701	1.157596
C	2.603538	-3.852973	1.185888
C	3.481059	-3.405050	0.213985
C	4.810865	-3.797514	0.302580
C	5.232360	-4.611978	1.343327
C	4.332453	-5.043507	2.311085
C	3.003207	-4.660007	2.242684
C	0.062483	-4.872381	0.715112
C	0.447083	-5.597535	-0.407993
C	-0.281057	-6.727058	-0.736590
C	-1.362979	-7.117313	0.049155
C	-1.730276	-6.381344	1.165397
C	-1.019557	-5.237804	1.504370
H	-4.268760	-3.777754	0.086473
H	-5.226945	-5.906058	-0.812463
H	-4.271846	-6.964942	-2.815615
H	-2.322893	-5.938513	-3.998927
H	1.294672	-5.283439	-1.010549
H	-0.006703	-7.308813	-1.610743
H	-1.929623	-8.003149	-0.221037
H	-2.580139	-6.685212	1.767727
H	-1.304619	-4.639875	2.365369
H	2.291602	-4.990124	2.995589
H	4.666980	-5.677516	3.125534
H	6.273417	-4.912671	1.404106
H	5.517370	-3.460831	-0.448961
H	3.139128	-2.770753	-0.596749

Im12 (**Ph2S=O**)

Mo	-6.243025	2.062899	1.849569
Cl	-4.370877	3.545992	1.712603
Cl	-5.141037	0.572486	0.230250
O	-7.383449	2.824562	0.958408
O	-6.627016	2.822588	3.813662
S	-6.011923	4.132536	4.427975
C	-6.753704	5.479253	3.505447
C	-6.950844	4.290375	5.953776
C	-8.100996	5.441570	3.173830
C	-8.626575	6.490419	2.438340
C	-7.813344	7.553195	2.057816
C	-6.469906	7.575108	2.404158
C	-5.924553	6.524457	3.129067
H	-4.869287	6.514563	3.387003
H	-5.839078	8.402863	2.097794
H	-8.234034	8.370161	1.479995
H	-9.675512	6.480118	2.160619
H	-8.723697	4.606397	3.481645
C	-6.559627	5.306756	6.815098
C	-7.260877	5.481163	7.997150
C	-8.322856	4.639285	8.305869
C	-8.688261	3.621429	7.435995
C	-7.999330	3.435064	6.244207
H	-8.265035	2.642114	5.553737
H	-9.514807	2.963460	7.684539
H	-8.867266	4.777497	9.234743
H	-6.973310	6.273163	8.680982
H	-5.725949	5.958959	6.564814

TS13 (**Ph2S=O**)

Mo	-6.735333	2.079471	1.960769
Cl	-4.917652	3.493602	1.498406
Cl	-5.841575	0.365336	0.420649
O	-7.969152	2.770905	1.123458
O	-6.915022	2.796309	3.711302
S	-6.000384	4.257125	4.457280
C	-6.599868	5.646029	3.538225
C	-7.012054	4.294812	5.929411
C	-7.950158	5.770297	3.227948
C	-8.354308	6.843084	2.449606
C	-7.422442	7.767406	1.992373
C	-6.076791	7.628659	2.309335
C	-5.654872	6.559529	3.081883
H	-4.603398	6.427099	3.320946
H	-5.351505	8.350102	1.947772
H	-7.747587	8.601877	1.378982
H	-9.402971	6.954761	2.193753
H	-8.670039	5.042259	3.589564
C	-7.390511	5.513139	6.484454
C	-8.075046	5.518011	7.689740
C	-8.367278	4.323244	8.334038
C	-7.973274	3.115396	7.774710
C	-7.285199	3.091317	6.570220
H	-6.979033	2.150638	6.126762
H	-8.201142	2.181146	8.278066
H	-8.903309	4.334400	9.277821
H	-8.378717	6.464099	8.126365
H	-7.157554	6.448381	5.985256

HOBcat

C	1.231238	0.000000	-0.619816
C	0.031418	0.000000	0.082979
C	-0.003298	0.000000	1.456980
C	1.226915	0.000000	2.115775
C	2.425143	0.000000	1.413008
C	2.448649	0.000000	0.017550
O	-1.014593	0.000000	-0.798034
B	-0.421837	0.000000	-2.047239
O	0.964874	0.000000	-1.963945
H	-0.945582	0.000000	1.992877
H	1.245909	0.000000	3.200607
H	3.363647	0.000000	1.957562
H	3.375735	0.000000	-0.544438
O	-1.125867	0.000000	-3.187704
H	-0.571038	0.000000	-3.968845

Ph_2S

C	2.834137	-1.410645	1.879719
C	1.678858	-0.827893	2.397404
C	1.772735	0.172264	3.359057
C	3.022316	0.587514	3.803909
C	4.173498	0.020049	3.278515
C	4.076402	-0.975948	2.312622
S	0.059463	-1.399171	1.892908
C	0.142444	-1.181365	0.118853
C	-0.423771	-2.160020	-0.692407
C	-0.439826	-1.991634	-2.071050
C	0.123394	-0.860792	-2.644053
C	0.694018	0.111819	-1.830932
C	0.695490	-0.037551	-0.453157
H	-0.845687	-3.056094	-0.245562
H	-0.882981	-2.759172	-2.698704
H	0.120003	-0.736078	-3.722512
H	1.132305	1.001934	-2.272846
H	1.128993	0.732267	0.179473
H	0.869625	0.629084	3.753715
H	3.091819	1.368352	4.555416
H	5.149028	0.352642	3.619925
H	4.975819	-1.425821	1.902617
H	2.756740	-2.199398	1.136246