Surporting Information

Mechanistic insights into hydrogen generation for catalytic hydrolysis and alcoholysis of silanes with high-valent oxorhenium(V) Complexes

1. Complete reference of 45.

2. Figure S1. The optimized structure of adducts **2*trans*** + H_2O-*anti*. **TS2**, **TS[2+2]** and **Int[2+2]**. Bond distances are shown in Å.

3. Figure S2. The optimized geometries of the ionic transition states **TS4*anti*** and the intermediates **4*anti*** with various alcohols, including CH_3OH, CH_3CH_2OH and t-BuOH for the oxorhenium(V) complex (**1**)-catalyzed the alcoholysis reactions.

4. Figure S3. The optimized structures of the ionic transition states **TS4*anti*** and the intermediates **4*anti*** with a varieties of silanes, including $EtMe_2SiH$, Et_2MeSiH, Et_3SiH, $PhMe_2SiH$, Ph_2MeSiH, Ph_3SiH and $BuMe_2SiH$ for the oxorhenium(V) complex (**1**)-catalyzed the hydrolysis reactions.

5. Figure S4. Optimized structures of the transition states **TS4anti-PhOH**, **TS5-PhOH** and the intermediates **4anti-PhOH, 4syn-PhOH** in oxorhenium(V) complex (1)-catalyzed the alcoholysis of phenol via the ionic mechanistic pathway.

6. Figure S5. Schematic free-energy surface (B3LYP) for the cationic high-valent oxorhenium complex $[Re(O)(hoz)_2]+$ (**1**) catalyzed the hydrolysis (black) and alcoholysis (blue) of silanes along the ionic mechanistic pathway.

7. Table S1. The calculated free energies of key intermediates and transition states at B3LYP and B3LYP-D levels of theory are listed for the oxorhenium(V) complex (**1**) catalyzing the hydrosilylation.

8. Figure S6. Isomers of η^1-silane-rhenium(V) adduct: **2trans-2, 2cis-2, 2cis-3, 2cis-4** (with ΔG (optimized in gas-phase) in the parenthesis, **2trans** is set to zero).

9. Figure S7.The energy plot versus d(H···Si) or d(Si···O(OH)) for searching the transition state **TS8*trans*, TS8*cis*** from complex **2*trans*+OH or 2*cis*+OH** (note: Taking Si···O(OH) separation as the reaction coordinate, the search for transition state in such an arrangement has been unsuccessful. The energy plot versus d(Si···O(OH)) went uphill, till to obtain the dissociative neutral rhenium hydride species (1H*trans*) and the solvated Me_3SiOH^+ ion.

10. Figure S8. The energy plot versus d(H···Si) for searching the transition state **TS9** and the rhenium(VII) intermediate **9** from complex **2*trans* or 2*cis*** (note: Taking H···Si separation as the reaction coordinate, the search for transition state in such an arrangement has been unsuccessful. The energy plot versus d(H···Si) goes uphill.

11. Figure S9. The energy plot versus d(H···Si) for searching the transition state **TS10** and the rhenium(VII) intermediat**e 10-2** from silane-rhenium complex **10** (note: Taking H···Si separation as the reaction coordinate, the search for transition state in such an arrangement has been unsuccessful. The energy plot versus d(H···Si) goes uphill.

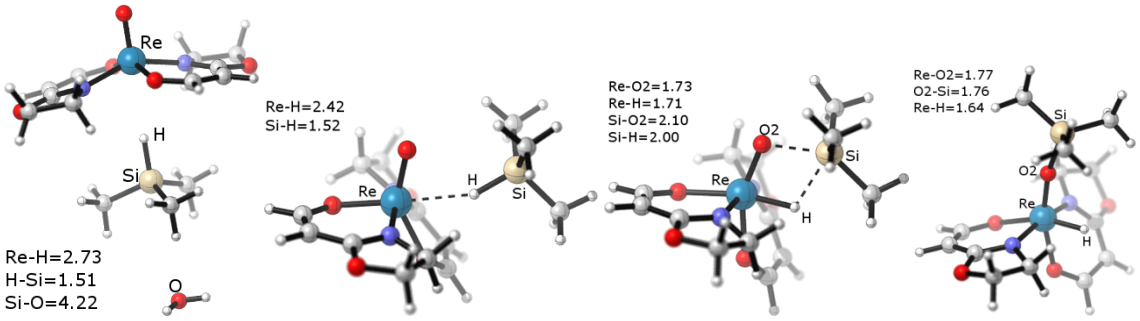
12. Equation 1 Two reactions for generation of **1Htrans/1Hcis** and **1-OHtrans/1OH-cis** with B $(C_6F_5)_4^-$.

13. Table S2. Cartesian coordinates for all optimized structures in XYZ format.

Complete reference of 45.

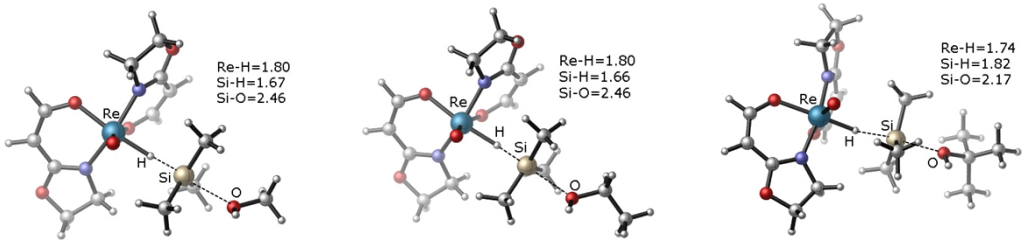
Frisch, M. J. et al. *Gaussian 09*; Gaussian, Inc. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, 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 optimized structure of adducts 2*trans* + H_2O-*anti,***TS2**, **TS[2+2]** and **Int[2+2]**. Bond distances are shown in Å.



2*trans* + H_2O-*anti* **TS2** **TS[2+2]** **Int[2+2]**

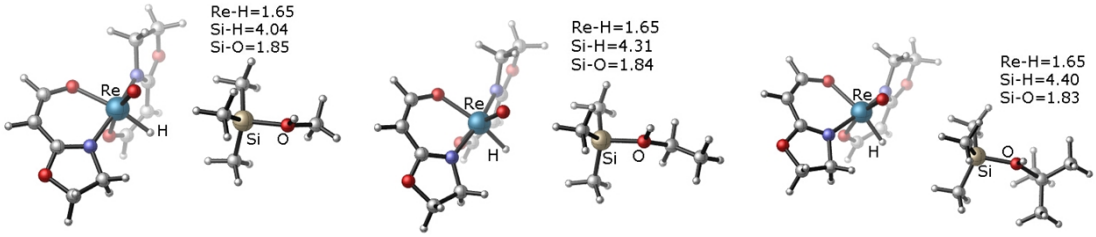
Figure S2. The optimized geometries of the ionic transition states **TS4*anti*** and the intermediates **4*anti*** with various alcohols, including CH_3OH, CH_3CH_2OH and t-BuOH for the oxorhenium(V) complex (**1**)-catalyzed the alcoholysis reactions.



