Supporting Information

Mechanistic insights into B-H bond activation with the high-valent oxo-molybdenum complex MoO_2Cl_2

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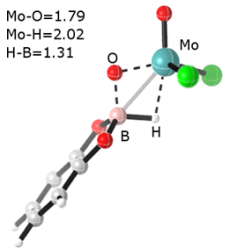
1. Complete reference of **27**.
2. **Figure S1**. The optimized structure of the isomer of the [2+2] addition transition state with higher free energy barrier.
3. **Table S1** The relative free energies of the key transition states obtained at M06(6-311++G(d,p)+ LANL2DZ), M06(6-311++G(d,p)+ SDD) calculation level for MoO_2Cl_2 mediated the hydrosilylation reaction are shown.
4. **Table S2**. Cartesian coordinates for all optimized structures in XYZ format.

Complete reference of 27

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.

Figure S1. The other optimized structure of the [2+2] transition state addition with higher free energy barrier.



TS[2+2]-ISO2

(which is 0.7 kcal/mol higher than TS[2+2] shown in the main text with the hydride coordinating at the equatorial plane).

Table S1 The relative free energies of the key transition states obtained at M06(6-311++G(d,p)+ LANL2DZ), M06(6-311++G(d,p)+ SDD) calculation level for MoO_2Cl_2 mediated the hydrosilylation reaction are shown.

	M06 *6-311G(d,p) +Lan2LDZ*	M06 *6-311G(d,p) +SDD*
TS22	26.1	25.6
Int22	-2.5	-1.9

These results have indicated that for the dependence on the basis set (for Mo atom, the triple-ζ SDD basis set with Stuttgart-Dresden ECP and Lan2LDZ basis set) is insignificant.

Table S2. Cartesian coordinates for each structure calculated. (XYZ format).

Optimized under solvent conditions

1

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

TS[2+2]

Cl	-0.640667	-1.668931	-0.267244
Mo	1.531516	-1.097921	-0.088199
O	2.027448	-1.402313	1.551945
B	3.697776	-1.040103	1.246272
O	4.014056	0.103259	1.991638
C	4.821333	-0.357143	2.983731
C	5.077593	-1.716809	2.789520
C	5.875559	-2.435645	3.652313
C	6.417946	-1.737598	4.728552
C	6.165928	-0.379386	4.919643
C	5.357061	0.340543	4.044207
O	1.564817	0.536789	-0.363622
Cl	2.244034	-2.380560	-1.856045
O	4.445393	-2.147573	1.665069
H	3.575992	-0.887685	0.010893
H	6.066069	-3.491557	3.495006
H	7.051910	-2.264249	5.434684
H	6.608717	0.128780	5.770239
H	5.153088	1.396716	4.181926

3

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

4 (Ph_2CO)

Mo	-0.400028	3.771663	0.278995
O	0.410360	5.201704	0.348496
Cl	-0.485011	3.261072	-2.014500
Cl	1.536989	2.331950	0.307143
H	-0.056715	3.254251	1.822385
O	-2.056475	4.234928	1.043094
B	-2.965520	3.480328	1.717289
O	-2.763643	2.965682	2.980545
O	-4.195148	3.135903	1.194955
C	-3.884277	2.215065	3.227085
C	-4.750843	2.315444	2.144938
O	-1.563892	1.744533	0.429640
C	-2.046986	0.606425	0.471776
C	-2.792204	0.105056	-0.693235
C	-3.433562	1.032561	-1.520834
C	-2.817181	-1.252375	-1.025233
C	-1.897549	-0.190226	1.699293
C	-2.865899	-1.117810	2.095609
C	-2.736616	-1.778136	3.306644
C	-1.637875	-1.531210	4.118915
C	-0.672641	-0.606253	3.733040
C	-0.808516	0.073539	2.537211
C	-4.112761	0.604507	-2.646315
C	-4.131025	-0.747372	-2.972513
C	-3.476816	-1.671884	-2.168898
C	-4.175705	1.441407	4.325710
C	-5.390711	0.755744	4.296954
C	-6.256350	0.853188	3.212109
C	-5.949953	1.643446	2.103197
H	-3.488734	1.365696	5.161919
H	-5.663350	0.130211	5.141084
H	-7.192284	0.303927	3.226221
H	-6.616138	1.727054	1.251331
H	-3.741235	-1.291927	1.477714
H	-3.500784	-2.481817	3.620949
H	-1.534948	-2.057164	5.063297
H	0.184057	-0.414471	4.370894
H	-0.066731	0.804066	2.228206
H	-2.289361	-1.973851	-0.409734
H	-3.477651	-2.723543	-2.436256
H	-4.654985	-1.081180	-3.863019
H	-4.625200	1.324004	-3.276623
H	-3.406513	2.085602	-1.257986

TS5 (Ph_2CO)

Mo	-0.236109	2.836507	1.988398
O	-0.163449	2.981994	3.650452
O	-1.881042	3.759792	1.831570
Cl	0.978915	0.850995	2.070165
C	-3.605812	1.558099	-0.760622
O	-0.136056	2.633291	-0.206811
C	-2.457337	3.612646	-1.278469
B	-3.213654	3.565323	1.918648
O	-3.788816	2.377430	2.339344
H	-1.387969	1.652487	1.178586
Cl	1.396576	4.355627	1.480023
C	-1.123936	1.795356	-0.235402
C	-0.801730	0.350365	-0.495922
C	-1.438373	-0.698498	0.162431
C	-1.107422	-2.009564	-0.138013
C	-0.143145	-2.280222	-1.101232
C	0.498922	-1.235591	-1.751811
C	0.178407	0.078684	-1.445528
C	-4.779320	2.090004	-1.270258
C	-4.790715	3.374460	-1.800739
C	-3.626494	4.131219	-1.809654
C	-2.434523	2.319847	-0.751559
O	-4.152173	4.521374	1.598442
C	-5.355528	3.884268	1.754714

C	-6.617254	4.364609	1.495407
C	-7.674002	3.476168	1.698131
C	-7.455739	2.175762	2.141299
C	-6.169688	1.700679	2.402908
C	-5.137567	2.585801	2.199360
H	-5.987854	0.687484	2.744501
H	-8.302967	1.513297	2.286797
H	-8.688406	3.809284	1.503568
H	-6.774304	5.377879	1.142072
H	-3.611506	0.549220	-0.361220
H	-5.689721	1.498242	-1.254745
H	-5.710770	3.786159	-2.204715
H	-3.630188	5.134430	-2.223875
H	-1.546241	4.201356	-1.265435
H	-2.158855	-0.487295	0.949963
H	-1.594732	-2.823355	0.389623
H	0.116213	-3.307915	-1.336208
H	1.260558	-1.443212	-2.497015
H	0.688715	0.901442	-1.936284

5 (Ph_2CO)

Mo	3.499626	3.664810	-1.468559
O	4.194548	2.737026	-0.304036
Cl	2.404617	2.047313	-2.784454
O	3.884588	5.387157	-0.906148
C	3.398393	6.683938	-1.221453
C	3.563910	6.918244	-2.704386
C	4.077639	7.719062	-0.362959
Cl	1.332114	4.094625	-0.622896
O	4.795569	3.725607	-2.854536
B	4.948292	3.912856	-4.179761
O	6.180025	4.084236	-4.785177
O	3.911372	3.936761	-5.094784
C	4.516359	4.164589	-6.298621
C	5.890778	4.262245	-6.109410
C	6.751724	4.530420	-7.148866
C	6.174427	4.688321	-8.408473
C	4.799131	4.579762	-8.598764
C	3.935764	4.312423	-7.537169
C	5.211587	7.439544	0.388221
C	5.810634	8.444265	1.139439
C	5.281072	9.725839	1.143734
C	4.144508	10.005424	0.393561
C	3.545701	9.006457	-0.356361
C	4.845213	7.043888	-3.241998
C	5.009813	7.240050	-4.603883
C	3.897768	7.309776	-5.437481
C	2.623397	7.173174	-4.907118
C	2.455530	6.973522	-3.541050
H	2.861933	4.235599	-7.669489
H	4.388558	4.707131	-9.595283
H	6.814243	4.897755	-9.259701
H	7.821463	4.611380	-6.990287
H	2.656835	9.222323	-0.945850
H	3.722534	11.005870	0.394916
H	5.751174	10.508085	1.731853
H	6.697573	8.219860	1.724295
H	5.626595	6.436529	0.390577
H	1.458493	6.866139	-3.119008
H	1.754549	7.221619	-5.556335
H	4.031771	7.465552	-6.504479
H	6.008273	7.338444	-5.019900
H	5.712184	6.995139	-2.586521
H	2.319636	6.668167	-0.980871

TS6 (Ph_2CO)

Mo	0.340753	0.882879	-2.680479
O	1.831428	0.559882	-2.061201
Cl	0.397006	-0.386394	-4.611659
Cl	0.542085	2.864850	-3.781599
O	-0.641696	1.541844	-1.249553
B	-1.634950	0.629699	-0.814674
O	-1.518993	0.051864	0.465831
O	-2.988178	0.885101	-1.104169
O	-0.959841	-0.520242	-2.028463
C	-1.199395	-1.898132	-2.359368
C	-2.639865	-2.220615	-2.052910
C	-0.172385	-2.794108	-1.723215
C	0.178113	-3.968398	-2.385123
C	1.092045	-4.846905	-1.823969
C	1.671349	-4.554459	-0.595573
C	1.330065	-3.383042	0.065744
C	0.410026	-2.504605	-0.492701
C	-3.033867	-2.935048	-0.927363
C	-4.378898	-3.211262	-0.713178
C	-5.334422	-2.773411	-1.618415
C	-4.947465	-2.049432	-2.741079
C	-3.607128	-1.775412	-2.953931
C	-3.683772	0.357628	-0.065168
C	-2.795795	-0.159028	0.880556
C	-3.233766	-0.758992	2.039616
C	-4.614208	-0.817924	2.231067
C	-5.501055	-0.295449	1.292448
C	-5.047641	0.305889	0.119092
H	-1.084545	-1.985281	-3.447833
H	-5.729458	0.709635	-0.621939
H	-6.569005	-0.358492	1.476210
H	-5.004124	-1.276304	3.134479
H	-2.533699	-1.158240	2.765762
H	-0.272593	-4.191203	-3.350273
H	1.359448	-5.758205	-2.350444
H	2.392485	-5.237864	-0.157364
H	1.782297	-3.148796	1.024885
H	0.139202	-1.593778	0.034226
H	-3.293352	-1.211783	-3.831224
H	-5.692289	-1.705723	-3.452562
H	-6.384300	-2.994788	-1.449774
H	-4.679429	-3.771599	0.167136
H	-2.289111	-3.290303	-0.219610

