Supporting Information

Heterolytic cleavage of Si−H bonds: Reduction of imines using silane/high-valent oxo-molybdenum MoO$_2$Cl$_2$ as a catalyst

Yiou Wang, Piao Gu, Wenmin Wang and Haiyan Wei*

1. Complete reference of 9.

2. 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) and M06(6-311++G(d,p)+ QVZP) and MP2(6-311G(d,p)+ LANL2DZ) calculation level for MoO$_2$Cl$_2$ mediated the hydrosilylation reaction are shown.

3. Table S2 The relative free energies of the key transition states obtained at B3LYP-D(6-311++G(2d,p)+ QVZP), M06(6-311++G(2d,p)+ QVZP) calculation level for MoO$_2$Cl$_2$ mediated the hydrosilylation reaction are shown.

4. Table S3 The relative free energies with different solvation, (CH$_2$Cl$_2$, THF and Toluene) of the key transition states and the intermediates obtained at M06(6-311++G(2d,p)+ QVZP) calculation level for MoO$_2$Cl$_2$ mediated the hydrosilylation reaction are shown.

5. Scheme S1 The energy profile for MoO$_2$Cl$_2$ catalyzing the hydrosilylation of imines process through the [2+2] addition pathway. The solvation energies are included in parentheses, and the gas-phase energies are the values without parentheses.

6. Figure S1. The calculated geometric structures of the transition states along the [2+2] addition pathway.

7. Figure S2 The calculated geometric structures of the transition states for the transformation between the ion pair of **5anti**, **5syn** and **6syn.** The solvation energies are included in parentheses, and the gas-phase energies are the values without parentheses

8. Figure S3 The calculated geometric structures of other two isomer of **TS4syn.** The solvation energies are included in parentheses, and the gas-phase energies are the values without parentheses.

9. Figure S4 The detailed scan plot for the ionic hydrosilylation pathway from the adduct **3+im**.

10. Figure S5 The IRC plot for the ionic hydrosilylation pathway from the transition state **TS4anti**.

11. Table S4 Cartesian coordinates for all optimized structures in XYZ format.

Complete reference of 9

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 relative free energies of the intermediates and transition states obtained at M06(6-311++G(d,p)+ LANL2DZ), M06(6-311++G(d,p)+ SDD) and M06(6-311++G(d,p)+ QVZP) calculation level for MoO_2Cl_2 mediated the hydrosilylation reaction are shown. The solvation energies are included in parentheses, and the gas-phase energies are the values without parentheses.

	M06 6-311++G(d,p) + LANL2DZ)	M06 (6-311++G(d,p)+ SDD	M06 (6-311++G(2d,p) + QVZP)	MP2 (6-311G(d,p)+ LANL2DZ
TS[2+2]	28.7(26.4)	29.1	30.9(29.0)	38.8 (35.9)
TS4anti	18.1(14.4)	20.4	25.4(21.4)	20.0(19.7)

These results have indicated that the ionic hydrosilylation pathway passing through **TS4anti** is the most favorable pathway at all level of calculation.

Table S2 The relative free energies of the key transition states obtained at B3LYP-D(6-311++G(2d,p)+ QVZP), M06(6-311++G(2d,p)+ QVZP) calculation level for MoO_2Cl_2 mediated the hydrosilylation reaction are shown.

	B3LYP (6-311++G(2d,p) + QVZP)	M06 (6-311++G(2d,p) + QVZP)	B3LYP-sol (6-311++G(2d,p) + QVZP)	M06-sol (6-311++G(2d,p) + QVZP)
3+im	11.1	14.3	13.0	17.2
TS4anti	25.7	25.4	17.0	21.4
4anti	25.4	25.3	13.4	16.5

Table S3 The relative free energies with different solvation, (CH_2Cl_2, THF and Toluene) of the key transition states and the intermediates obtained at M06(6-311++G(2d,p)+ QVZP) calculation level for MoO_2Cl_2 mediated the hydrosilylation reaction are shown.