TS4anti (15.4 kcal/mol)
1+HSiMe$_3$+CH$_3$OH

TS4anti (15.8 kcal/mol)
1+HSiMe$_3$+CH$_3$CH$_2$OH

TS4anti (17.2 kcal/mol)
1+HSiMe$_3$+t-BuOH

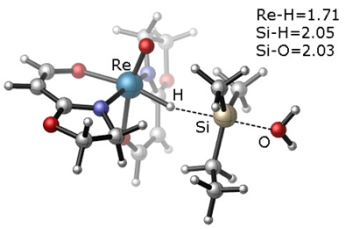


4anti (15.8 kcal/mol)
1+HSiMe$_3$+CH$_3$OH

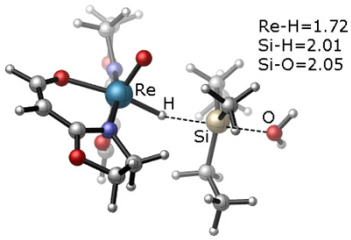
4anti (15.4 kcal/mol)
1+HSiMe$_3$+CH$_3$CH$_2$OH

4anti (15.9 kcal/mol)
1+HSiMe$_3$+t-BuOH

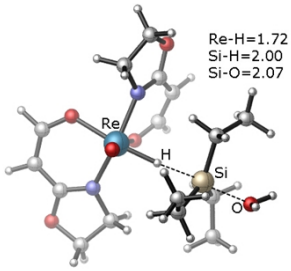
Figure S3. The optimized structures of the ionic transition states TS4anti and the intermediates 4anti with a varieties of silanes, including EtMe2SiH, Et2MeSiH, Et3SiH, PhMe2SiH, Ph2MeSiH, Ph3SiH and BuMe2SiH for the oxorhenium(V) complex (1)-catalyzed the hydrolysis reactions. Bond distances are shown in Å.



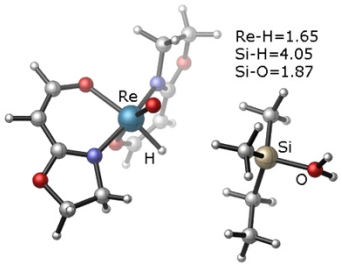
TS4anti (14.0 kcal/mol)
1+EtMe$_2$SiH+H$_2$O



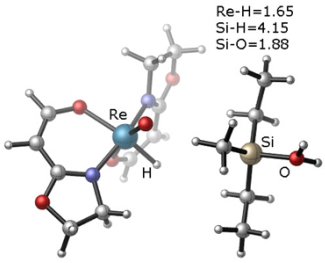
TS4anti (14.8 kcal/mol)
1+ Et$_2$MeSiH+ H$_2$O



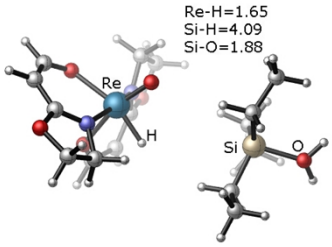
TS4anti (16.5 kcal/mol)
1+ Et$_3$SiH+ H$_2$O



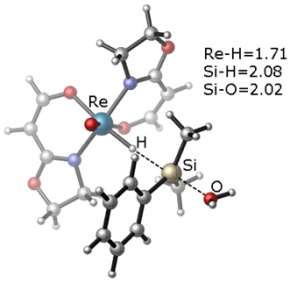
4anti (16.1 kcal/mol)
1+EtMe$_2$SiH+H$_2$O



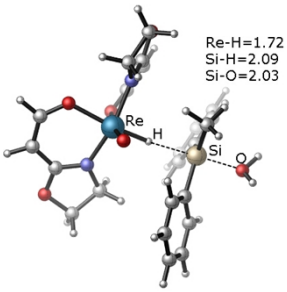
4anti (15.9 kcal/mol)
1+ Et$_2$MeSiH+ H$_2$O



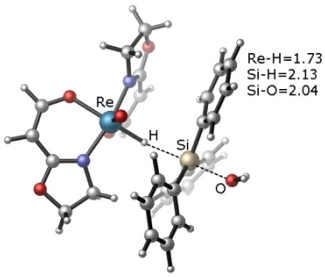
4anti (18.9 kcal/mol)
1+ Et$_3$SiH+ H$_2$O



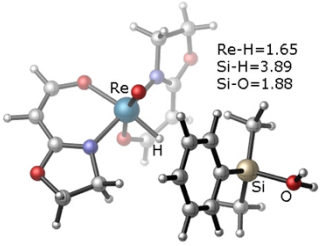
TS4anti (15.2 kcal/mol)
1+PhMe$_2$SiH+H$_2$O



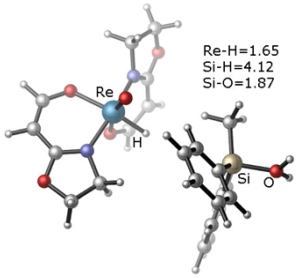
TS4anti (13.3 kcal/mol)
1+ Ph$_2$MeSiH+ H$_2$O



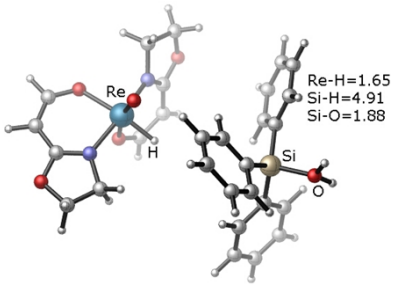
TS4anti (13.5 kcal/mol)
1+ Ph$_3$SiH+ H$_2$O



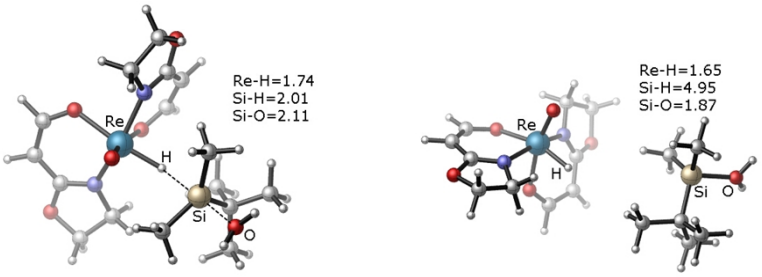
4anti (17.6 kcal/mol)
1+PhMe$_2$SiH+H$_2$O



4anti (17.2 kcal/mol)
1+ Ph$_2$MeSiH+ H$_2$O



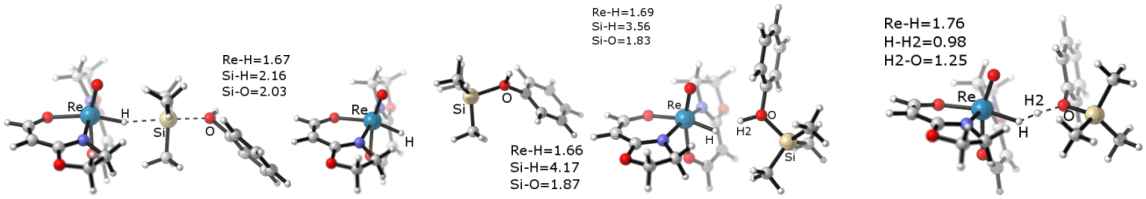
4anti (19.1 kcal/mol)
1+ Ph$_3$SiH+ H$_2$O



TS4anti (20.7 kcal/mol)
1+BuMe$_2$SiH + H$_2$O

4anti (19.5 kcal/mol)
1+BuMe$_2$SiH + H$_2$O

Figure S4. Optimized structures of the transition states **TS4*anti*-PhOH**, **TS5-PhOH** and the intermediates **4*anti*-PhOH**, 4*syn*-PhOH in oxorhenium(V) complex (**1**)-catalyzed the alcoholysis of phenol via the ionic mechanistic pathway. Bond distances are shown in Å.