7

Mo	-1.132953	0.229464	0.362122
O	-2.667477	0.171383	1.000248
O	-1.056887	1.650384	-0.500784
Cl	-0.879843	-1.541284	-1.029002
Cl	0.343461	0.287031	2.079118
H	1.595872	0.868256	-0.830931
B	2.614817	0.279419	-0.863894
O	3.668693	0.634630	-1.671250
O	2.896905	-0.832443	-0.105138
C	4.647565	-0.287038	-1.402442
C	4.178511	-1.180305	-0.450140
C	5.911622	-0.383715	-1.937220
H	4.573152	-2.912274	0.764437

C	6.702365	-1.432483	-1.470068
H	6.878046	-3.132386	-0.175472
H	7.707826	-1.550402	-1.861224
H	6.267395	0.321664	-2.680198
C	6.231857	-2.329091	-0.514660
C	4.948687	-2.219645	0.019215

7+Ph_2CO

Mo	-2.466463	0.162478	-1.219856
O	-0.898648	0.475555	-1.684248
O	-2.400282	-0.392909	0.344808
Cl	-3.731995	2.038774	-1.362036
Cl	-3.313885	-1.479203	-2.526188
H	-0.056968	-1.688810	-0.198077
B	1.048284	-1.992016	0.064307
O	2.019483	-2.239263	-0.885515
O	1.484368	-2.311585	1.336645
C	3.118703	-2.622792	-0.172366
C	2.794090	-2.668792	1.178038
C	4.376984	-2.941220	-0.630301
C	5.316183	-3.313293	0.331762
C	4.990888	-3.360603	1.683719
C	3.711424	-3.036921	2.136109
O	1.914584	0.415621	0.225774
C	1.345131	1.491818	0.295408
C	1.803298	2.620437	-0.558620
C	0.191613	1.672292	1.217767
C	2.352688	2.313484	-1.804904
C	1.770793	3.948721	-0.132601
C	2.278033	4.952685	-0.944403
C	2.799498	4.641182	-2.192835
C	2.833878	3.319911	-2.624053
C	0.097134	0.826711	2.324392
C	-0.987923	0.912406	3.179321
C	-2.005127	1.824607	2.923416
C	-1.929923	2.658223	1.816268
C	-0.832249	2.590308	0.969692
H	3.242787	3.075843	-3.599641
H	2.388720	1.274692	-2.119416
H	1.372533	4.196867	0.846885
H	2.265601	5.982605	-0.601078
H	3.184844	5.430757	-2.831139
H	4.619785	-2.900665	-1.686743
H	6.322530	-3.570990	0.016438
H	5.748264	-3.654254	2.403863
H	3.446457	-3.071517	3.187473
H	-0.780474	3.242196	0.101730
H	-2.726669	3.367067	1.612278
H	-2.860551	1.884602	3.589753
H	-1.048899	0.259124	4.044243
H	0.887467	0.103566	2.500107

TS8 (Ph_2CO)

Mo	0.138541	1.015968	0.162377
O	0.018688	0.656222	1.781072
O	1.527272	0.276480	-0.390129
Cl	0.376467	3.258769	-0.046881
Cl	-1.701958	0.346615	-0.971841
H	-0.223466	-1.834601	0.636198
B	-0.008083	-2.806670	-0.011766
O	-0.299536	-4.089324	0.512559
O	-0.233758	-2.802738	-1.405497
C	-0.408013	-4.109408	-1.736423
C	-0.450652	-4.885890	-0.578324
C	-0.550347	-4.670355	-2.985361
C	-0.642413	-6.247600	-0.626558
C	-0.741132	-6.053976	-3.044871
C	-0.786710	-6.825572	-1.891002
O	1.864555	-2.785630	-0.013642
C	1.472055	-2.543878	2.833859
C	2.693653	-2.212931	0.704521
C	1.149246	-2.154422	4.121691
C	2.370193	-1.785887	2.076180
C	1.698212	-0.994798	4.655701
C	2.578713	-0.227211	3.904052
C	2.924618	-0.624668	2.623427
C	4.044986	-1.995195	0.156175
C	4.191143	-1.841200	-1.225390
C	5.449324	-1.680902	-1.776738
C	6.573932	-1.704994	-0.958776
C	6.438796	-1.881766	0.411557
C	5.178468	-2.015715	0.972324
H	5.558019	-1.543448	-2.847866
H	3.305615	-1.839792	-1.852905
H	5.077079	-2.169637	2.042046
H	7.318378	-1.918042	1.046357
H	7.561913	-1.590728	-1.394682
H	-0.516132	-4.058412	-3.881048
H	-0.855364	-6.531412	-4.013360
H	-0.936472	-7.898164	-1.969447
H	-0.678736	-6.840295	0.281910
H	3.609895	-0.022305	2.034012
H	2.998941	0.683496	4.318631
H	1.436921	-0.686909	5.663631
H	0.465050	-2.755210	4.712282
H	1.048417	-3.450586	2.413499

8 (Ph_2CO)

C	-5.961344	3.424395	2.479638
C	-5.410049	2.164491	2.758945
C	-5.149516	1.270800	1.710839
C	-5.428676	1.638852	0.407567
C	-5.952963	2.897311	0.139536
C	-6.217223	3.790031	1.174284
C	-5.164479	1.807976	4.143176
C	-4.168252	0.831127	4.532299
O	-5.911842	2.388712	4.994790
B	-5.755081	2.737682	6.439235
O	-6.288111	1.781575	7.359671
C	-7.087557	2.491896	8.199599
C	-7.772574	2.047639	9.306436
C	-8.531211	2.991189	10.005834
C	-8.584757	4.317097	9.597737
C	-7.883535	4.759323	8.471994
C	-7.142798	3.823755	7.787448
O	-6.380928	3.999009	6.680625
O	-3.414988	4.009996	4.876845
Mo	-2.793943	3.758130	6.419348
O	-2.091134	2.245408	6.461462
Cl	-3.642566	4.549000	8.476210
Cl	-1.009404	5.240261	6.531484
H	-4.472573	2.819228	6.622423
H	-6.623699	4.771799	0.956126
H	-6.158653	4.110445	3.296781

H	-4.768778	0.277662	1.923297
H	-5.243954	0.941084	-0.402139
H	-6.163940	3.185203	-0.885874
H	-7.915090	5.793906	8.146518
H	-9.179600	5.027785	10.163318
H	-9.084366	2.678313	10.886046
H	-7.719311	1.009956	9.619054
C	-2.966016	0.716257	3.816572
C	-2.022681	-0.216494	4.200627
C	-2.273675	-1.051305	5.283144
C	-3.463727	-0.948779	5.994112
C	-4.405015	-0.004539	5.633591
H	-2.759407	1.392587	2.993302
H	-1.083002	-0.286938	3.663250
H	-1.532015	-1.787243	5.577996
H	-3.655756	-1.608471	6.833436
H	-5.338008	0.069490	6.181818

TS9 (Ph_2CO)

Mo	-0.210906	0.036328	-0.034328
O	0.012326	-0.012177	1.622209
Cl	1.717606	0.816629	-1.166670
Cl	-1.083434	2.347901	-0.313709
O	-0.209138	-1.578568	-0.561306
H	-1.929551	-0.067075	-0.243548
B	-2.792298	-0.474396	-1.732771
O	-3.831975	0.431912	-1.684676
O	-1.834477	-0.128185	-2.679341
C	-2.252729	1.091053	-3.152516
C	-3.458285	1.429820	-2.553182
O	-2.987605	-1.846329	-1.457646
C	-2.889507	-2.624113	-0.430616
C	-1.951050	-4.312409	-1.938133
C	-3.090532	-2.112696	0.900935
C	-1.621961	1.917555	-4.050069
C	-2.263514	3.122832	-4.335671
C	-3.472563	3.462231	-3.737431
C	-4.099508	2.614001	-2.823781
C	-2.599276	-3.999297	-0.729971
C	-2.976352	-5.029686	0.147865
C	-2.700849	-6.342962	-0.177395
C	-2.041412	-6.639087	-1.364900
C	-1.665713	-5.625211	-2.243068
C	-2.321220	-2.609079	1.966772
C	-2.441466	-2.042955	3.220481
C	-3.341450	-1.004859	3.431567
C	-4.123555	-0.520934	2.387141
C	-3.991835	-1.057465	1.123548
H	-1.146629	-5.867639	-3.163859
H	-1.651915	-3.512146	-2.606300
H	-3.519869	-4.797760	1.057465
H	-3.006177	-7.141521	0.489764
H	-1.821506	-7.672751	-1.613537
H	-0.671072	1.647175	-4.496269
H	-1.803870	3.812646	-5.036201
H	-3.939303	4.410980	-3.982335
H	-5.035852	2.874435	-2.342973
H	-1.584216	-3.385185	1.788264
H	-1.819883	-2.399735	4.034300
H	-3.431184	-0.563545	4.419203
H	-4.831734	0.281312	2.562125
H	-4.607319	-0.684577	0.312180

9 (Ph_2CO)

Mo	0.226975	0.281061	-0.379037
Cl	1.134911	1.407896	1.551486
O	1.631120	0.102193	-1.321409
O	-0.327319	-1.232032	0.089345
Cl	-1.541545	2.006298	-0.146800
H	-0.653663	0.378271	-1.832157
B	0.606568	1.271782	-3.985874
O	0.861579	2.447792	-3.337969
O	-0.651853	1.196383	-4.510731
C	-0.327021	3.137368	-3.414806
C	-1.247184	2.380580	-4.124454
O	1.638471	0.373952	-4.213415
C	1.957738	-0.837795	-3.864795
C	4.251236	-0.025564	-3.589947
H	6.289679	0.565847	-3.342630
C	0.949262	-1.823997	-3.591447
C	-0.280302	-1.798440	-4.269600
C	-1.254857	-2.723778	-3.957454
C	3.368139	-1.096480	-3.818800
C	3.878133	-2.389986	-4.024951
C	-0.639539	4.367880	-2.889834
C	-2.534564	2.806856	-4.345756
C	-1.941220	4.814474	-3.106624
C	-2.865986	4.053185	-3.816093
C	5.241938	-2.602673	-3.992818
C	6.103486	-1.539916	-3.745792
C	5.608678	-0.253811	-3.542999
C	-1.029402	-3.657603	-2.951023
C	0.182424	-3.688465	-2.270287
C	1.177522	-2.789638	-2.593805
H	3.852581	0.967029	-3.410485
H	3.206598	-3.209757	-4.256065
H	5.638243	-3.596383	-4.170093
H	7.174611	-1.713391	-3.714825
H	0.085620	4.943687	-2.325970
H	-2.241411	5.777771	-2.707120
H	-3.871895	4.434904	-3.957717
H	-3.248620	2.201668	-4.892617
H	2.105681	-2.778623	-2.032637
H	0.342218	-4.405601	-1.472795
H	-1.809002	-4.367344	-2.692444
H	-2.196711	-2.718712	-4.494887
H	-0.451689	-1.080826	-5.063162