	M06-gas (6-311++G(2d,p) + QVZP)	M06- CH_2Cl_2 (6-311++G(2d,p) + QVZP)	M06-THF (6-311++G(2d,p) + QVZP)	M06-Toluene (6-311++G(2d,p) + QVZP)
3+im	14.3	17.2	16.4	20.0
TS4anti	25.4	21.4	21.9	27.9
4anti	25.3	16.5	17.8	25.9
5anti	28.6	12.0	12.8	23.7
TS5syn	33.6	30.7	32.0	37.7
5syn	15.9	7.5	8.4	16.8
6syn	16.6	7.8	8.4	17.0
TS7	19.6	12.5	13.4	21.2
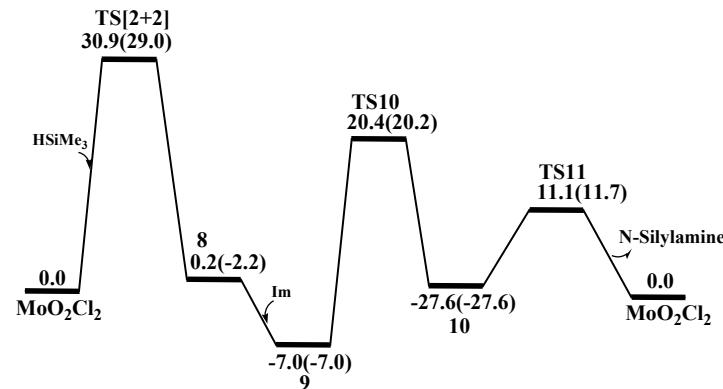
Scheme S1 The energy profile for MoO_2Cl_2 catalyzing the hydrosilylation of imines process through the [2+2] addition pathway. The solvation energies are included in parentheses, and the gas-phase energies are the values without parentheses.

Figure S1. The calculated geometric structures of the transition states along the [2+2] addition pathway.

Mo-H=1.77
Si-H=1.85
Si-O=2.06

TS[2+2]

Mo-N=2.22
Mo-H=1.79
C-H=1.61
N-C=1.36

TS10

Mo-O=1.77
Mo-N=2.22
O-Si=1.85
Si-N=2.26

TS11

Mo-H=1.70
H-Si=2.57
Mo-H-Si=151.2

TS(**5anti→5syn**) 31.1(12.8) kcal/mol

Mo-H=1.71
H-Si=2.17
H-C=2.57

TS(**5syn→6syn**) 16.7 (6.3) kcal/mol

Figure S2 The calculated geometric structures of the transition states for the transformation between the ion pair of **5anti**, **5syn** and **6syn.** The solvation energies are included in parentheses, and the gas-phase energies are the values without parentheses.

Mo-H=1.91
H-Si=1.65
Si-N=2.27

Mo-H=1.93
H-Si=1.67
Si-N=2.29

TS4syn-ISO2 28.7(29.2) kcal/mol   **TS4syn-ISO3** 32.5(29.8) kcal/mol
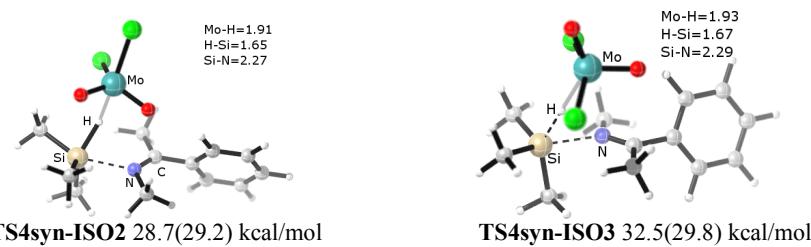
Figure S3 The calculated geometric structures of other two isomer of **TS4syn.** The solvation energies are included in parentheses, and the gas-phase energies are the values without parentheses.