TS4*anti*-PhOH **4*anti*-PhOH** **4*syn*-PhOH** **TS5-PhOH**

Figure S5. Schematic free-energy surface (B3LYP level) for the cationic high-valent oxorhenium complex $[Re(O)(hoz)_2]^+$ (**1**) catalyzed the hydrolysis (black) and alcoholysis (blue) of silanes along the ionic mechanistic pathway .

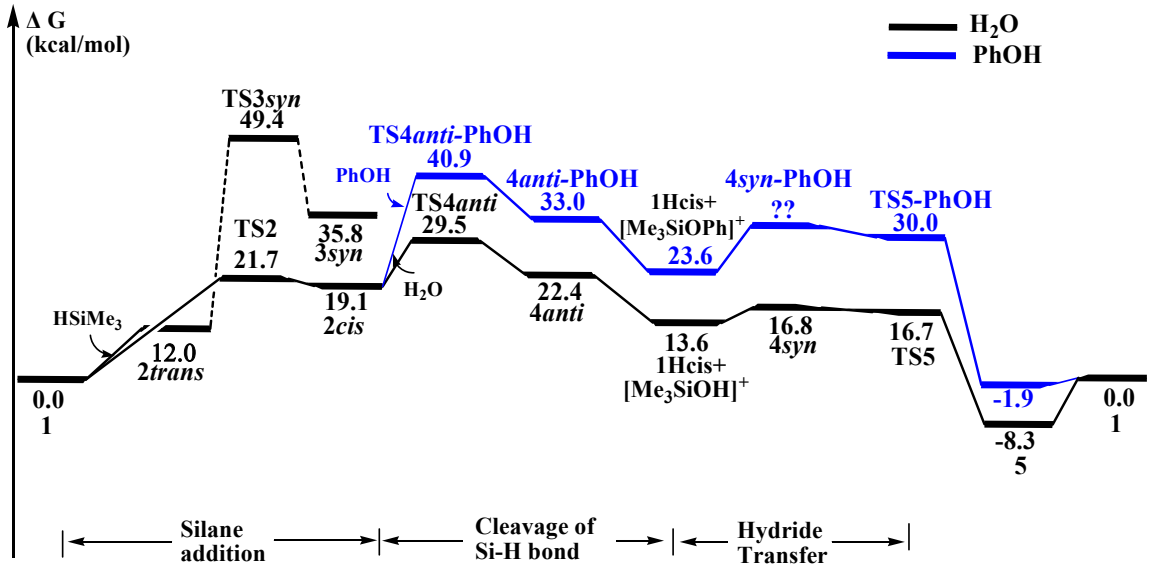
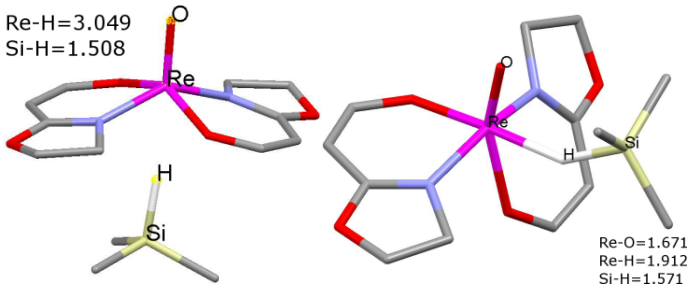


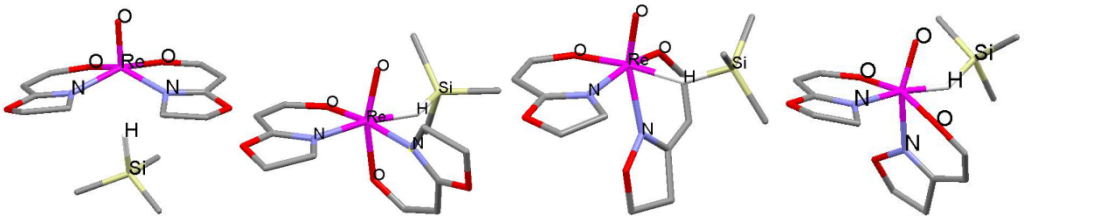
Table S1 The calculated free energies of key intermediates and transition states at B3LYP and B3LYP-D levels of theory are listed for oxorhenium(V) complex (**1**) catalyzing the hydrosilylation. (a---H2O, b---PhOH)

	SMD//B3LYP 6-311G(d,p) Lan2L2DZ	SMD//B3LYP-D 6-311G(d,p) Lan2L2DZ
1	0.0	0.0
2trans	12.0	3.5
TS2	21.7	13.2
2cis	19.1	10.0
TS4anti[a]	29.5	15.7
4anti	22.4	17.2
TS4syn	45.1	31.8
4syn	16.8	13.8
TS5	16.7	8.7
5	-8.3	-10.8
TS4anti[b]	40.9	23.9
4anti	33.0	25.0
TS4syn	55.2	37.3
TS5	30.0	13.7
5	-1.9	-7.5
TS3syn[a]	49.4	34.4
3syn	35.8	28.2

Figure S6. Isomers of η^1-silane-rhenium(V) adduct: 2*trans*-2, 2*cis*-2, 2*cis*-3, 2*cis*-4 (with ΔG (optimized in the gas-phase) in the parenthesis, 2*trans* is set to zero).



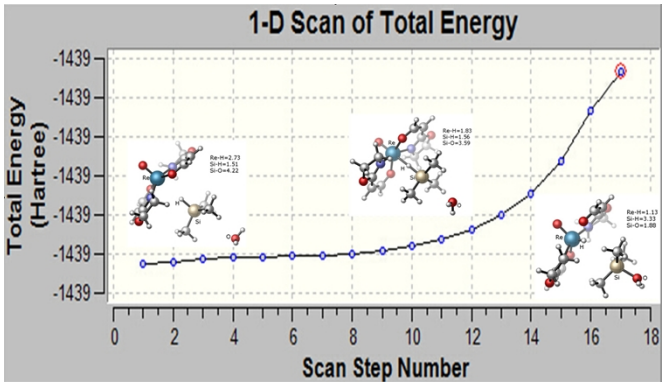
2_*trans*(0.0kcal/mol) **2*cis*(6.5 kcal/mol)**



2_*trans*-2 (13.2kcal/mol) **2_*cis*-2** (7.7 kcal/mol) **2_*cis*-3**(47.5kcal/mol) **2_*cis*-4** (44.3 kcal/mol)

Figure S7.The energy plot versus d(Si···O(OH)) for searching the transition state TS8*trans*, TS8*cis* from complex 2*trans*+OH or 2*cis*+OH (note: Taking Si···O(OH) separation as the reaction coordinate, the search for transition state in such an arrangement has been unsuccessful. The energy plot versus d(H···Si) or d(Si···O(OH)) goes uphill, till to obtain the dissociative neutral rhenium hydride species (1H*trans*) and the solvated Me_3SiOH^+ ion.