10 (Ph_2CO)

Mo	0.233334	0.823402	-0.181521
O	0.332818	0.190908	1.370719
O	1.380366	2.048905	-0.366986
Cl	-1.836988	2.053223	-0.297642
Cl	-1.000449	-0.694516	-1.780654
H	1.313382	-0.278960	-0.895011
B	0.553220	0.618566	-3.957658
O	0.156991	1.812556	-3.416778
O	-0.278460	0.151556	-4.933748
C	-1.046798	2.069755	-4.031179
C	-1.311197	1.066275	-4.952688
O	1.827826	0.147579	-3.664748
C	2.380332	-0.906213	-3.140257
C	1.834025	-3.047597	-2.067543
C	1.719552	-2.181203	-3.168997

C	0.930288	-2.550255	-4.270385
C	0.287466	-3.770343	-4.272707
C	0.391608	-4.613542	-3.170702
C	1.156506	-4.249607	-2.068073
C	-2.446021	1.060937	-5.727347
C	-3.324794	2.126417	-5.536656
C	-3.058515	3.134649	-4.614924
C	-1.902490	3.126821	-3.835987
C	3.677221	-0.687844	-2.567017
C	4.034183	0.605518	-2.139308
C	5.267338	0.821400	-1.565396
C	6.166967	-0.234191	-1.432745
C	5.837314	-1.509633	-1.877371
C	4.598601	-1.743078	-2.439321
H	5.532861	1.811175	-1.210616
H	3.318575	1.416498	-2.222804
H	4.355745	-2.728199	-2.822082
H	6.554012	-2.318888	-1.791701
H	7.138858	-0.056928	-0.982572
H	-1.685732	3.905116	-3.113140
H	-3.768484	3.946555	-4.495275
H	-4.238705	2.167096	-6.120366
H	-2.643545	0.268437	-6.440396
H	2.396719	-2.737449	-1.193363
H	1.214509	-4.902628	-1.204250
H	-0.134692	-5.562908	-3.170095
H	-0.302063	-4.068381	-5.132756
H	0.857684	-1.897174	-5.132219

TS11 (Ph_2CO)

Mo	-0.230691	0.344012	-0.225091
O	-0.579653	0.535160	1.399331
Cl	2.125679	0.099436	-0.458691
Cl	0.130710	2.677816	-1.046602
O	-0.768308	-1.195095	-0.664437
H	-1.765903	0.927492	-0.849181
B	-1.316637	1.277849	-3.509286
O	-0.299416	0.427645	-3.132534
O	-0.976240	2.113775	-4.531792
O	-2.598814	1.166405	-3.030364
C	0.753985	0.785807	-3.954538
C	0.338628	1.802874	-4.800715
C	-3.158617	1.390218	-1.852195
C	-3.179549	5.374303	-0.451975
C	-3.317528	3.023445	0.009690
C	-4.065203	0.350668	-1.404834
C	2.023881	0.264894	-4.001859
C	1.170337	2.356034	-5.744112
C	2.879630	0.818915	-4.953646
C	2.464182	1.839913	-5.802438
C	-3.026346	5.116072	-1.807347
C	-3.004700	3.810596	-2.263126
C	-3.167112	2.753431	-1.359065
C	-3.320313	4.327712	0.456054
C	-5.208602	0.652213	-0.651547
C	-6.063703	-0.362381	-0.262554
C	-5.787033	-1.677461	-0.612419
C	-4.658817	-1.984968	-1.368996
C	-3.806216	-0.979788	-1.772172
H	-4.446582	-3.014291	-1.637041
H	-2.914569	-1.217257	-2.343080
H	-5.447140	1.681831	-0.409821
H	-6.955746	-0.125528	0.307340
H	-6.458146	-2.471381	-0.299720
H	2.337883	-0.525719	-3.329817
H	3.895065	0.443900	-5.029334
H	3.161501	2.245540	-6.528305
H	0.833131	3.150292	-6.400555
H	-3.373295	2.202744	0.719054
H	-3.413498	4.535411	1.516516
H	-3.179741	6.399543	-0.095260
H	-2.918226	5.934628	-2.510652
H	-2.898330	3.607687	-3.323595

$Ph_2CHOBcat$

C	0.299295	-1.890004	0.384187
C	1.013885	-0.926850	-0.318691
C	0.647691	0.419993	-0.286014
C	-0.451949	0.741448	0.474676
C	-1.165969	-0.222371	1.177738
C	-0.815458	-1.551475	1.153746
O	-1.020641	1.968684	0.676766
B	-2.095764	1.724353	1.517240
O	-2.203100	0.378540	1.841225
O	-2.918190	2.696697	1.928622
H	1.198209	1.179654	-0.830364
H	1.875557	-1.225875	-0.907061
H	0.612480	-2.928080	0.335825
H	-1.380634	-2.293972	1.706647
C	-3.971634	2.405457	2.849080
C	-3.424779	2.334487	4.256183
C	-5.048497	3.453801	2.715746
C	-3.624435	1.200751	5.034375
C	-3.131219	1.143715	6.332414
C	-2.425926	2.218065	6.853591
C	-2.216850	3.352159	6.075905
C	-2.717675	3.412491	4.785574
H	-4.165449	0.354189	4.617460
H	-3.292928	0.254168	6.933912
H	-2.035712	2.173824	7.866038
H	-1.664283	4.194500	6.481536
H	-2.561111	4.302336	4.180432
C	-6.291717	3.203017	3.293134
C	-7.305031	4.144933	3.218247
C	-7.086323	5.351710	2.563533
C	-5.850882	5.604797	1.986629
C	-4.833714	4.660038	2.060381
H	-6.462714	2.257494	3.804534
H	-8.271179	3.936237	3.667992
H	-7.879923	6.090240	2.501648
H	-5.673792	6.544065	1.470741
H	-3.871638	4.856165	1.599077
H	-4.408515	1.428419	2.597257

TS8 (PhCHO)

Mo	0.936842	0.030807	-0.777761
O	1.111601	0.136700	0.874552
Cl	2.949462	-0.456132	-1.689924
O	-0.098902	-1.238928	-1.058921
Cl	0.132662	1.973144	-1.632872
H	-1.643723	0.558753	0.606462
B	-2.608592	0.868823	-0.009980
O	-3.251865	2.092531	0.192891
O	-2.855302	0.386202	-1.300012

O	-3.842707	-0.364545	1.053456
C	-3.323375	-1.192065	1.783412
C	-4.062796	-2.153520	2.585957
C	-5.459257	-2.203832	2.539057
C	-6.134940	-3.128014	3.311467
C	-5.423143	-3.999969	4.132679
C	-4.035943	-3.952076	4.184648
C	-3.354066	-3.028724	3.409699
C	-3.790237	1.232622	-1.815642
C	-4.031897	2.263770	-0.911555
C	-4.933911	3.267627	-1.181506
C	-5.597598	3.207030	-2.408950
C	-5.352597	2.180476	-3.313204
C	-4.434675	1.166609	-3.029874
H	-2.217643	-1.243591	1.866807
H	-7.218565	-3.176491	3.280449
H	-5.994051	-1.514718	1.892701
H	-2.268668	-2.974502	3.435165
H	-3.490712	-4.634320	4.828413
H	-5.958804	-4.723872	4.739523
H	-4.236073	0.360370	-3.728420
H	-5.884935	2.162870	-4.259302
H	-6.319196	3.978720	-2.659098
H	-5.115966	4.065735	-0.469371

8 (PhCHO)

Mo	-5.956273	3.890976	2.471388
O	-6.142547	2.271955	2.089925
Cl	-6.086815	4.972036	0.435323
O	-4.376910	4.136145	2.972763
Cl	-7.659396	5.220400	3.400430
H	-6.158254	3.212644	4.293805
B	-6.761790	2.537168	5.193282
O	-8.061773	2.120453	4.803974
O	-6.847081	3.298710	6.393120
C	-8.905647	2.678102	5.711500
C	-8.175989	3.386959	6.666572
C	-10.278710	2.617098	5.750646
O	-5.844941	1.324572	5.370430
C	-4.607794	1.365514	5.171376
C	-3.751265	0.266461	5.437018
C	-3.360499	-1.975151	6.200745
C	-4.238814	-0.941380	5.967397
C	-2.004944	-1.815249	5.908675
C	-1.515607	-0.624264	5.383758
C	-2.386196	0.420497	5.147464
C	-8.793280	4.054684	7.698310
C	-10.189388	3.994547	7.748799
C	-10.915173	3.292316	6.796708
H	-4.158261	2.285837	4.772837
H	-3.718531	-2.913340	6.610195
H	-5.296001	-1.045954	6.187405
H	-2.031873	1.362245	4.738001
H	-0.459473	-0.518512	5.162659
H	-1.320625	-2.637035	6.096000
H	-10.836028	2.069495	4.997688
H	-11.998697	3.267169	6.860533
H	-10.712479	4.510675	8.547933
H	-8.215945	4.604769	8.434188

TS9 (PhCHO)

Mo	-0.658403	-0.446893	-0.054849
O	-1.462224	-0.693766	1.421585
Cl	1.332746	0.616791	0.681918
O	-0.268478	-1.937877	-0.700433
Cl	-0.691089	1.258940	-1.803403
H	-2.275704	-0.377553	-0.705566
B	-3.882365	0.070029	-0.405712
O	-3.729876	1.339169	0.119581
O	-4.358788	0.066814	-1.697940
O	-4.145518	-1.057870	0.424850
C	-4.001089	-1.035438	1.694252
C	-4.130707	-2.211213	2.457284
C	-4.387516	-3.457830	1.853005
C	-4.494485	-4.576912	2.644656
C	-4.344050	-4.465102	4.028373
C	-4.087326	-3.238080	4.633178
C	-3.980029	-2.107347	3.852432
C	-4.358325	1.394848	-2.046805
C	-3.982872	2.164522	-0.951829
C	-3.886245	3.532629	-1.016877
C	-4.187227	4.116264	-2.247776
C	-4.561374	3.347764	-3.344779
C	-4.655327	1.958243	-3.264634
H	-3.824861	-0.076978	2.187703
H	-4.690282	-5.545433	2.198464
H	-4.496974	-3.524636	0.775895
H	-3.775512	-1.136945	4.295169
H	-3.970323	-3.174735	5.708909
H	-4.426352	-5.355298	4.644279
H	-4.939138	1.348538	-4.115216
H	-4.784410	3.837740	-4.287069
H	-4.122467	5.194613	-2.350015
H	-3.582980	4.120493	-0.157694

10 (PhCHO)