Figure S4 The detailed scan plot for the ionic hydrosilylation pathway from the adduct **3+im**. (The first maximum point corresponds to the transition state TS4anti, the first minimum point corresponds to the first intermediate 4anti. The maximum point corresponds to the second transition state 5anti, and then the laste point corresponds to the syn intermediate 5syn)
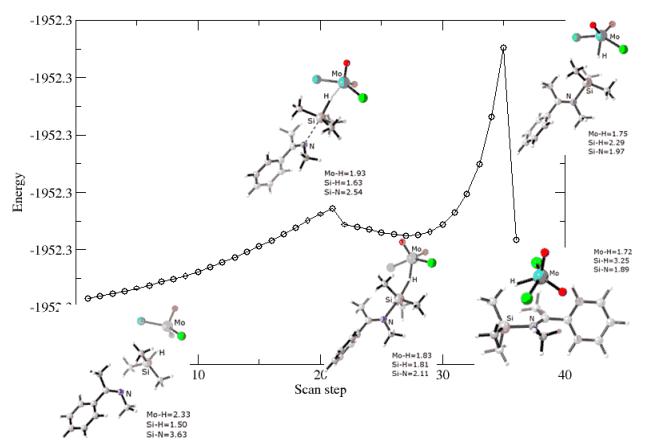
Figure S5 The IRC plot for the ionic hydrosilylation pathway from the transition state **TS4anti**. (From the last point of the IRC calculation (both forward and reverse calculations), we optimization the structures, which leads to the adduct of **3+im**, and **4anti**, respectively.
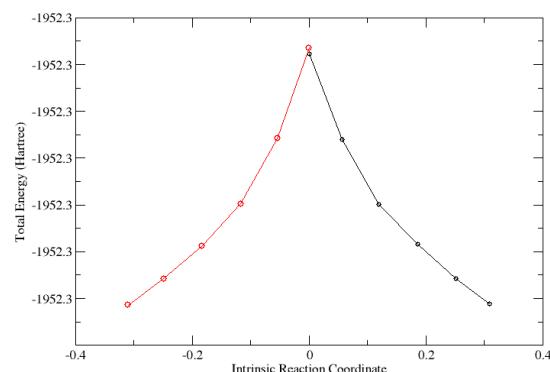
Table S4 Cartesian coordinates for each structure calculated. (XYZ format).

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]

O	1.148240	-1.255720	-0.355794
Mo	-0.130813	-0.193612	0.206998
Cl	-0.568068	2.100787	-0.181769
Si	2.791967	-0.023091	-0.292424
O	-0.519644	-0.586312	1.769440
Cl	-1.912639	-0.675526	-1.179527
H	1.339261	0.713545	0.582210
C	3.525836	1.503586	0.533511
C	2.638268	0.336592	-2.107912
C	3.765910	-1.487219	0.308376
H	4.832805	-1.238784	0.327526
H	3.465294	-1.744666	1.329030
H	3.598574	-2.363916	-0.320698
H	4.563795	1.611422	0.188978
H	2.974285	2.409745	0.262184
H	3.538761	1.420082	1.624313
H	3.564168	0.789449	-2.479159
H	2.417764	-0.565044	-2.683698
H	1.832895	1.060790	-2.281630

3+im

|			
Mo	-0.063877	0.060200	0.681809
O	-1.459775	0.105039	1.582720
O	1.163957	0.078383	1.802947
Cl	0.286856	2.026780	-0.452645
Cl	0.232176	-1.979071	-0.333937
H	-1.729238	0.045575	-0.952987
Si	-2.169094	-0.046524	-2.392311
N	-3.467127	-0.601116	-5.732579
C	-3.263967	-1.600094	-6.492967
C	-4.142317	-2.032458	-7.620803
C	-4.726395	-3.297565	-7.618439
C	-5.532774	-3.702918	-8.672233
C	-5.745883	-2.856154	-9.751141
C	-5.156185	-1.599241	-9.768833
C	-4.364076	-1.187992	-8.707225
C	-3.139826	1.516931	-2.719949
C	-3.192216	-1.605771	-2.499640
H	-4.020912	-1.589314	-1.784842
C	-0.636069	-0.101742	-3.458424
C	-4.667989	0.192923	-5.839934
C	-2.041742	-2.439179	-6.278512
H	-4.561593	-3.965498	-6.776704
H	-5.993511	-4.685762	-8.652435
H	-6.370213	-3.176305	-10.579451
H	-5.315430	-0.935189	-10.612860
H	-3.903742	-0.203030	-8.718758
H	-0.080407	-1.036848	-3.331040
H	-0.940899	-0.015324	-4.507154
H	0.037847	0.730328	-3.229027
H	-2.578298	-2.487151	-2.284094

H	-3.600965	-1.708118	-3.510147
H	-2.569668	2.396042	-2.401461
H	-3.335423	1.611702	-3.793056
H	-4.098122	1.525656	-2.191283
H	-5.080090	0.330534	-4.832612
H	-4.414982	1.194350	-6.209382
H	-5.450984	-0.227246	-6.484346
H	-1.424796	-2.458649	-7.184201
H	-1.454085	-2.056247	-5.442128
H	-2.319898	-3.479574	-6.072587