Scan for TS8trans



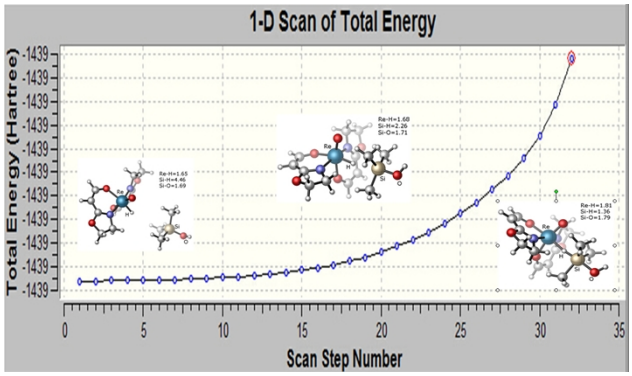


Figure S8. The energy plot versus d(H···Si) for searching the transition state TS9 and the rhenium(VII) intermediate 9 from complex 2*trans* or 2*cis* (note: Taking H···Si separation as the reaction coordinate, the search for transition state in such an arrangement has been unsuccessful. The energy plot versus d(H···Si) goes uphill.

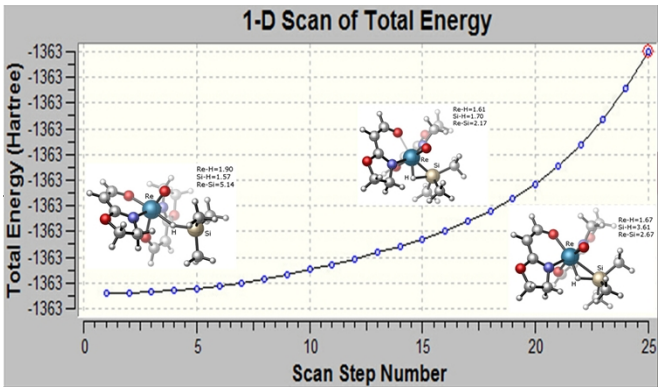
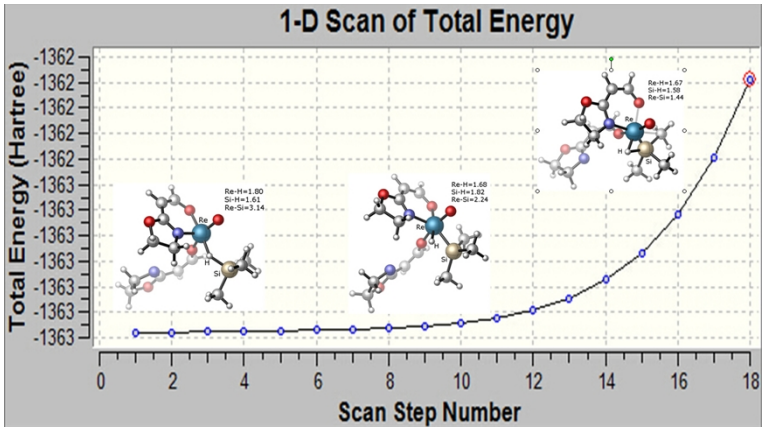


Figure S9. The energy plot versus d(H···Si) for searching the transition state TS10 and the rhenium(VII) intermediate 10-2 from silane-rhenium complex 10 (note: Taking H···Si separation as the reaction coordinate, the search for transition state in such an arrangement has been unsuccessful. The energy plot versus d(H···Si) goes uphill.



Equation 1 Two reactions for the generation of 1Htrans/1Hcis and 1-OHtrans/1OH-cis with B $(C_6F_5)_4^-$.

$$1 + H_2O + B(C_6F_5)_4^- \rightarrow 1\text{-OH}\textit{trans} + HB(C_6F_5)_2 + (C_6F_5)_2 ; \quad \Delta G = 11.3 \text{ kcal/mol}$$

$$1 + H_2O + B(C_6F_5)_4^- \rightarrow 1\text{-OH}\textit{cis} + HB(C_6F_5)_2 + (C_6F_5)_2 ; \quad \Delta G = 12.0 \text{ kcal/mol}$$

The reaction to generate the rhenium hydroxo complex (**1-OH**) with the cation $B(C_6F_5)_4^-$ under the experimental environment is calculated to be endergonic too.

Table S2. Cartesian coordinates for all optimized structures in XYZ format.

Optimized under solvent conditions

1	**$[Re(O)(hoz)_2]^+$**		
Re	0.296861	-0.151071	0.250688
O	-0.399832	-0.176016	2.141266
O	1.947518	-0.171142	0.420922
N	-0.418747	-2.041126	0.067553
O	0.052078	-0.117609	-1.752635
N	-0.352693	1.763131	0.305852
C	-0.650258	-1.229841	2.879594
C	-0.783834	-2.514617	2.452895
C	-0.722844	-2.853765	1.080279
O	-1.021507	-4.087472	0.726741
C	-0.813529	-4.224119	-0.721440
C	-0.664126	-2.781963	-1.204210
C	-0.167959	0.925003	-2.514841
C	-0.427876	2.200174	-2.114003
C	-0.515345	2.562580	-0.749315
O	-0.808625	3.812421	-0.450152
C	-0.702119	3.979640	1.006538
C	-0.676222	2.546204	1.533246
H	-0.770257	-0.998909	3.936892
H	-1.002123	-3.300200	3.161504
H	0.085988	-4.824112	-0.857190
H	-1.679665	-4.743102	-1.123879
H	0.167781	-2.654272	-1.890384
H	-1.573646	-2.402187	-1.671385
H	-0.141022	0.695671	-3.579040
H	-0.595277	2.971977	-2.851339
H	-1.559806	4.562436	1.331446
H	0.222502	4.526504	1.192809
H	0.086344	2.394731	2.292592
H	-1.640146	2.224295	1.927473

2trans			
Re	0.005838	0.002168	0.024002
O	0.021510	0.008633	1.682210
O	1.981505	-0.070215	-0.413587
N	-0.025865	1.958826	-0.517365
O	-1.966220	0.076236	-0.381199
N	0.018209	-1.958001	-0.504340
H	-0.112715	-0.114814	-2.719409
Si	-0.315290	-0.187225	-4.209020
C	-2.760704	-0.946462	-0.584818
C	-2.411788	-2.255464	-0.729097
C	-1.065506	-2.699220	-0.713468
O	-0.824395	-3.975224	-0.950300
C	0.613811	-4.217947	-0.768666
C	1.216934	-2.813033	-0.718944
C	2.763307	0.956979	-0.638723
C	2.400685	2.261428	-0.793396
C	1.053273	2.700634	-0.752547
O	0.804954	3.976080	-0.985619
C	-0.627944	4.217640	-0.765447
C	-1.229459	2.812642	-0.707712
C	0.361448	1.398468	-4.967009
C	-2.163577	-0.353298	-4.531072
C	0.619311	-1.693678	-4.846186
H	-3.812722	-0.671050	-0.644553
H	-3.181116	-2.995581	-0.895847
H	0.948778	-4.821251	-1.608492
H	0.725499	-4.770674	0.163947
H	1.922958	-2.690695	0.098698
H	1.704684	-2.531721	-1.652991
H	3.817052	0.690842	-0.710722
H	3.162124	3.005165	-0.979333
H	-0.715066	4.764644	0.173221
H	-0.984969	4.826159	-1.592174
H	-1.735351	2.533680	-1.632516
H	-1.919457	2.688172	0.123146
H	1.430097	1.517574	-4.762072
H	-0.153771	2.282587	-4.577975
H	0.231071	1.392184	-6.054592
H	-2.721729	0.484412	-4.101219
H	-2.367555	-0.370178	-5.607215
H	-2.563847	-1.277885	-4.104224
H	0.499081	-1.789224	-5.930831
H	0.248548	-2.618294	-4.392522
H	1.691606	-1.619457	-4.639319