C	0.240424	0.995867	0.096179
C	0.440200	0.686486	1.419806
C	1.245968	1.455343	2.248658
C	1.894412	2.580138	1.799219
C	1.698508	2.907743	0.458676
C	0.891834	2.135615	-0.372349
O	1.256909	0.902158	3.512966
B	0.414663	-0.158881	3.394629
O	-0.073111	-0.372562	2.142308
O	0.181890	-1.003368	4.487757
C	-0.917667	-1.658193	4.627286
H	-1.616343	-1.699932	3.787945
C	-1.211532	-2.323080	5.820265
C	-0.356675	-2.247546	6.943774
C	-0.712232	-2.901545	8.097743
C	-1.905078	-3.627943	8.144513
C	-2.755650	-3.707580	7.043989
C	-2.416768	-3.054204	5.881276
Cl	-1.939143	1.269321	4.356718
Mo	-0.477256	2.200505	6.236135
Cl	-0.143592	3.924895	4.593715
O	-1.336094	2.899243	7.498754
O	1.094051	1.856718	6.741419
H	-0.969087	0.610180	6.563594
H	-0.074273	-2.852344	8.972718
H	0.560901	-1.671292	6.888111
H	-3.060179	-3.089519	5.007291
H	-3.676715	-4.275220	7.107774

H	-2.177085	-4.138553	9.063311
H	2.517363	3.176006	2.456195
H	2.184866	3.790334	0.056282
H	0.762857	2.427525	-1.409536
H	-0.392430	0.387449	-0.539834

TS11 (PhCHO)

Mo	-0.608201	-0.364754	0.294162
O	-1.065777	-0.841846	1.833747
O	0.956540	-0.903083	-0.020578
Cl	-0.305888	1.991851	0.280858
Cl	-2.518181	0.144969	-1.195840
H	-1.135470	-1.840616	-0.498451
B	-0.750641	-0.879851	-3.474517
O	-0.062281	0.294511	-3.505324
O	-1.856807	-0.916433	-4.269676
C	-0.832840	1.093573	-4.321890
C	-1.918072	0.361843	-4.786568
O	-0.258676	-1.972892	-2.764238
C	-0.980157	-2.781645	-2.050107
C	-0.407814	-3.980017	-1.548738
C	-1.266661	-4.903777	-0.929968
C	0.966271	-4.248222	-1.667750
C	-0.757022	-6.089937	-0.447352
C	0.604939	-6.351856	-0.570263
C	1.463305	-5.435877	-1.177354
C	-0.637588	2.410054	-4.662425
C	-1.591188	2.973978	-5.509128
C	-2.675884	2.239687	-5.978197
C	-2.864271	0.904743	-5.621575
H	-2.066425	-2.657861	-2.060517
H	2.521119	-5.658943	-1.261901
H	1.621557	-3.526619	-2.143410
H	-2.323784	-4.669605	-0.839796
H	-1.410092	-6.813422	0.027642
H	1.006247	-7.284751	-0.186443
H	0.208439	2.973328	-4.285256
H	-1.484047	4.012493	-5.804927
H	-3.397740	2.716681	-6.633122
H	-3.709299	0.324886	-5.975250

TS8 ($PhCOCH_3$)

Mo	0.494864	1.183836	-0.779168
O	1.312279	1.643566	0.615361
O	0.687027	2.354523	-1.970203
Cl	1.665397	-0.736002	-1.572883
Cl	-1.450786	-0.346502	-0.765276
H	-0.906539	2.013392	-0.195257
O	-2.852916	1.974082	1.091636
B	-3.699655	0.974305	0.639977
O	-3.938774	-0.101068	1.450632
O	-4.472174	0.996301	-0.490149
C	-4.848764	-0.849460	0.745840
C	-5.173204	-0.188265	-0.431206
C	-2.279565	2.965245	0.459462
C	-1.468293	3.824317	1.292013
C	-1.257183	3.488263	2.639069
C	-0.456279	4.283711	3.431950
C	0.149571	5.414531	2.894239
C	-0.847167	4.963663	0.757850
C	-0.047476	5.752669	1.559672
C	-6.066023	-0.702352	-1.340664
C	-6.632939	-1.934700	-1.017311
C	-6.308847	-2.598502	0.161872
C	-5.401607	-2.064316	1.075970
C	-2.753922	3.340963	-0.887627
H	-0.294835	4.021089	4.471775
H	-1.719857	2.599404	3.051859
H	-0.978355	5.230383	-0.284578
H	0.432433	6.631726	1.143750
H	0.785815	6.034080	3.518451
H	-5.139126	-2.574732	1.995773
H	-6.769893	-3.557280	0.376452
H	-7.342252	-2.384925	-1.704206
H	-6.308827	-0.176660	-2.257220
H	-2.959274	2.463800	-1.502116
H	-3.699866	3.887335	-0.757886
H	-2.051402	3.992072	-1.404553

8 ($PhCOCH_3$)

Mo	-6.216117	3.203105	2.155127
O	-6.577833	1.570885	2.181809
Cl	-6.365391	3.786472	-0.084220
O	-4.591848	3.401929	2.527455
Cl	-7.825373	4.838562	2.734701
H	-6.383120	3.130765	4.062113
B	-6.715513	2.566396	5.178148
O	-7.994031	1.949892	5.079880
O	-6.756778	3.562924	6.200175
C	-8.794305	2.635238	5.934671
C	-8.054292	3.607172	6.607152
C	-10.140609	2.467941	6.164291
O	-5.642526	1.527584	5.330008
C	-4.402976	1.704085	5.534552
C	-3.576312	0.520279	5.512429
C	-3.357410	-1.836350	5.041738
C	-4.132945	-0.697381	5.081816
C	-2.024773	-1.782816	5.440883
C	-1.465242	-0.588049	5.877268
C	-2.230256	0.561272	5.907640
C	-8.631141	4.446288	7.531906
C	-9.997944	4.281726	7.773135
C	-10.735796	3.313926	7.104058
C	-3.880394	3.060978	5.772564
H	-3.785718	-2.771412	4.697532
H	-5.170379	-0.727739	4.767848
H	-1.779887	1.483897	6.254074
H	-0.427440	-0.554138	6.190113
H	-1.417138	-2.681866	5.409199
H	-10.708114	1.711293	5.632665
H	-11.796456	3.211621	7.311406
H	-10.489081	4.925589	8.496118
H	-8.045825	5.201520	8.046121
H	-2.796556	3.104299	5.827698
H	-4.217518	3.725142	4.968546
H	-4.318232	3.452327	6.697429

TS9 ($PhCOCH_3$)

Mo	0.148728	0.363934	0.239691
O	-0.840922	-0.058156	1.522776
O	1.760504	0.426880	0.754401
Cl	0.177753	-1.492954	-1.256177
Cl	-0.923202	1.546360	-1.607214
H	0.103429	2.062729	0.624248

B	0.540365	3.606354	1.222528
O	-0.513606	3.805976	2.093235
O	0.413410	4.328078	0.050810
O	1.777840	3.208647	1.788680
C	2.888629	2.882675	1.227593
C	3.081132	3.066644	-0.217479
C	3.916219	2.414213	2.110006
C	3.608149	2.150759	3.457458
C	5.225966	2.208807	1.643503
C	6.202107	1.762182	2.510008
C	5.883021	1.499960	3.838190
C	4.587408	1.691735	4.310527
C	-1.418279	4.519038	1.351778
C	-0.860262	4.837987	0.119287
C	-1.547127	5.551028	-0.833951
C	-2.840994	5.947221	-0.497903
C	-3.400923	5.631262	0.736158
C	-2.694309	4.903869	1.693146
H	4.347988	1.476803	5.346062
H	2.595863	2.293552	3.816972
H	5.482172	2.411511	0.609819
H	7.214583	1.611378	2.152358
H	6.652487	1.137375	4.512747
H	-3.123223	4.645879	2.655022
H	-4.413178	5.952639	0.959751
H	-3.425016	6.510096	-1.218910
H	-1.102640	5.783358	-1.795350
H	3.819248	2.375667	-0.620973
H	2.144627	2.975843	-0.768481
H	3.445820	4.092721	-0.375389

10 ($PhCOCH_3$)

Mo	0.331990	1.147359	0.027898
O	0.387493	0.688604	1.643064
O	1.401097	2.423473	-0.245028
Cl	-1.813595	2.185380	-0.307627
Cl	-0.701092	-0.578446	-1.528385
H	1.496127	0.030344	-0.503383
O	1.812551	0.490621	-3.278532
B	0.536346	0.839211	-3.726985
O	-0.187082	0.206792	-4.695584
O	0.006574	2.026576	-3.312003
C	-1.186309	2.103801	-3.994342
C	-1.307160	1.002873	-4.830668
C	2.406040	-0.652749	-3.180538
C	3.695165	-0.628507	-2.571529
C	4.208081	0.574166	-2.044009
C	1.779104	-1.884952	-3.675912
C	5.444683	0.583734	-1.438446
C	6.184112	-0.593483	-1.354241
C	5.691163	-1.787344	-1.874478
C	4.452799	-1.811548	-2.476823
C	-2.152489	3.079782	-3.930691
C	-3.264984	2.898840	-4.750613
C	-3.386225	1.791662	-5.585195
C	-2.397463	0.810932	-5.644127
H	5.838283	1.504567	-1.023038
H	3.621694	1.483918	-2.103919
H	4.066068	-2.742402	-2.876565
H	6.277976	-2.696046	-1.801243
H	7.157267	-0.581533	-0.873107
H	-2.049903	3.937816	-3.276329
H	-4.057218	3.640137	-4.732686
H	-4.271596	1.686038	-6.203674
H	-2.479505	-0.056234	-6.289700
H	0.754600	-1.733572	-4.005751
H	2.371242	-2.261472	-4.520371
H	1.804003	-2.653467	-2.897494

TS11 ($PhCOCH_3$)

Mo	0.494864	1.183836	-0.779168
O	1.312279	1.643566	0.615361
O	0.687027	2.354523	-1.970203
Cl	1.665397	-0.736002	-1.572883
Cl	-1.450786	-0.346502	-0.765276
H	-0.906539	2.013392	-0.195257
O	-2.852916	1.974082	1.091636
B	-3.699655	0.974305	0.639977
O	-3.938774	-0.101068	1.450632
O	-4.472174	0.996301	-0.490149
C	-4.848764	-0.849460	0.745840
C	-5.173204	-0.188265	-0.431206
C	-2.279565	2.965245	0.459462
C	-1.468293	3.824317	1.292013
C	-1.257183	3.488263	2.639069
C	-0.456279	4.283711	3.431950
C	0.149571	5.414531	2.894239
C	-0.847167	4.963663	0.757850
C	-0.047476	5.752669	1.559672
C	-6.066023	-0.702352	-1.340664
C	-6.632939	-1.934700	-1.017311
C	-6.308847	-2.598502	0.161872
C	-5.401607	-2.064316	1.075970
C	-2.753922	3.340963	-0.887627
H	-0.294835	4.021089	4.471775
H	-1.719857	2.599404	3.051859
H	-0.978355	5.230383	-0.284578
H	0.432433	6.631726	1.143750
H	0.785815	6.034080	3.518451
H	-5.139126	-2.574732	1.995773
H	-6.769893	-3.557280	0.376452
H	-7.342252	-2.384925	-1.704206
H	-6.308827	-0.176660	-2.257220
H	-2.959274	2.463800	-1.502116
H	-3.699866	3.887335	-0.757886
H	-2.051402	3.992072	-1.404553