TS4anti

Mo	3.510907	-0.308961	0.059057
O	3.905095	-0.850368	1.591861
O	4.845960	-0.457286	-0.929822
Cl	3.577706	2.014622	0.488351
Cl	2.278911	-2.206693	-0.653385
H	1.842175	0.398069	-0.588740
Si	0.249839	0.652264	-0.324326
N	-2.260556	0.757576	0.065427
C	-3.003946	-0.264992	0.243562
C	-4.494129	-0.247800	0.177589
C	-5.261624	-0.540758	1.301498
C	-6.646747	-0.550896	1.217805
C	-7.272785	-0.294467	0.005955
C	-6.511760	-0.018905	-1.122493
C	-5.128252	0.010969	-1.035824
C	0.262378	2.503253	-0.578318
C	-0.288216	-0.323187	-1.832212
C	0.355998	0.093322	1.463656
C	-2.860906	2.063628	-0.136517
C	-2.423760	-1.620253	0.490821
H	1.149130	0.682305	1.941993
H	-4.773797	-0.747155	2.250887
H	-7.238993	-0.765449	2.101726
H	-8.355976	-0.311825	-0.060290
H	-6.997976	0.175592	-2.073239
H	-4.527995	0.230343	-1.916404
H	-0.454672	-1.381942	-1.622901
H	-1.206215	0.104484	-2.248866
H	0.499264	-0.266706	-2.590256
H	0.630148	-0.962535	1.556326
H	-0.569665	0.270055	2.015116
H	1.256370	2.820008	-0.906374
H	-0.462746	2.814307	-1.335185
H	0.048713	3.034770	0.354364
H	-2.299839	2.803867	0.439772
H	-2.776390	2.349638	-1.192438
H	-3.915748	2.114600	0.150433
H	-2.736629	-2.300685	-0.310179
H	-1.336765	-1.616991	0.553909
H	-2.832785	-2.036146	1.418689

4anti

Mo	-0.180211	-0.179486	-0.634294
O	-0.282532	-0.532350	1.001429
O	1.408220	0.059613	-1.125678
Cl	-0.856874	2.093703	-0.585902
Cl	-0.415313	-2.408213	-1.483606
H	-1.643061	-0.088912	-1.735321

Electronic Supplementary Material (ESI) for Catalysis Science & Technology
This journal is © The Royal Society of Chemistry 2013

Si	-2.625497	-0.198821	-3.255880
N	-3.607337	-0.678129	-5.063241
C	-3.294572	-1.687751	-5.792635
C	-3.928865	-1.975065	-7.105810
C	-4.622361	-3.165395	-7.311714
C	-5.179792	-3.440107	-8.551761
C	-5.020727	-2.544671	-9.600010
C	-4.312462	-1.366097	-9.405338
C	-3.775709	-1.076646	-8.160725
C	-3.418224	1.471458	-2.987645
C	-3.555399	-1.594437	-2.403215
H	-3.635986	-1.367083	-1.336338
C	-0.953943	-0.041502	-4.111941
C	-4.739626	0.168868	-5.421583
C	-2.227548	-2.652663	-5.402457
H	-4.744327	-3.871494	-6.494583
H	-5.734252	-4.360888	-8.701001
H	-5.446994	-2.766972	-10.572946
H	-4.178812	-0.668515	-10.225783
H	-3.222896	-0.153444	-8.004480
H	-0.267275	-0.858567	-3.875491
H	-1.038174	0.053686	-5.199654
H	-0.502604	0.882279	-3.729267
H	-3.070376	-2.569036	-2.483916
H	-4.567118	-1.666029	-2.820364
H	-2.882662	1.978861	-2.179061
H	-3.346089	2.109718	-3.874044
H	-4.469283	1.396477	-2.692170
H	-5.335928	0.346688	-4.523289
H	-4.387080	1.141381	-5.778178
H	-5.372637	-0.282791	-6.187140
H	-1.407610	-2.593653	-6.128142
H	-1.826322	-2.502488	-4.402274
H	-2.623469	-3.671166	-5.477201