TS2			
C	0.399968	1.312172	-4.465186
C	0.420639	0.253884	-3.358753
N	0.358191	1.073503	-2.124690
C	0.583166	2.333200	-2.455550
O	0.687263	2.564823	-3.750946
Re	0.094173	0.351319	-0.228347
O	-1.569144	0.364774	-0.087791
C	0.759061	3.420366	-1.556042
C	0.836087	3.233097	-0.216739
O	0.719375	2.094580	0.445484
N	0.632433	-0.283558	1.649333
C	1.347767	-1.346815	1.974484
O	1.495225	-1.545452	3.277133
C	0.661322	-0.561458	3.978109
C	0.340590	0.470541	2.895500
C	2.017765	-2.210472	1.070202
C	2.152748	-1.876456	-0.242555
O	1.629199	-0.826627	-0.828540
H	-0.648345	-1.888462	-0.774785
H	2.768694	-2.491133	-0.896514
H	1.338820	-0.335133	-3.349631
H	-0.577476	1.430851	-4.932007
H	-0.435693	-0.415972	-3.409993
H	0.982689	1.351092	2.943392
H	-0.701384	0.786123	2.915625
H	-0.221130	-1.087737	4.343063
H	1.243871	-0.174875	4.810226
H	1.169373	1.188594	-5.222775
H	1.032329	4.077251	0.440793
H	0.894638	4.409771	-1.968362
H	2.528297	-3.077130	1.465124
Si	-1.636816	-3.032457	-0.882599
C	-2.389254	-3.281457	0.820942
C	-0.664491	-4.537898	-1.452979
C	-2.932894	-2.529642	-2.147669
H	-3.135471	-4.083022	0.799051
H	-1.629250	-3.555214	1.558972
H	-2.889104	-2.372771	1.169826
H	-1.334072	-5.392376	-1.600506
H	-0.156232	-4.348184	-2.403634
H	0.091086	-4.830918	-0.718107

H	-3.713044	-3.295610	-2.217146
H	-3.416882	-1.587475	-1.873844
H	-2.497827	-2.411491	-3.144938

2cis

C	0.314092	1.124133	-4.536844
C	0.193114	0.081936	-3.420817
N	0.236933	0.906876	-2.191391
C	0.607343	2.130094	-2.529190
O	0.733449	2.340215	-3.829786
Re	-0.014857	0.203533	-0.279485
O	-1.662663	0.412274	-0.061856
C	0.912469	3.199427	-1.645620
C	0.995767	3.021221	-0.301673
O	0.776112	1.914813	0.372651
N	0.433204	-0.463315	1.631402
C	1.232709	-1.443093	1.994798
O	1.314029	-1.647007	3.308403
C	0.347436	-0.756135	3.957277
C	-0.022510	0.239585	2.854548
C	2.056322	-2.215005	1.131902
C	2.276660	-1.822201	-0.155544
O	1.702997	-0.807694	-0.745893
H	-0.538805	-1.534112	-0.843417
H	3.014367	-2.348646	-0.760134
H	1.026689	-0.623004	-3.406562
H	-0.634535	1.348726	-5.023883
H	-0.743700	-0.470634	-3.469853
H	0.504846	1.191169	2.943155
H	-1.094126	0.430588	2.805582
H	-0.495600	-1.368696	4.278449
H	0.838983	-0.309710	4.817857
H	1.076062	0.901851	-5.279873
H	1.291174	3.855140	0.333145
H	1.146891	4.162772	-2.074629
H	2.617692	-3.036845	1.552573
Si	-1.517097	-2.761157	-0.833978
C	-1.980763	-3.096273	0.943107
C	-0.474885	-4.100577	-1.620079
C	-2.959861	-2.228189	-1.893865
H	-2.644971	-3.967186	0.980739
H	-1.105171	-3.318302	1.557898
H	-2.515682	-2.251165	1.383587
H	-1.090259	-4.993080	-1.781247
H	-0.084868	-3.786204	-2.592392
H	0.367582	-4.385668	-0.985128
H	-3.697039	-3.038179	-1.932384
H	-3.453574	-1.343226	-1.484882
H	-2.649702	-2.012901	-2.920032

TS4anti (H_2O)

Re	0.464957	0.328296	-0.513239
O	0.542620	-0.289418	-2.069422
O	1.679007	-0.876129	0.696335
N	-1.144837	-0.710155	0.233068
O	0.122058	1.527074	1.169866
H	-0.492566	1.589873	-1.123793
Si	-1.499540	2.939819	-2.336575
O	-2.613202	4.269660	-3.333628
H	-2.756128	5.149645	-2.945287
H	-2.504545	4.375870	-4.294098
C	0.148300	3.675939	-2.816786
N	2.192680	1.500354	-0.629876
C	-2.145274	1.526439	-3.370958
C	-2.343237	3.445873	-0.745440
C	0.534812	2.728354	1.428625
C	1.597689	3.357162	0.836985
C	2.444584	2.655657	-0.060751
O	3.666879	3.150492	-0.302832
C	4.311320	2.268143	-1.274057
C	3.446868	1.005188	-1.241730
C	1.326507	-1.949321	1.328574
C	0.060478	-2.447717	1.490422
C	-1.091038	-1.786666	1.004795
O	-2.278709	-2.259871	1.382335
C	-3.314516	-1.496493	0.687755
C	-2.559156	-0.280096	0.151422
H	-2.034395	2.834121	0.100543
H	-3.428521	3.358908	-0.854757
H	-2.106168	4.488479	-0.508088
H	0.361474	4.573610	-2.229382
H	0.139573	3.956117	-3.874952
H	0.961192	2.966016	-2.664019
H	-2.134931	1.807318	-4.429691
H	-1.531402	0.632129	-3.263023
H	-3.176350	1.284285	-3.099983
H	1.902242	4.338541	1.171266
H	4.290404	2.771119	-2.242408
H	5.339155	2.116309	-0.952688
H	3.254348	0.603730	-2.236598
H	3.869320	0.214680	-0.617147
H	2.153425	-2.494813	1.789049
H	-0.085892	-3.348608	2.068931
H	-3.715439	-2.133971	-0.101558
H	-4.092253	-1.262672	1.411048
H	-2.702095	0.608465	0.770826
H	-2.827691	-0.044676	-0.876600
H	-0.003195	3.246757	2.224766