8 ($PhCHO\text{-}OCH_3$)

C	-10.849799	3.572171	6.783260
C	-10.279565	2.802337	5.765149
C	-8.906771	2.725470	5.734328
C	-8.114186	3.391859	6.669883
C	-8.666536	4.152571	7.673932
C	-10.061659	4.231214	7.716991
O	-8.120251	2.046787	4.859065
B	-6.787927	2.363964	5.228665
O	-5.934055	1.138034	5.342794
C	-4.669139	1.214564	5.372803
C	-3.847720	0.097793	5.567123
C	-4.374379	-1.201778	5.765301
C	-3.530571	-2.257826	5.932504
C	-2.132046	-2.060354	5.902386
C	-1.595895	-0.775677	5.714112
C	-2.451618	0.284401	5.550756

O	-6.800089	3.154351	6.415505
Mo	-5.902758	3.544629	2.479682
Cl	-7.497623	5.089720	3.306142
O	-6.204440	1.924468	2.181949
Cl	-6.003099	4.521077	0.372767
O	-4.298589	3.709767	2.934682
H	-6.182480	3.053147	4.301976
H	-4.195500	2.195136	5.239183
H	-3.899485	-3.266393	6.084336
H	-5.449310	-1.347532	5.781077
H	-2.053935	1.284220	5.400916
H	-0.525053	-0.615894	5.695938
O	-1.404894	-3.151910	6.059290
H	-10.885362	2.286063	5.027704
H	-11.930719	3.655902	6.840456
H	-10.534561	4.822656	8.494966
H	-8.040527	4.666767	8.395798
C	0.017703	-3.060084	6.003804
H	0.387310	-4.077465	6.121999
H	0.344096	-2.663381	5.037640
H	0.400913	-2.436232	6.817165

TS9 (PhCHO-OCH$_3$)

Mo	0.178045	0.346602	0.525151
O	-0.099431	-0.303836	2.043343
O	1.737123	0.996246	0.465733
Cl	0.321673	-1.499335	-0.969671
Cl	-1.780156	0.991727	-0.769145
H	-0.320886	1.943799	1.063261
B	-0.065848	3.506104	1.331083
O	1.064890	3.376902	2.191046
C	2.268880	3.386292	1.738507
C	3.362415	3.133216	2.558110
C	3.226042	2.816236	3.934772
C	4.332186	2.548012	4.679481
C	5.614828	2.580677	4.083782
C	5.765698	2.890785	2.719625
C	4.649019	3.162448	1.975153
O	-1.289365	3.837001	1.895555
C	-1.992765	4.378576	0.852818
C	-3.312827	4.761905	0.820034
C	-3.786647	5.266988	-0.391407
C	-2.961797	5.376442	-1.505504
C	-1.623148	4.984450	-1.460906
C	-1.168587	4.489481	-0.262715
O	0.079922	4.009779	0.042024
O	6.616468	2.303153	4.892830
C	7.952833	2.301115	4.388278
H	2.424187	3.619252	0.682734
H	4.266680	2.300430	5.733278
H	2.239464	2.785989	4.384658
H	4.743540	3.396808	0.918753
H	6.745120	2.909431	2.258014
H	-3.950071	4.663183	1.692019
H	-4.824177	5.577362	-0.463587
H	-3.366764	5.769187	-2.432566
H	-0.973258	5.052760	-2.326447
H	8.588014	2.032773	5.230664
H	8.066725	1.557923	3.593634
H	8.230950	3.293807	4.022075

10 (PhCHO-OCH$_3$)

Mo	5.395055	-1.661775	-2.405342
Cl	3.086131	-0.864591	-3.172761
Cl	5.342595	0.468336	-1.291298
O	6.993719	-1.691885	-2.943838
O	5.185776	-2.876514	-1.266774
H	4.901222	-2.532831	-3.774948
O	4.357619	-1.169262	-6.001908
B	4.463936	0.144063	-5.558041
O	5.583874	0.558602	-4.896039
O	3.565034	1.135032	-5.824980
C	4.128668	2.248081	-5.236055
C	5.352660	1.901207	-4.681047
C	6.152276	2.814994	-4.038970
C	5.662900	4.118566	-3.970435
C	4.434873	4.466836	-4.524889
C	3.635076	3.529045	-5.176704
C	3.208839	-1.747036	-6.186152
C	3.116301	-3.110575	-6.384967
C	4.249694	-3.962096	-6.320177
C	4.112366	-5.309289	-6.487696
C	2.830959	-5.851546	-6.732881
C	1.694702	-5.015355	-6.800921
C	1.833828	-3.673843	-6.623725
O	2.601876	-7.133351	-6.908772
C	3.682669	-8.068194	-6.829046
H	4.430678	-7.862537	-7.599945
H	4.140154	-8.043797	-5.836116
H	3.239075	-9.046469	-7.004038
H	0.729975	-5.474039	-6.986299
H	0.969296	-3.017966	-6.662925
H	4.980560	-5.953720	-6.427765
H	5.228975	-3.537496	-6.125831
H	7.103550	2.528140	-3.604775
H	6.254386	4.877890	-3.469344
H	4.087759	5.492087	-4.447240
H	2.677106	3.788705	-5.612819
H	2.310564	-1.126491	-6.195646

TS11 (PhCHO-OCH$_3$)

C	-3.108839	1.580879	-4.399869
C	-2.076631	0.679641	-4.301616
C	-0.862966	0.868239	-4.950586
C	-0.619244	1.970093	-5.735123
C	-1.658958	2.893522	-5.843997
C	-2.873399	2.704313	-5.192508
O	-0.024843	-0.184095	-4.666259
B	-0.757229	-0.956513	-3.810241
O	-0.257710	-2.143815	-3.309204
C	-0.955194	-2.936712	-2.534312
C	-0.325056	-4.021195	-1.901027
C	-1.125552	-4.982324	-1.244536
C	-0.544736	-6.029734	-0.590205
C	0.858889	-6.144059	-0.557281
C	1.667265	-5.186778	-1.197283
C	1.077267	-4.138584	-1.855878
O	-2.031043	-0.501818	-3.594928
Cl	0.330141	0.199503	-1.337650
Mo	-1.217200	-0.830938	0.281092
Cl	-0.587312	1.014767	1.666161
O	-2.890080	-0.719410	0.172657
O	-0.788451	-2.190655	1.171042
H	-1.179843	-1.808897	-1.167122

H	-2.043734	-2.902094	-2.607005
H	2.747012	-5.265000	-1.168404
H	1.693733	-3.388354	-2.340553
H	-2.206632	-4.874488	-1.262181
H	-1.134079	-6.783564	-0.080062
O	1.330203	-7.186365	0.106798
H	0.332690	2.109790	-6.235090
H	-1.512655	3.782320	-6.449278
H	-3.656240	3.448269	-5.298424
H	-4.048982	1.423910	-3.883024
C	2.740330	-7.369044	0.213447
H	2.880256	-8.268179	0.811330
H	3.191638	-7.514079	-0.772985
H	3.206858	-6.518729	0.720222

8 (Ph_2CO-OCH_3)

C	-4.536492	0.051848	5.489646
C	-4.302202	0.924784	4.418287
C	-3.127342	0.796738	3.662975
C	-2.210087	-0.189609	3.972394
C	-2.459739	-1.062090	5.023952
C	-3.621706	-0.943290	5.777629
C	-5.270467	1.958876	4.091869
O	-5.936015	2.572173	4.996390
B	-5.709572	2.831582	6.444232
O	-6.255882	4.109988	6.783145
C	-7.038557	3.901213	7.868998
C	-7.048787	2.545059	8.198055
C	-7.770980	2.063848	9.264917
C	-8.502005	2.994453	10.009841
C	-8.492093	4.343718	9.684032
C	-7.751710	4.823747	8.599316
O	-6.271361	1.852345	7.324993
C	-5.552635	2.345369	2.739973
C	-6.115271	3.615816	2.487677
C	-6.397706	4.010984	1.209818
C	-6.156796	3.139902	0.132491
C	-5.627743	1.864333	0.366946
C	-5.326813	1.481921	1.655256
O	-3.304078	4.313446	5.106508
Mo	-2.708991	3.714581	6.559042
Cl	-0.868365	5.077577	6.971318
O	-2.054591	2.204855	6.281141
Cl	-3.517950	4.078141	8.753843
H	-4.418277	2.827523	6.583969
H	-6.803483	4.994176	0.996369
H	-6.291471	4.291364	3.318064
H	-4.950338	0.479668	1.830739
H	-5.466181	1.170681	-0.449215
O	-6.468273	3.610872	-1.069652
H	-7.735235	5.876663	8.337727
H	-9.068098	5.043142	10.282210
H	-9.084837	2.652304	10.859523
H	-7.768347	1.007203	9.511905
H	-2.919679	1.503305	2.865312
H	-1.290899	-0.270675	3.401868
H	-1.739875	-1.838929	5.262863
H	-3.813017	-1.629737	6.595598
H	-5.446390	0.140767	6.074006
C	-6.220395	2.800904	-2.213048
H	-6.539621	3.388857	-3.072499
H	-5.154065	2.570028	-2.306707
H	-6.800861	1.873187	-2.172932

TS9 (Ph_2CO-OCH_3)

Mo	-0.076620	0.353687	-0.077595
O	-0.104046	0.233283	1.604254
O	1.379071	-0.289803	-0.574506
Cl	-1.728913	-1.205497	-0.634410
Cl	-0.834175	1.717170	-1.941698
H	0.486736	2.076803	0.286897
B	-0.010546	3.124224	0.975539
O	0.750254	3.089794	2.229580
C	1.882030	2.564888	2.537399
C	2.122394	2.369553	3.930934
C	1.034226	2.366856	4.834060
C	1.244208	2.210654	6.174265
C	2.552955	2.076680	6.674058
C	3.645028	2.093495	5.795583
C	3.424398	2.233740	4.445302
O	-1.409529	2.933152	1.182419
C	-2.017289	3.865567	0.398568
C	-1.058512	4.674543	-0.206632
C	-1.403677	5.687458	-1.068974
C	-2.767056	5.871044	-1.315482
C	-3.723532	5.062843	-0.714924
C	-3.360787	4.035625	0.160501
O	0.186923	4.281056	0.176067
O	2.655136	1.948340	7.989888
C	3.945249	1.800209	8.573825
C	2.847843	2.211099	1.506668
C	3.013026	3.034561	0.384102
C	3.899507	2.672949	-0.612303
C	4.611334	1.482800	-0.512605
C	4.445669	0.655639	0.590731
C	3.577207	1.017869	1.604169
H	0.419766	2.186053	6.878782
H	0.024785	2.465807	4.449741
H	4.277373	2.281880	3.776806
H	4.659494	2.014028	6.166197
H	-4.098501	3.391171	0.626888
H	-4.774606	5.226536	-0.931487
H	-3.081176	6.658598	-1.993381
H	-0.647000	6.305840	-1.540116
H	3.415394	0.351531	2.445594
H	4.985104	-0.283360	0.654575
H	5.294967	1.195034	-1.305226
H	4.034764	3.319346	-1.472859
H	2.458793	3.964153	0.305428
H	3.782146	1.731629	9.648361
H	4.432871	0.885168	8.222022
H	4.578059	2.667315	8.358508