5anti

Mo	0.089653	-0.007451	0.132233
O	-0.207988	-0.119973	1.792419
O	1.715066	0.048199	-0.307872
H	-1.185050	0.105795	-1.060113
Si	-3.430873	0.380612	-1.645331
N	-5.204761	1.099366	-2.086489
C	-5.581765	2.283988	-1.740315
C	-6.963103	2.779080	-1.942700
C	-8.029476	2.126557	-1.323499
C	-9.316392	2.623230	-1.451934
C	-9.550020	3.759319	-2.215815
C	-8.492984	4.408807	-2.837926
C	-7.199380	3.932836	-2.687841
C	-3.541215	-1.393849	-2.181816
C	-3.511677	0.528540	0.216556
C	-2.403825	1.415548	-2.802847
Cl	-0.427648	-2.263376	-0.457736
Cl	-0.396427	2.356743	-0.058435
C	-6.076145	0.221118	-2.867818
C	-4.663656	3.236789	-1.060167
H	-1.729211	0.728144	-3.325942
H	-6.374006	4.448145	-3.171331
H	-8.674081	5.295826	-3.435837
H	-10.559743	4.142149	-2.322655
H	-10.139827	2.121478	-0.954568
H	-7.844290	1.238929	-0.723727

H	-2.916439	1.355153	0.614195
H	-4.547766	0.630299	0.562534
H	-3.108115	-0.395201	0.644957
H	-1.755196	2.102665	-2.249251
H	-2.938729	1.991077	-3.567060
H	-2.604123	-1.868965	-1.860004
H	-4.358718	-1.937505	-1.697521
H	-3.618073	-1.517388	-3.266252
H	-5.489037	-0.206749	-3.683555
H	-6.434298	-0.605406	-2.247417
H	-6.929018	0.759454	-3.280922
H	-5.006009	3.381389	-0.028180
H	-3.617378	2.934860	-1.044222
H	-4.744206	4.216290	-1.542317

5syn

C	-1.297976	5.142584	5.331204
C	-1.556452	4.251367	4.301422
C	-0.668741	3.201931	4.060157
C	0.469557	3.057782	4.857434
C	0.735273	3.972882	5.862572
C	-0.153358	5.011957	6.105128
C	-0.936024	2.196877	3.009189
N	-1.077068	2.497688	1.754532
Si	-1.387520	1.245142	0.373045
C	-2.712767	0.017928	0.826900
C	-1.033939	0.796566	3.493903
C	0.306910	0.475535	0.175945
C	-1.800673	2.190098	-1.168993
Mo	-4.856322	3.688679	1.806243
O	-6.522963	3.455551	1.722341
O	-4.290540	4.984213	2.755244
Cl	-4.344732	1.994162	3.460592
Cl	-4.420052	4.637718	-0.333513
H	-3.765540	2.592187	1.046256
H	-3.404503	-0.054985	-0.019627
H	-2.295082	-0.977655	1.013039
H	-3.306206	0.325405	1.693358
H	-2.682664	2.830582	-1.066685
H	0.302211	-0.191628	-0.693531
H	-0.966472	2.788369	-1.547207
H	0.629351	-0.111802	1.040927
H	-2.028074	1.435407	-1.933004
H	1.061634	1.247985	-0.011588
H	-1.023829	0.042693	2.709126
H	-0.229419	0.595352	4.206025
H	-1.977309	0.713482	4.048260
H	1.167020	2.244526	4.674911
H	1.633046	3.868520	6.463028
H	0.046392	5.719929	6.903359
H	-2.003347	5.944258	5.523083
H	-2.462454	4.369054	3.711414
C	-0.890248	3.875690	1.271869
H	-0.233330	3.850793	0.398507
H	-1.851498	4.303127	0.967205
H	-0.439264	4.501320	2.039829

6syn

Mo	0.424061	-1.369019	-0.153376
O	-0.140453	-1.426519	1.435124
O	2.024776	-0.850929	-0.378407
Cl	-0.579447	0.759376	-0.804884