4anti (H_2O)

Re	0.452036	0.160631	-0.091547
O	0.187500	-0.134664	-1.721822
O	1.841665	-1.202338	0.750736
N	-1.028604	-1.004324	0.734947
O	0.521537	0.988347	1.876751
H	-0.527548	1.492517	-0.150249
Si	-1.828358	3.652849	-3.232832
O	-2.619934	4.871924	-4.414861
H	-2.683106	5.821833	-4.198027
H	-2.535689	4.763367	-5.381531
C	-0.022512	4.069831	-3.279977
N	2.138932	1.368295	-0.331861
C	-2.301494	2.059963	-4.050126
C	-2.714789	4.090312	-1.667046
C	0.936793	2.161013	2.210174
C	1.807280	2.950426	1.494942
C	2.472180	2.438468	0.353135
O	3.619883	3.020549	-0.037027
C	4.074998	2.323001	-1.236550
C	3.262938	1.025509	-1.229228
C	1.569056	-2.359654	1.251653
C	0.332305	-2.892176	1.524466
C	-0.871031	-2.180255	1.323619
O	-1.997655	-2.714238	1.806560

C	-3.113065	-1.875680	1.371382
C	-2.430635	-0.577489	0.941729
H	-2.340541	3.452673	-0.858815
H	-3.792451	3.928973	-1.754559
H	-2.534978	5.128530	-1.372068
H	0.169890	5.088900	-2.932488
H	0.393585	3.955204	-4.285062
H	0.514927	3.384373	-2.615487
H	-1.903657	1.992479	-5.067229
H	-1.876234	1.227379	-3.479371
H	-3.386167	1.928548	-4.085250
H	2.144881	3.890489	1.907730
H	3.849829	2.957331	-2.096255
H	5.149863	2.180550	-1.150284
H	2.894663	0.756120	-2.219358
H	3.817251	0.178286	-0.817128
H	2.444971	-2.967603	1.495335
H	0.265907	-3.872255	1.975201
H	-3.606503	-2.390384	0.544978
H	-3.796706	-1.772784	2.210917
H	-2.465063	0.191807	1.717635
H	-2.846691	-0.170836	0.021150
H	0.589351	2.528018	3.180242

1Hcis

Re	0.324602	1.117176	-4.534589
O	0.200013	-0.020653	-3.309847
N	0.459843	2.781493	-3.278988
O	-1.582267	1.925330	-5.031795
N	0.129267	-0.087858	-6.190065
O	0.976248	2.545802	-5.975764
H	1.971192	0.978567	-4.539888
C	-2.411120	1.438787	-5.889904
C	-2.197264	0.425107	-6.793910
C	-0.951158	-0.223689	-6.943037
O	-0.803397	-1.054233	-7.981334
C	0.504635	-1.696282	-7.859466
C	1.237570	-0.816317	-6.846847
C	1.747469	3.559289	-5.778270
C	1.960490	4.196531	-4.579017
C	1.190211	3.859664	-3.437412
O	1.093123	4.756858	-2.439349
C	0.288103	4.146112	-1.385433
C	-0.397331	2.972780	-2.090721
H	0.966126	3.822814	-0.592906
H	-0.394838	4.903759	-1.007296
H	-0.413778	2.068850	-1.481745
H	-1.418387	3.203363	-2.406555
H	-3.396442	1.914736	-5.892942
H	-2.991314	0.145933	-7.471930
H	0.954461	-1.719604	-8.849550
H	0.337602	-2.712713	-7.498595
H	1.910754	-0.099033	-7.323477
H	2.235245	3.963473	-6.670031
H	1.799282	-1.395642	-6.115702
H	2.580994	5.080484	-4.539511

$SiMe_3OH^+$

C	0.026389	0.000002	-0.045212
Si	0.009149	-0.000002	1.828322
O	1.635504	-0.000002	2.266073
H	1.831312	0.000000	3.209620
C	-0.849664	-1.534234	2.493474
C	-0.849666	1.534227	2.493480
H	-0.833196	-1.563128	3.588535
H	-1.900119	-1.557276	2.182260
H	-0.374795	-2.450547	2.127776
H	-0.374800	2.450542	2.127783
H	-1.900122	1.557268	2.182269
H	-0.833196	1.563118	3.588541
H	0.537367	0.885137	-0.437302
H	0.537370	-0.885129	-0.437305
H	-0.993016	0.000001	-0.445912

4syn (H_2O)

Re	-1.686417	-0.195569	-0.310322
O	-3.202228	-0.912498	-0.272004
N	-0.613906	-1.859516	0.352111
O	-1.145168	0.591746	1.582624
N	-2.193397	1.724658	-0.847019
O	0.273005	0.470827	-0.828907
H	-1.486157	-0.662680	-1.887010
Si	-1.921417	-2.675896	-6.252446
C	-0.417617	-2.493265	-5.184706
O	-3.219793	-3.412726	-5.126935
C	-2.794919	-1.100701	-6.700088
C	-1.771605	-3.923845	-7.613740
C	1.272897	-0.255388	-1.192111
C	1.450362	-1.591805	-0.918551
C	0.575204	-2.264938	-0.029330
O	1.013906	-3.377507	0.584761
C	-0.075016	-3.871397	1.423151
C	-1.034578	-2.681327	1.507008
C	-1.421927	1.770353	2.027823
C	-1.955601	2.830288	1.335621
C	-2.240887	2.779281	-0.046867
O	-2.565705	3.924011	-0.656197
C	-2.932201	3.611420	-2.036143
C	-2.383877	2.198082	-2.235796
H	-3.182417	-4.254585	-4.634541
H	-3.883732	-2.801317	-4.754666
H	2.068668	0.269632	-1.728235
H	2.366746	-2.084933	-1.210679
H	-0.515329	-4.735398	0.921821
H	0.351233	-4.171862	2.377643
H	-2.079212	-2.976639	1.406942
H	-0.918523	-2.104975	2.428362
H	-1.180589	1.926327	3.082998
H	-2.105036	3.772469	1.843540
H	-4.020337	3.661172	-2.105009
H	-2.481819	4.366039	-2.677110
H	-1.423306	2.190903	-2.757335
H	-3.079887	1.550324	-2.767010
H	-0.027461	-3.460704	-4.858084
H	-0.611009	-1.875035	-4.304218
H	0.368081	-2.001978	-5.770466
H	-2.971351	-0.463409	-5.828614
H	-2.171669	-0.533048	-7.399692
H	-3.750295	-1.296342	-7.195307
H	-2.721163	-4.076961	-8.132756
H	-1.047731	-3.547616	-8.346097
H	-1.401135	-4.886994	-7.253821

TS5 (H_2O)