10 (Ph_2CO-OCH_3)

C	4.554853	-1.708132	-2.338398
C	3.624395	-0.656122	-2.521729
C	3.998566	0.652319	-2.141674
C	5.224766	0.905676	-1.586034
C	6.136664	-0.151361	-1.415429
C	5.785493	-1.458240	-1.801832
C	2.350275	-0.881216	-3.095696
C	1.700063	-2.169467	-3.160472
C	1.770902	-3.041187	-2.062835
C	1.108586	-4.252217	-2.103686

C	0.396447	-4.616741	-3.240235
C	0.334540	-3.765334	-4.337984
C	0.967266	-2.538809	-4.296977
O	1.773577	0.176607	-3.605579
B	0.501242	0.623546	-3.912500
O	-0.305688	0.148437	-4.908548
C	-1.347907	1.049524	-4.949661
C	-1.118462	2.054221	-4.020134
C	-1.991677	3.101270	-3.847059
C	-3.126503	3.098664	-4.656849
C	-3.357650	2.089324	-5.586324
C	-2.462313	1.033481	-5.753861
O	0.070803	1.810442	-3.374839
Cl	-1.071193	-0.694695	-1.755254
Mo	0.183930	0.805227	-0.156219
Cl	-1.836727	2.106562	-0.329030
O	0.235027	0.156637	1.391576
O	1.375056	1.995010	-0.306769
H	1.240467	-0.320122	-0.862905
H	5.475675	1.911721	-1.273117
H	3.283917	1.461702	-2.246908
H	4.309677	-2.711579	-2.668653
H	6.520674	-2.246023	-1.678811
O	7.347681	-0.010414	-0.905363
H	-1.803265	3.880275	-3.117245
H	-3.847663	3.903025	-4.554805
H	-4.255856	2.120691	-6.194504
H	-2.632135	0.239936	-6.472886
H	2.287719	-2.731853	-1.160159
H	1.135757	-4.910736	-1.242225
H	-0.119617	-5.571279	-3.269111
H	-0.214578	-4.059989	-5.225770
H	0.921554	-1.876808	-5.154045
C	7.796658	1.287039	-0.517662
H	8.807401	1.151118	-0.136532
H	7.819964	1.964277	-1.377117
H	7.163015	1.702024	0.272090

TS11 (Ph_2CO-OCH_3)

C	-3.876379	-1.072175	-1.838446
C	-4.010080	0.261778	-1.410228
C	-5.059101	0.583581	-0.523521
C	-5.923755	-0.384321	-0.089540
C	-5.774643	-1.712562	-0.520764
C	-4.738587	-2.049893	-1.404818
C	-3.087756	1.247995	-1.891216
C	-3.083796	2.649289	-1.468983
C	-3.091068	2.998731	-0.113374
C	-3.102303	4.328084	0.257587
C	-3.096846	5.322220	-0.715707
C	-3.078912	4.983916	-2.061320
C	-3.064620	3.652785	-2.442250
O	-2.537839	0.971029	-3.074810
B	-1.269123	1.202245	-3.543751
O	-0.986213	2.076216	-4.553088
C	0.365135	1.925311	-4.770682
C	0.866449	0.963154	-3.907375
C	2.191861	0.601047	-3.904444
C	3.010550	1.261736	-4.819935
C	2.508290	2.228156	-5.685271
C	1.159899	2.581276	-5.679457
O	-0.170414	0.477950	-3.130783
Mo	-0.252195	0.128840	-0.294614
O	-0.898567	-1.308373	-0.905999
O	-0.645742	0.174266	1.330872
Cl	2.089682	-0.261237	-0.474900
Cl	0.263397	2.512285	-0.830592
H	-1.725566	0.873419	-0.901777
H	-4.603445	-3.071315	-1.739930
H	-3.057621	-1.341124	-2.496602
H	-5.212624	1.609616	-0.209048
H	-6.747532	-0.148076	0.575436
O	-6.663754	-2.576121	-0.046340
H	2.574999	-0.149805	-3.222290
H	4.066424	1.013875	-4.854052
H	3.179914	2.720687	-6.380918
H	0.754675	3.332476	-6.348254
H	-3.034429	2.221941	0.644370
H	-3.089660	4.593830	1.309326
H	-3.096023	6.366776	-0.420058
H	-3.077539	5.759614	-2.819784
H	-3.075197	3.392862	-3.495507
C	-6.606669	-3.932712	-0.473627
H	-7.427299	-4.441299	0.030307
H	-6.744830	-4.008261	-1.557265
H	-5.659719	-4.399687	-0.183894

Optimized under gas phase

1

Mo	0.109824	-0.384989	0.246467
O	-0.062374	0.719808	1.475190
O	1.662329	-0.219766	-0.321355
Cl	-1.365225	0.078476	-1.412072
Cl	-0.190556	-2.482006	1.054927

TS[2+2]

Cl	-0.648563	-1.616072	-0.271164
Mo	1.531182	-1.088644	-0.096235
O	2.029285	-1.419135	1.537440
B	3.693651	-1.051169	1.249429
O	4.001721	0.093093	1.997178
C	4.811667	-0.362835	2.987690
C	5.077998	-1.720525	2.791283
C	5.885279	-2.432283	3.650704
C	6.425762	-1.732203	4.726027
C	6.162042	-0.377696	4.920566
C	5.344525	0.335845	4.048568
O	1.597261	0.544672	-0.370941
Cl	2.227328	-2.405442	-1.834133
O	4.447538	-2.154732	1.668249
H	3.585606	-0.896754	0.012862
H	6.082774	-3.485495	3.487689
H	7.067339	-2.253864	5.428531
H	6.602834	0.132372	5.770685
H	5.130343	1.389479	4.186098

3

Cl	-4.262063	-2.363754	-0.772910
Mo	-3.047115	-0.434153	-0.983782
H	-4.482922	-0.153100	-1.773010
O	-3.188325	0.186342	0.535066
Cl	-1.136254	-1.541939	-1.608792
O	-2.681908	1.111747	-2.007724
B	-3.038317	1.781266	-3.122886

O	-2.524713	3.012010	-3.468755
O	-3.954948	1.316960	-4.047175
C	-4.015311	2.300837	-4.998203
C	-3.141273	3.324833	-4.649540
C	-2.985439	4.447088	-5.429633
C	-3.755063	4.508556	-6.589494
C	-4.632042	3.485148	-6.936368
C	-4.780989	2.351626	-6.139625
H	-5.458891	1.546584	-6.398291
H	-5.213345	3.569929	-7.848343
H	-3.668119	5.375281	-7.236073
H	-2.299671	5.236973	-5.146319

4 (Ph_2CO)

Mo	-0.313127	3.874112	0.314864
O	0.490032	5.299436	0.468410
Cl	-0.713606	3.434266	-1.938310
Cl	1.535216	2.434370	0.286912
H	-0.144188	3.246560	1.851774
O	-2.010836	4.304093	1.027875
B	-2.911746	3.528922	1.675657
O	-2.745290	3.031711	2.955124
O	-4.115549	3.133871	1.116601
C	-3.839371	2.239400	3.163473
C	-4.667880	2.295846	2.047629
O	-1.570211	1.718220	0.466036
C	-2.070894	0.597912	0.510292
C	-2.835986	0.097473	-0.649421
C	-3.459006	1.032519	-1.480268
C	-2.892505	-1.259825	-0.972024
C	-1.924467	-0.208267	1.740797
C	-2.900473	-1.117494	2.153410
C	-2.763794	-1.779626	3.362542
C	-1.648271	-1.551934	4.156097
C	-0.674831	-0.644020	3.753274
C	-0.817739	0.036748	2.558443
C	-4.153400	0.610118	-2.598926
C	-4.205484	-0.742472	-2.914676
C	-3.567763	-1.675026	-2.108074
C	-4.140744	1.458592	4.254151
C	-5.319001	0.715891	4.182958
C	-6.143945	0.766078	3.064472
C	-5.830710	1.565802	1.964753
H	-3.481811	1.419225	5.114216
H	-5.595759	0.083120	5.020215
H	-7.053297	0.174270	3.045963
H	-6.462181	1.615193	1.084674
H	-3.790630	-1.269212	1.550648
H	-3.536313	-2.467639	3.690938
H	-1.538330	-2.079410	5.098821
H	0.195028	-0.465566	4.376807
H	-0.074626	0.758772	2.232685
H	-2.377395	-1.986002	-0.350889
H	-3.592878	-2.728197	-2.368047
H	-4.740681	-1.070706	-3.800446
H	-4.648138	1.337006	-3.234591
H	-3.397828	2.085607	-1.223350

TS5 (Ph_2CO)

Mo	-0.225398	2.870999	1.963445
O	-0.239274	3.011405	3.621848
O	-1.846162	3.854563	1.749757
Cl	0.880229	0.845473	2.075191
C	-3.622508	1.631099	-0.824831
O	-0.136363	2.645812	-0.247878
C	-2.440125	3.675247	-1.291095
B	-3.162814	3.614246	1.866559
O	-3.676898	2.387781	2.274422
H	-1.416602	1.718797	1.150849
Cl	1.452281	4.315223	1.473303
C	-1.142831	1.833423	-0.248599
C	-0.858646	0.374527	-0.481830
C	-1.538371	-0.642133	0.182668
C	-1.236056	-1.967568	-0.078995
C	-0.256224	-2.284729	-1.010839
C	0.429832	-1.272473	-1.666273
C	0.137365	0.055931	-1.397289
C	-4.782320	2.186870	-1.339612
C	-4.769460	3.480104	-1.845847
C	-3.594971	4.219405	-1.827291
C	-2.442448	2.375990	-0.783543
O	-4.158702	4.525982	1.584214
C	-5.323732	3.828164	1.752486
C	-6.613533	4.247901	1.529581
C	-7.622002	3.306463	1.737202
C	-7.331947	2.011107	2.149902
C	-6.018593	1.596661	2.374384
C	-5.034391	2.533382	2.167027
H	-5.777520	0.589671	2.696186
H	-8.142597	1.306418	2.303029
H	-8.655419	3.593603	1.573414
H	-6.824463	5.259239	1.201213
H	-3.642801	0.613773	-0.448910
H	-5.700981	1.608149	-1.342721
H	-5.679180	3.911577	-2.252086
H	-3.580635	5.229824	-2.222684
H	-1.517342	4.243833	-1.250170
H	-2.265566	-0.391527	0.952955
H	-1.754130	-2.756217	0.457080
H	-0.016850	-3.323696	-1.214236
H	1.207179	-1.517716	-2.382977
H	0.685876	0.859343	-1.878123