Cl	0.662332	-3.676159	-0.690554
H	-0.673575	-1.666540	-1.435526
Si	-3.373742	-0.227181	-3.130062
N	-1.666879	-0.631982	-3.797369
C	-1.092280	-1.802539	-3.747869
C	-0.985446	0.526633	-4.392853
C	-1.856360	-3.021272	-3.369539
C	0.318321	-2.028396	-4.110496
C	0.676800	-3.138642	-4.880852
C	2.010585	-3.423667	-5.116454
C	3.001670	-2.633735	-4.548767
C	1.324647	-1.226144	-3.565316
C	2.656327	-1.541690	-3.765694
C	-3.692954	-1.063923	-1.497465
C	-4.507705	-0.778910	-4.507172
C	-3.446669	1.620518	-2.930123
H	-4.211111	-0.347451	-0.850461
H	-4.323596	-1.953621	-1.588447
H	-2.764120	-1.335996	-0.986703
H	-2.692175	1.974816	-2.221386
H	-5.542517	-0.506566	-4.272138
H	-3.359813	2.181966	-3.863961
H	-4.477965	-1.860531	-4.671624
H	-4.430471	1.850092	-2.502525
H	-4.244230	-0.284858	-5.449240
H	-2.861188	-2.815752	-3.007928
H	-1.937398	-3.663917	-4.254769
H	-1.300817	-3.581396	-2.607881
H	-0.086329	-3.781135	-5.308692
H	2.277502	-4.279669	-5.727355
H	4.046873	-2.880154	-4.706166
H	3.420153	-0.942905	-3.281813
H	1.071492	-0.386642	-2.925058
H	-1.705885	1.071230	-5.008682
H	-0.615851	1.190832	-3.606166
H	-0.158279	0.206424	-5.024594

TS7

Mo	0.288537	-1.501230	-0.218429
O	-0.550245	-1.702713	1.225877
O	1.881196	-0.980514	-0.023167
Cl	-0.624192	0.645316	-0.842706
Cl	0.671055	-3.750918	-0.845400
H	-0.546770	-1.700511	-1.789121
Si	-3.336151	-0.216232	-3.114228
N	-1.630443	-0.617853	-3.703324
C	-1.008955	-1.773158	-3.499984
C	-0.967603	0.494372	-4.394937
C	-1.831081	-3.001202	-3.259441
C	0.387989	-2.003779	-3.956076
C	0.685562	-3.125501	-4.727818
C	1.995095	-3.396453	-5.099270
C	3.022894	-2.567091	-4.680678
C	1.430992	-1.165020	-3.555195
C	2.737278	-1.451760	-3.901648
C	-3.732323	-0.987908	-1.459363
C	-4.463376	-0.830974	-4.471917
C	-3.450917	1.639508	-2.988269
H	-4.250023	-0.235045	-0.854472
H	-4.395422	-1.854127	-1.552619
H	-2.845915	-1.281309	-0.890965
H	-2.713806	2.042996	-2.287848

H	-5.495194	-0.521682	-4.270299
H	-3.356788	2.159698	-3.945284
H	-4.455626	-1.922003	-4.558032
H	-4.445533	1.872015	-2.588697
H	-4.177123	-0.410980	-5.442674
H	-2.714651	-2.803858	-2.654777
H	-2.168948	-3.380505	-4.233518
H	-1.237033	-3.771693	-2.765647
H	-0.102916	-3.802161	-5.040749
H	2.210978	-4.273165	-5.701193
H	4.049663	-2.795411	-4.948134
H	3.537562	-0.812127	-3.545040
H	1.222436	-0.308239	-2.919768
H	-1.698307	0.985589	-5.043678
H	-0.579929	1.229932	-3.684452
H	-0.153676	0.129749	-5.020306

TS4syn

Mo	-4.579897	2.374750	2.320535
O	-6.240756	2.462652	2.149563
O	-4.124156	2.998859	3.809216
Cl	-4.070050	4.209254	0.916338
Cl	-4.459567	0.062118	2.755783
H	-3.134007	1.737551	1.209109
Si	-1.846361	1.305497	0.230494
N	-1.050115	2.796142	1.778674
C	-0.571548	4.049486	1.216318
C	-0.938789	2.557967	3.031174
C	-0.491617	3.569381	4.025445
C	-1.281190	4.694042	4.258997
C	-0.898704	5.620215	5.216779
C	0.275878	5.437695	5.934853
C	1.064442	4.319156	5.703618
C	0.675592	3.379008	4.760362
C	-1.285279	1.229596	3.612500
C	-2.810225	-0.262547	-0.209795
C	-0.086827	0.628321	0.346274
C	-2.062168	2.455904	-1.223343
H	-3.854551	-0.037418	-0.451612
H	-2.334628	-0.717587	-1.088725
H	-2.810434	-1.005091	0.594010
H	-3.127561	2.562903	-1.448719
H	0.080196	-0.017443	-0.524822
H	-1.638050	3.455556	-1.131374
H	0.058307	0.005903	1.235691
H	-1.586461	1.960889	-2.080254
H	0.680100	1.408312	0.352726
H	-1.641074	0.506369	2.877324
H	-0.400231	0.820267	4.114136
H	-2.055214	1.351013	4.383160
H	1.291751	2.500951	4.583520
H	1.982670	4.174100	6.263856
H	0.575339	6.167609	6.680387
H	-1.522737	6.488083	5.404253
H	-2.205661	4.826970	3.702122
H	0.004149	3.823881	0.313080
H	0.064886	4.606647	1.908207
H	-1.422539	4.673361	0.926653