Re	1.328332	0.197681	-0.257313
O	-0.141699	-0.258352	-0.928319
O	2.728826	-0.563758	-1.523781
N	1.699550	-1.383275	0.987478
O	2.736959	1.133415	0.916432
N	1.564278	1.925112	-1.403388
C	2.957287	2.404537	1.100315
C	2.589576	3.402432	0.243049
C	2.032835	3.092953	-1.027694
O	2.059342	4.025127	-1.983584
C	1.409303	3.459508	-3.168047
C	1.358932	1.958425	-2.869228
C	3.288250	-1.741561	-1.475616
C	3.186181	-2.670863	-0.481555
C	2.459424	-2.432441	0.711232
O	2.558502	-3.321223	1.691644
H	0.818106	-3.591249	2.778672
C	1.667327	-2.907378	2.780234
C	1.289087	-1.471932	2.406866
H	3.523033	2.652746	1.998427
H	2.869842	4.425393	0.448629
H	0.419747	3.912173	-3.246199
H	2.012937	3.724154	-4.032758
H	0.400650	1.508697	-3.129066
H	2.156393	1.397963	-3.361243
H	3.912995	-1.966827	-2.340229
H	3.725425	-3.603445	-0.565265
H	2.223469	-3.000234	3.709813
H	1.838605	-0.726695	2.986634
H	0.221084	-1.283516	2.504158
H	0.418724	0.932356	1.054567
H	-0.233184	1.574272	0.728008
O	-1.224552	2.345956	0.546918
H	-1.681702	2.085704	-0.268112
Si	-2.143886	3.216626	1.769910
C	-0.906616	3.429970	3.146341
C	-3.594749	2.137001	2.232588
C	-2.657640	4.821839	0.970644
H	-0.020787	3.975406	2.808459
H	-0.584203	2.469157	3.558410
H	-1.357801	4.003883	3.962567
H	-3.262328	1.178446	2.642575
H	-4.209578	2.630616	2.992809
H	-4.238104	1.934465	1.370389
H	-3.240802	5.424597	1.675252
H	-3.281691	4.654195	0.087076
H	-1.786728	5.410460	0.667811

5 (H_2O)

Re	-1.494016	-0.330155	0.002556
O	-2.742969	-1.368569	-0.326925
N	-0.017169	-1.470580	0.806480
O	-1.854205	0.221149	1.912870
N	-2.105828	1.505164	-0.594483
O	-0.446082	-0.284839	-1.722249
Si	-2.278629	-2.416495	-6.645697
C	-1.611652	-3.084444	-5.018395
C	-1.318244	-0.899849	-7.182253
C	-2.204682	-3.763603	-7.954553
C	0.568860	-1.046212	-2.054552
C	1.254646	-1.906369	-1.253111
C	0.961678	-2.061818	0.124024
O	1.735200	-2.852386	0.842459
C	1.178011	-2.942087	2.199600
C	0.152271	-1.809284	2.247086
C	-2.549506	1.256957	2.315251
C	-3.012074	2.287521	1.555658
C	-2.751728	2.388221	0.167071
O	-3.163350	3.467450	-0.468508
C	-2.885240	3.299847	-1.902068
C	-1.940751	2.098844	-1.951385
H	0.867759	-0.936300	-3.095707
H	2.079416	-2.473286	-1.659736
H	0.734097	-3.932989	2.293289
H	2.003752	-2.829437	2.897256
H	0.517131	-0.935036	2.786828
H	-0.795263	-2.122551	2.678071
H	-2.745959	1.254947	3.386399
H	-3.572368	3.085241	2.021390
H	-3.842824	3.119194	-2.389812
H	-2.447972	4.229012	-2.258093
H	-0.900297	2.389510	-2.096996
H	-2.219102	1.380730	-2.718082
H	-2.185356	-3.951650	-4.673639
H	-1.648258	-2.325915	-4.229369
H	-0.569234	-3.403951	-5.127280
H	-1.406001	-0.094621	-6.445581
H	-0.253608	-1.129719	-7.297437
H	-1.680306	-0.517555	-8.141908
H	-1.174690	-4.107662	-8.100960
H	-2.573943	-3.403493	-8.920353
H	-2.803174	-4.636322	-7.670921
H	-4.524010	-2.528741	-6.230887
O	-3.858762	-1.867193	-6.451087

TS3syn

Re	1.323315	0.237229	-0.731936
N	2.072250	0.411397	-2.654625
O	3.115709	0.764448	-0.035019
O	0.395871	1.631265	-0.799052
N	0.967642	-0.381668	1.181567
O	-0.222705	-1.004772	-1.387059
C	1.378166	0.044621	-3.912965
C	2.250131	0.704192	-4.986891
O	3.469949	1.078940	-4.263378
C	3.232653	0.953107	-2.964813
C	4.243038	1.387926	-2.060456
C	4.134808	1.248797	-0.714270
C	1.748594	0.003542	2.385304
C	1.008882	-0.713350	3.519685
O	-0.204154	-1.237194	2.877958
C	-0.106674	-1.046177	1.574129
C	-1.157434	-1.553787	0.757762
C	-1.150159	-1.511130	-0.600394
H	0.359810	0.430023	-3.908926
H	1.347222	-1.041177	-4.015575
H	2.541779	0.040467	-5.797082
H	1.820742	1.622522	-5.386926
H	5.142812	1.813041	-2.481335
H	4.962110	1.560921	-0.078988
H	1.730767	1.088612	2.494226
H	2.782258	-0.320212	2.286106
H	0.689245	-0.057332	4.325980
H	1.548567	-1.569321	3.923015

H	-1.986620	-2.028719	1.262757
H	-1.980303	-1.965219	-1.140482
H	2.156909	-1.565554	-0.963259
Si	2.840048	-3.150769	-1.161635
C	4.371249	-2.445404	-1.993332
C	2.876528	-3.301720	0.724065
C	2.824484	-4.988599	-1.683662
H	4.168721	-2.197994	-3.039752
H	5.164919	-3.200239	-1.987117
H	4.741180	-1.546366	-1.496849
H	3.209563	-2.378668	1.202960
H	1.883892	-3.550009	1.114308
H	3.550170	-4.116136	1.012075
H	3.720506	-5.467428	-1.273520
H	1.962560	-5.538620	-1.288690
H	2.850395	-5.132052	-2.769402
O	1.227132	-3.001227	-2.361828
H	0.782869	-3.811798	-2.658462
H	0.567543	-2.291254	-2.158578

3syn

Re	-0.059390	0.097826	-0.324205
O	-0.443329	-0.139259	1.307333
O	1.971226	0.157095	-0.407877
N	-0.011295	2.151225	-0.440283
O	-2.360545	-0.179282	-0.295938
N	0.120645	-1.824569	-1.032826
H	-0.901838	0.363773	-1.790626
Si	-1.940745	-0.214359	-5.357724
O	-2.497305	-1.569650	-4.273455
H	-2.372736	-1.679027	-3.243829
C	-0.112887	-0.132697	-5.044739
C	-2.897349	1.282497	-4.813724
C	-2.430305	-0.865837	-7.027451
C	-2.889022	-1.155304	-0.871081
C	-2.268595	-2.224423	-1.567601
C	-0.888873	-2.566191	-1.457594
O	-0.550274	-3.804033	-1.821104
C	0.911830	-3.902095	-1.794210
C	1.339628	-2.670925	-0.997260
C	2.753921	1.185803	-0.218076
C	2.392237	2.495987	-0.117264
C	1.048312	2.921378	-0.270330
O	0.801232	4.228785	-0.277611
C	-0.653285	4.410552	-0.303593
C	-1.180247	3.028319	-0.693340
H	-3.987258	-1.194852	-0.854436
H	-2.915058	-3.063876	-1.803898
H	1.255429	-3.887619	-2.829794
H	1.167620	-4.851044	-1.328853
H	1.581660	-2.908327	0.041494
H	2.183476	-2.148820	-1.441393
H	3.809782	0.924478	-0.147326
H	3.149568	3.250965	0.037476
H	-0.957029	4.720051	0.697265
H	-0.872397	5.196742	-1.022191
H	-1.457091	2.967518	-1.747737
H	-2.027941	2.714950	-0.087104
H	0.107307	0.060378	-3.991047
H	0.386019	-1.058616	-5.344354
H	0.318848	0.686793	-5.629373
H	-2.711907	1.522273	-3.763196
H	-2.594426	2.148020	-5.413340
H	-2.165939	-0.128752	-7.793550
H	-3.972897	1.141354	-4.953680
H	-3.509035	-1.034578	-7.098852
H	-1.911966	-1.797449	-7.270975
H	-3.199360	-2.169218	-4.582264