5 (Ph_2CO)

Mo	0.213365	1.641161	0.652611
O	-0.188297	1.743238	2.261361
O	-0.933750	0.428008	-0.304098
Cl	1.949665	3.160185	0.323462
C	3.488098	-1.126698	-2.114583
O	1.416766	0.232516	0.608886
C	4.117961	0.169455	-0.172339
B	-2.237844	0.087691	-0.401998
O	-2.715387	-0.765348	-1.397225
H	1.038650	-0.803900	-1.109581
Cl	-1.221509	3.283098	-0.242986
C	1.776397	-0.834966	-0.298440
C	1.607333	-2.143185	0.453518
C	0.415752	-2.865615	0.300985
C	0.219336	-4.058544	0.998161
C	1.209073	-4.533625	1.860177
C	2.397579	-3.814827	2.019800
C	2.597871	-2.627279	1.318383
C	4.760725	-0.941660	-2.652971
C	5.715259	-0.197048	-1.954970

C	5.389819	0.359427	-0.717587
C	3.160107	-0.577562	-0.868453
O	-3.247775	0.478048	0.471965
C	-4.385959	-0.139197	-0.001257
C	-5.675524	-0.077804	0.497196
C	-6.647893	-0.819105	-0.190354
C	-6.324659	-1.578116	-1.322012
C	-5.013734	-1.631002	-1.818808
C	-4.062953	-0.896186	-1.132166
H	-4.752433	-2.212767	-2.696323
H	-7.104829	-2.137710	-1.829422
H	-7.674026	-0.801753	0.164553
H	-5.913556	0.515000	1.373801
H	2.746769	-1.703938	-2.662490
H	5.004444	-1.372490	-3.620189
H	6.704790	-0.046907	-2.377691
H	6.123404	0.948254	-0.173983
H	3.861994	0.614286	0.783736
H	-0.357496	-2.493217	-0.366350
H	-0.704905	-4.614573	0.867661
H	1.057369	-5.461467	2.404956
H	3.171123	-4.183536	2.687756
H	3.527960	-2.078775	1.433006

TS6 (Ph_2CO)

Mo	0.457688	0.785978	-2.534862
O	1.891067	0.395652	-1.828028
Cl	0.574977	-0.454475	-4.474450
Cl	0.747999	2.758237	-3.605746
O	-0.580892	1.441658	-1.152265
B	-1.653646	0.586135	-0.793589
O	-1.622258	-0.050116	0.461663
O	-2.972369	0.928844	-1.130409
O	-0.993112	-0.546657	-2.049071
C	-1.219562	-1.921526	-2.386074
C	-2.636069	-2.268657	-2.000391
C	-0.149918	-2.802072	-1.801787
C	0.242579	-3.937103	-2.504098
C	1.203110	-4.789947	-1.983878
C	1.787412	-4.508960	-0.756281
C	1.403623	-3.376129	-0.053521
C	0.436502	-2.524896	-0.570363
C	-2.949603	-3.010482	-0.868289
C	-4.274840	-3.291726	-0.563066
C	-5.292150	-2.830966	-1.383366
C	-4.985973	-2.083987	-2.514726
C	-3.665407	-1.805381	-2.818609
C	-3.740041	0.426928	-0.128640
C	-2.924925	-0.172690	0.832040
C	-3.445359	-0.757823	1.963394
C	-4.831661	-0.719939	2.109861
C	-5.645425	-0.120966	1.153201
C	-5.109037	0.466132	0.008256
H	-1.156526	-1.995745	-3.480771
H	-5.730573	0.933386	-0.747550
H	-6.720488	-0.108560	1.301069
H	-5.283400	-1.161800	2.992174
H	-2.798595	-1.216298	2.703171
H	-0.210089	-4.149299	-3.470515
H	1.504630	-5.670662	-2.542279
H	2.546435	-5.170594	-0.350692
H	1.860097	-3.150524	0.905229
H	0.127085	-1.646007	-0.010696
H	-3.416910	-1.213848	-3.697378
H	-5.780017	-1.720305	-3.159662
H	-6.327439	-3.049273	-1.139656
H	-4.511698	-3.866296	0.326973
H	-2.154143	-3.375186	-0.224082

7

Mo	-2.175315	0.208189	-0.091532
Cl	-3.963672	-0.569137	-1.229939
Cl	-1.695634	-1.149109	1.645615
O	-2.491235	1.744758	0.460241
O	-0.865263	0.331316	-1.108409
H	0.484826	1.487582	1.245288
B	1.477462	1.009828	0.830172
O	2.591959	1.735987	0.482634
O	1.667695	-0.341190	0.656049
C	2.946474	-0.460453	0.176276
C	3.508469	0.804022	0.071476
C	4.793692	0.997275	-0.381969
C	5.505844	-0.147284	-0.734127
C	4.942049	-1.415436	-0.629193
H	3.187687	-2.579871	-0.080556
C	3.639160	-1.598172	-0.167861
H	5.528732	-2.282553	-0.913557
H	6.523654	-0.045782	-1.097534
H	5.219840	1.991065	-0.458383

7+Ph_2CO

Mo	-2.846409	-0.822542	-0.398219
O	-1.601766	0.196562	-0.828162
O	-2.667026	-1.161858	1.220592
Cl	-4.830146	0.225116	-0.723926
Cl	-2.732622	-2.730916	-1.611284
H	-0.232014	-1.851661	0.479587
B	0.925697	-2.049222	0.437741
O	1.614122	-2.353541	-0.716605
O	1.714663	-2.185585	1.562959
C	2.894254	-2.600093	-0.303922
C	2.955472	-2.498500	1.080633
C	3.999064	-2.920056	-1.059433
C	5.190048	-3.140936	-0.366478
C	5.250953	-3.042103	1.019363
C	4.124304	-2.716576	1.774797
O	1.588355	0.393189	0.164038
C	1.219837	1.549726	0.253875
C	2.012362	2.630298	-0.395386
C	-0.024328	1.883106	0.999091
C	2.810902	2.287754	-1.487162
C	2.045610	3.936512	0.093750
C	2.855543	4.886976	-0.509507
C	3.624704	4.543870	-1.612299
C	3.601591	3.242523	-2.100949
C	-0.396924	1.057498	2.059462
C	-1.593832	1.270641	2.721979
C	-2.445789	2.287987	2.307871
C	-2.090122	3.102239	1.240747
C	-0.877675	2.910099	0.596254
H	4.209000	2.973435	-2.959296
H	2.794484	1.259835	-1.835950
H	1.456338	4.203573	0.965772
H	2.888287	5.898218	-0.116148

H	4.251171	5.291445	-2.089533
H	3.935446	-2.997468	-2.139121
H	6.086950	-3.397391	-0.921695
H	6.194538	-3.223671	1.525648
H	4.157045	-2.638559	2.855737
H	-0.611902	3.532500	-0.252627
H	-2.760756	3.888701	0.908888
H	-3.391569	2.444678	2.818004
H	-1.876015	0.626749	3.548543
H	0.264143	0.245147	2.348546

TS8 (Ph_2CO)

Mo	0.092167	-0.333753	0.482393
Cl	0.541303	-0.699085	2.673145
O	1.569260	-0.170795	-0.286451
O	-0.635518	-1.717273	-0.092189
Cl	-1.231232	1.503193	0.512298
H	-0.524771	0.021291	-1.968256
B	-0.192717	0.769677	-2.854771
O	0.001486	2.135625	-2.509826
O	-0.909722	0.698769	-4.089742
O	1.379386	0.254417	-3.219299
C	-0.370116	2.835494	-3.611807
C	-0.921403	1.973630	-4.561024
C	-0.275901	4.189270	-3.839505
C	-0.754231	4.668627	-5.061361
C	-1.304104	3.811524	-6.003776
C	-1.399315	2.438140	-5.764456
C	1.951582	-0.829882	-3.008970
C	1.211263	-2.081261	-2.813085
C	3.420504	-0.811170	-2.989600
C	4.061959	0.380062	-2.637307
C	5.442040	0.447144	-2.634550
C	6.192479	-0.662233	-3.008257
C	1.674569	-3.052308	-1.918684
C	0.950143	-4.213291	-1.719359
C	-0.227420	-4.424240	-2.425019
C	-0.691794	-3.466634	-3.316463
C	0.013845	-2.291034	-3.503833
C	5.562671	-1.841562	-3.381333
C	4.180188	-1.921683	-3.365449
H	5.938808	1.366736	-2.343811
H	3.455608	1.235081	-2.357197
H	3.685321	-2.836909	-3.674366
H	6.150678	-2.699718	-3.689357
H	7.276576	-0.604392	-3.013431
H	0.151783	4.848150	-3.091513
H	-0.694072	5.731187	-5.274720
H	-1.667548	4.212235	-6.944814
H	-1.829851	1.757635	-6.491277
H	2.583274	-2.871130	-1.352650
H	1.298780	-4.952799	-1.006275
H	-0.792225	-5.338449	-2.271302
H	-1.614470	-3.632331	-3.862241
H	-0.351283	-1.532655	-4.190088

8 (Ph_2CO)

C	-5.908596	3.477102	2.524322
C	-5.411617	2.201706	2.817564
C	-5.218919	1.276507	1.786495
C	-5.513707	1.626749	0.480633
C	-5.985130	2.901313	0.195537
C	-6.180120	3.825955	1.216057
C	-5.152383	1.862586	4.213695
C	-4.166174	0.857035	4.582832
O	-5.858658	2.467619	5.062247
B	-5.629733	2.791100	6.558279
O	-6.198247	1.798285	7.419966
C	-7.083539	2.467263	8.208390
C	-7.862886	1.972935	9.227370
C	-8.696145	2.878382	9.889446
C	-8.728534	4.218311	9.531089
C	-7.931970	4.711461	8.494738
C	-7.117629	3.813237	7.845091
O	-6.259271	4.041471	6.821075
O	-3.332170	3.940087	4.780685
Mo	-2.612932	3.819902	6.297745
O	-2.027405	2.267150	6.488883
Cl	-3.433890	4.896984	8.173181
Cl	-0.736709	5.123873	6.127260
H	-4.377155	2.846497	6.660802
H	-6.545027	4.821157	0.986113
H	-6.050740	4.182134	3.336481
H	-4.871158	0.274579	2.016154
H	-5.380695	0.903643	-0.316852
H	-6.207034	3.176444	-0.830898
H	-7.943966	5.756889	8.206876
H	-9.382322	4.899369	10.066514
H	-9.325198	2.525005	10.700161
H	-7.823719	0.923822	9.499934
C	-2.983943	0.720444	3.842051
C	-2.050230	-0.231193	4.201748
C	-2.296779	-1.069606	5.282287
C	-3.466594	-0.943127	6.018896
C	-4.395458	0.025726	5.685947
H	-2.784719	1.400119	3.019685
H	-1.121798	-0.314547	3.647379
H	-1.563588	-1.820634	5.559208
H	-3.651458	-1.596027	6.864876
H	-5.304251	0.137893	6.268458