TS(5anti→5syn)

Mo	-3.358071	-0.579476	0.118864

O	-3.567414	-0.832913	1.783186
O	-4.609729	-1.067855	-0.906573
H	-1.935751	0.092361	-0.514599
Si	0.259501	1.398168	-0.230042
N	2.155723	1.037806	-0.244684
C	2.652219	-0.151618	-0.122548
C	4.105533	-0.394559	0.014340
C	4.808141	0.173628	1.077970
C	6.153255	-0.107967	1.251020
C	6.811286	-0.936772	0.351564
C	6.118581	-1.499341	-0.711374
C	4.764849	-1.246811	-0.870391
C	0.102144	3.247143	-0.096583
C	-0.234196	0.667406	1.408330
C	-0.168904	0.877865	-1.966162
Cl	-3.641122	1.811734	0.077752
Cl	-1.784378	-2.386553	-0.269481
C	3.010744	2.209889	-0.448544
C	1.795417	-1.363232	-0.062971
H	-1.109937	1.357728	-2.253947
H	4.225034	-1.695875	-1.699271
H	6.631214	-2.146909	-1.414795
H	7.867192	-1.149294	0.483489
H	6.689727	0.320683	2.090993
H	4.291320	0.817581	1.784834
H	-0.420625	-0.407933	1.417361
H	0.550804	0.905965	2.139983
H	-1.154222	1.162318	1.737338
H	-0.292280	-0.198194	-2.109525
H	0.620424	1.245537	-2.637534
H	-0.978578	3.429065	-0.013855
H	0.567961	3.661273	0.803082
H	0.456546	3.793625	-0.975194
H	2.592077	2.800847	-1.267007
H	3.016509	2.837202	0.447369
H	4.032392	1.924879	-0.698149
H	1.805576	-1.752759	0.963321
H	0.756264	-1.225686	-0.363600
H	2.240479	-2.149119	-0.680640
TS5syn→6syn			
Mo	-2.036528	-1.041736	0.037707
O	-3.537958	-0.267863	-0.052430
Cl	-1.586335	-0.762591	2.379672
Cl	-1.334566	-0.673698	-2.253512
H	-0.605193	-0.102907	0.123815
O	-2.015927	-2.732738	-0.024822
Si	0.211607	2.947591	-0.087459
N	1.375698	1.492431	-0.359808
C	1.817377	0.660934	0.536983
C	2.519949	-0.588695	0.190209
C	1.932449	-1.523526	-0.667266
C	2.568302	-2.730875	-0.906543
C	3.802577	-2.999537	-0.331358
C	4.398830	-2.066870	0.507260
C	3.749862	-0.876618	0.787808
C	1.692385	1.302551	-1.784800
C	-0.837414	2.815292	1.440897
C	-0.881602	2.977992	-1.587851
C	1.392399	4.389888	-0.000765
C	1.604604	0.903074	1.982361
H	-1.418484	2.029770	-1.710667

H	0.965185	-1.324047	-1.122386
H	2.089451	-3.464447	-1.546236
H	4.299860	-3.943405	-0.531341
H	5.364638	-2.273691	0.956325
H	4.214794	-0.155759	1.454669
H	-1.237208	1.812133	1.621454
H	-0.338474	3.163184	2.349483
H	-1.698103	3.473561	1.267767
H	-0.360052	3.203438	-2.521532
H	-1.630355	3.762907	-1.428681
H	0.831125	5.325517	0.096530
H	2.054055	4.310528	0.868747
H	2.016389	4.471406	-0.896543
H	0.856989	0.812141	-2.294911
H	1.860710	2.283931	-2.235760
H	2.595871	0.704076	-1.899434
H	1.470122	1.955439	2.230463
H	0.704099	0.343988	2.289573
H	2.434477	0.491930	2.559737