TS9 (Ph_2CO)

Mo	0.032458	0.256780	-0.710188
Cl	0.342554	2.094569	0.708316
O	1.673880	-0.096859	-1.099035
O	-0.539457	-1.113998	0.051307
Cl	-2.030835	1.308220	-1.449167
H	-0.162124	-0.098223	-2.398271
B	0.800815	0.864804	-3.774682
O	0.891438	2.083141	-3.137504
O	-0.172595	0.824043	-4.741525
O	1.933256	0.028848	-3.815688
C	-0.159878	2.804460	-3.657267
C	-0.802317	2.047070	-4.625933
C	-0.590320	4.058132	-3.301591
C	-1.710049	4.539494	-3.976941
C	-2.352917	3.783243	-4.950433
C	-1.908195	2.507888	-5.296240
C	2.331355	-1.039367	-3.211690
C	1.434176	-2.154182	-3.032276
C	3.750021	-1.090511	-2.922843
C	4.420191	0.105984	-2.634467
C	5.773829	0.086742	-2.371753
C	6.474093	-1.115630	-2.415726

C	1.605644	-3.031266	-1.950069
C	0.688257	-4.037334	-1.731203
C	-0.394380	-4.189006	-2.591607
C	-0.568214	-3.330591	-3.669524
C	0.331904	-2.305154	-3.885100
C	5.820476	-2.302503	-2.717417
C	4.459005	-2.295746	-2.964667
H	6.289637	1.007715	-2.123070
H	3.849029	1.026853	-2.577321
H	3.947483	-3.215661	-3.227964
H	6.374625	-3.233531	-2.765564
H	7.540532	-1.124951	-2.213361
H	-0.096677	4.617842	-2.515657
H	-2.096105	5.521741	-3.726333
H	-3.227418	4.189627	-5.447515
H	-2.411708	1.901347	-6.039808
H	2.408791	-2.854826	-1.242896
H	0.794592	-4.687250	-0.870110
H	-1.119384	-4.975688	-2.408749
H	-1.418875	-3.450179	-4.330884
H	0.191392	-1.622783	-4.717154

9 (Ph_2CO)

Mo	-0.054259	0.466887	-0.600812
Cl	1.020914	2.493703	-0.112495
O	1.303303	-0.414389	-1.525971
O	-0.205040	-0.486429	0.734293
Cl	-2.163720	1.427983	-0.607310
H	-0.937694	-0.392820	-1.740276
B	0.563542	0.734695	-3.965706
O	0.167969	1.564564	-2.912424
O	0.281841	1.307866	-5.184273
O	1.112467	-0.478508	-3.846628
C	-0.370066	2.686302	-3.517470
C	-0.295957	2.516185	-4.891698
C	-0.899290	3.812763	-2.937232
C	-1.368917	4.790951	-3.813556
C	-1.298576	4.626358	-5.191667
C	-0.755252	3.476000	-5.762290
C	1.667740	-1.087714	-2.695040
C	1.155584	-2.510281	-2.606759
C	3.180442	-0.972364	-2.799209
C	3.792362	0.220328	-2.419795
C	5.161094	0.373013	-2.567380
C	5.924165	-0.659486	-3.096815
C	1.322607	-3.205088	-1.411632
C	0.890467	-4.516281	-1.306185
C	0.294373	-5.142814	-2.393486
C	0.132417	-4.452591	-3.584382
C	0.561277	-3.136033	-3.693986
C	5.314441	-1.845241	-3.477292
C	3.943960	-2.004352	-3.327656
H	5.634763	1.301065	-2.263727
H	3.194615	1.023328	-1.995441
H	3.468771	-2.936014	-3.619929
H	5.907783	-2.654889	-3.890074
H	6.997046	-0.539138	-3.209691
H	-0.946106	3.924497	-1.860262
H	-1.798667	5.699544	-3.405907
H	-1.674273	5.410304	-5.840748
H	-0.692592	3.334836	-6.835002
H	1.790085	-2.711647	-0.564073
H	1.016504	-5.051303	-0.370473
H	-0.045461	-6.170270	-2.309299
H	-0.333829	-4.937643	-4.436142
H	0.437148	-2.592575	-4.623675

10 (Ph_2CO)

Mo	0.300831	0.743431	-0.240018
O	0.385825	0.135032	1.317113
O	1.542342	1.866484	-0.482027
Cl	-1.680212	2.048234	-0.380077
Cl	-0.948595	-0.694673	-1.911566
H	1.332555	-0.451345	-0.911831
B	0.501926	0.635901	-3.896027
O	0.099479	1.832469	-3.378123
O	-0.254861	0.193571	-4.945690
C	-1.081989	2.085664	-4.034914
C	-1.293823	1.103584	-4.992148
O	1.787973	0.170703	-3.584129
C	2.330675	-0.876502	-3.059773
C	1.840382	-3.047487	-2.019796
C	1.688392	-2.165423	-3.101956
C	0.878115	-2.526759	-4.187476
C	0.249718	-3.755500	-4.194056
C	0.389245	-4.613006	-3.109885
C	1.178517	-4.257081	-2.021834
C	-2.393724	1.107291	-5.815126
C	-3.296610	2.152754	-5.630899
C	-3.089867	3.130389	-4.662992
C	-1.969251	3.114971	-3.835538
C	3.649793	-0.666884	-2.512197
C	3.998804	0.605264	-2.028938
C	5.258536	0.813062	-1.506549
C	6.185752	-0.224059	-1.486143
C	5.855472	-1.480224	-1.981185
C	4.590183	-1.708295	-2.485899
H	5.517576	1.784576	-1.100886
H	3.253158	1.394132	-2.005046
H	4.334008	-2.678210	-2.898713
H	6.589225	-2.278740	-1.977005
H	7.177227	-0.051225	-1.079142
H	-1.803300	3.852303	-3.059280
H	-3.823991	3.919520	-4.540495
H	-4.185832	2.197813	-6.250744
H	-2.549480	0.331336	-6.555418
H	2.410814	-2.735456	-1.151378
H	1.259111	-4.918463	-1.166579
H	-0.131686	-5.565260	-3.107250
H	-0.367284	-4.040781	-5.038694
H	0.754238	-1.849304	-5.023954

TS11 (Ph_2CO)

Mo	0.335924	0.707798	-0.375239
O	0.521618	-0.047686	1.104959
O	1.573556	1.846717	-0.560959
Cl	-1.611707	2.055349	-0.308486
Cl	-1.027639	-0.722360	-1.920061
H	1.371902	-0.367190	-1.248881
B	0.572442	0.638962	-3.999376
O	0.137691	1.778051	-3.385944
O	-0.202124	0.233950	-5.047400
C	-1.063876	2.042003	-4.007071
C	-1.265249	1.116974	-5.020841

O	1.847973	0.145881	-3.718645
C	2.329379	-0.861374	-3.053292
C	1.736318	-3.001411	-1.971413
C	1.666309	-2.144516	-3.080592
C	0.930038	-2.526066	-4.208996
C	0.294735	-3.752738	-4.232463
C	0.360112	-4.588988	-3.126673
C	1.076331	-4.211223	-1.995309
C	-2.380749	1.139500	-5.822020
C	-3.309443	2.143331	-5.553840
C	-3.112801	3.062039	-4.527895
C	-1.976223	3.028145	-3.722834
C	3.645847	-0.649259	-2.493756
C	4.031084	0.649348	-2.123580
C	5.285634	0.864214	-1.592740
C	6.173668	-0.197503	-1.448705
C	5.807354	-1.482232	-1.829908
C	4.546172	-1.713866	-2.345444
H	5.571410	1.860979	-1.275841
H	3.313812	1.460671	-2.193663
H	4.264393	-2.709683	-2.670153
H	6.509850	-2.302311	-1.729297
H	7.161241	-0.020683	-1.034114
H	-1.818847	3.715500	-2.900004
H	-3.867815	3.818070	-4.340956
H	-4.211555	2.201465	-6.153658
H	-2.528518	0.407717	-6.607489
H	2.243055	-2.668853	-1.070961
H	1.096642	-4.854607	-1.122872
H	-0.162521	-5.540193	-3.139166
H	-0.266482	-4.052107	-5.110574
H	0.870422	-1.868011	-5.068110

MoO_2Cl2+Ph2CHOBcat

B	0.550396	0.701803	-3.806198
O	1.780197	0.198759	-3.699933
C	2.093267	-0.774938	-2.699198
C	3.563059	-0.703091	-2.381346
C	4.461766	-0.013714	-3.183754
C	5.813004	0.001634	-2.860452
C	6.272220	-0.666134	-1.736385
C	5.373683	-1.353082	-0.929105
C	4.027530	-1.370785	-1.251321
O	-0.471013	0.552492	-2.855829
C	-1.577371	1.123696	-3.446737
C	-1.205419	1.674362	-4.665039
C	-2.102639	2.357898	-5.451538
C	-3.407983	2.458072	-4.970496
C	-3.780945	1.891157	-3.757880
C	-2.861584	1.204039	-2.965282
O	0.119318	1.431350	-4.897812
C	1.660123	-2.140982	-3.172090
C	0.637975	-2.815546	-2.516428
C	0.229311	-4.068948	-2.954238
C	0.836596	-4.647199	-4.057503
C	1.854980	-3.972742	-4.722090
C	2.267418	-2.727714	-4.279708
Mo	0.179623	2.099662	-0.273683
Cl	-1.149843	0.337419	0.278764
O	0.432468	2.918504	1.148907
O	1.685456	1.580360	-0.753990
Cl	-0.629607	3.642779	-1.727673
H	1.532987	-0.541157	-1.784393
H	6.509717	0.544337	-3.492238
H	4.096941	0.518149	-4.055776
H	3.321562	-1.910193	-0.622436
H	5.724883	-1.873194	-0.043243
H	7.328040	-0.649453	-1.484536
H	-3.136163	0.763718	-2.012900
H	-4.807193	1.983261	-3.418675
H	-4.148909	2.987462	-5.560324
H	-1.800012	2.791511	-6.397645
H	0.155709	-2.351209	-1.658896
H	-0.567648	-4.591044	-2.433901
H	0.518320	-5.626078	-4.402630
H	2.331839	-4.425828	-5.585746
H	3.070739	-2.200143	-4.787992