TS4anti (PhOH)

Re	-1.632036	0.107017	-0.319785
O	-1.427744	0.099794	-1.983403
O	-3.686466	0.246254	0.088011
N	-1.517629	2.122841	0.062724
H	0.033436	-0.118996	-0.157385
N	-1.995521	-1.939550	-0.109252
O	-1.355998	-0.031231	1.758789
Si	2.112926	-0.582229	-0.487645
O	4.074487	-1.093581	-0.660390
C	5.243231	-0.398913	-0.240685
H	4.222602	-2.054366	-0.622436
C	-0.975343	-1.043478	2.470215
C	-1.030704	-2.359710	2.091919
C	-1.666571	-2.736523	0.880622
O	-2.068066	-4.008338	0.738593
C	-2.658942	-4.134184	-0.592725
C	-2.896138	-2.683220	-1.018876
C	-4.380717	1.332288	0.200532
C	-3.918082	2.621391	0.258487
C	-2.541323	2.942663	0.254725
O	-2.200456	4.206927	0.507556
C	-0.751729	4.328025	0.346154
C	-0.273408	2.875661	0.337464
C	2.085129	0.599165	-1.929552
C	2.299538	0.059417	1.254779
C	1.618358	-2.349015	-0.828175
C	6.014436	-0.923608	0.787042
C	7.161566	-0.232017	1.173627
C	7.506389	0.965398	0.548073
C	6.708808	1.470436	-0.477333
C	5.566958	0.783066	-0.888403
H	2.380415	1.608614	-1.633599
H	1.086150	0.646186	-2.365854
H	1.380029	0.521530	1.613419
H	3.094074	0.810327	1.295427
H	2.562448	-0.754558	1.936200
H	2.772313	0.250736	-2.705488
H	2.151178	-2.722532	-1.709388
H	1.846757	-2.999707	0.021010
H	0.550826	-2.422087	-1.034985
H	-0.749291	-3.136165	2.788865
H	-0.624697	-0.803509	3.476314
H	-1.936621	-4.649044	-1.228661
H	-3.564937	-4.727984	-0.497716
H	-3.926098	-2.355277	-0.859698
H	-2.624619	-2.501656	-2.058645
H	-5.459526	1.173603	0.269555
H	-4.621446	3.432821	0.378884
H	-0.571850	4.844823	-0.597907
H	-0.377200	4.922635	1.176206
H	0.465532	2.684249	-0.438601
H	0.133692	2.562743	1.302123
H	5.729602	-1.849089	1.275056
H	7.779256	-0.630296	1.969818

H	8.396325	1.501193	0.856245
H	6.977202	2.395736	-0.973272
H	4.953452	1.152279	-1.699498

4anti (PhOH)

C	2.375162	-2.870907	0.844172
N	2.978775	-1.691470	0.185497
C	4.279690	-1.908835	0.069206
O	4.674222	-3.130413	0.442019
C	3.479364	-3.922850	0.727311
Re	1.989653	0.067484	-0.215906
N	1.342544	2.051879	-0.133860
C	0.957302	2.736707	0.918666
O	0.591480	4.004751	0.660346
C	0.609108	4.175558	-0.789753
C	1.425081	2.978127	-1.283187
C	0.995515	2.304317	2.267646
C	1.778334	1.235192	2.635980
O	2.414781	0.447243	1.839990
C	5.273721	-1.000673	-0.359148
C	5.024352	0.332289	-0.578378
O	3.898569	0.955030	-0.482726
O	1.277457	-0.313918	-1.686502
C	-2.599191	-1.761104	-2.217812
Si	-3.279653	-0.778304	-0.799110
C	-3.032374	-1.509269	0.885834
O	-5.105082	-1.012466	-1.125267
C	-3.036420	1.055686	-0.905976
H	0.632986	-0.422309	0.595941
C	-6.226514	-0.632819	-0.295087
H	-5.370217	-1.559758	-1.888290
H	-1.978232	-1.391459	1.161969
H	-3.266906	-2.576749	0.904503
H	-3.628337	-1.000339	1.647924
H	-3.569405	1.589771	-0.115315
H	-3.344447	1.452025	-1.877070
H	-1.967735	1.264641	-0.781767
H	-2.926922	-1.368156	-3.184826
H	-1.505699	-1.697976	-2.194679
H	-2.870021	-2.818885	-2.153259
H	0.565015	2.944059	3.024956
H	-0.425069	4.154965	-1.139559
H	1.056795	5.143276	-1.004798
H	0.999196	2.519811	-2.175964
H	2.470856	3.227861	-1.480185
H	5.872819	0.965129	-0.853953
H	6.284727	-1.371711	-0.449515
H	3.331623	-4.604735	-0.111765
H	3.666474	-4.486574	1.638569
H	2.136884	-2.624839	1.881992
H	1.460660	-3.165675	0.331289
H	1.924355	1.047489	3.703604
C	-6.751977	-1.577735	0.569268
C	-7.834809	-1.198251	1.361544
C	-8.350886	0.094356	1.273308
C	-7.793935	1.017991	0.390014
C	-6.713687	0.656611	-0.415206
H	-6.335092	-2.575766	0.621150
H	-8.270055	-1.915363	2.046980
H	-9.191465	0.381620	1.893837
H	-8.198306	2.020487	0.319531
H	-6.270982	1.353106	-1.115609

$SiMe_3OPh^+$

Si	0.000325	-0.010264	1.835998
C	-0.783998	1.557113	2.507971
C	-0.895325	-1.519429	2.501376
C	0.048077	-0.009429	-0.034039
O	1.638386	-0.065141	2.284858
H	-0.270493	2.453265	2.146130
H	-0.776480	1.581635	3.602215
H	-1.829424	1.622408	2.185880
H	-0.876055	-1.557009	3.594943
H	-1.946728	-1.498044	2.192994
H	-0.459386	-2.448748	2.121612
H	-0.966960	0.008245	-0.444944
H	0.548143	-0.902540	-0.421536
H	0.578993	0.867435	-0.417554
C	2.188333	-0.038089	3.537531
C	2.379757	-1.226293	4.250487
C	2.983863	-1.193622	5.506261
C	3.401459	0.016373	6.060525
C	3.215299	1.198281	5.343382
C	2.612108	1.176280	4.087224
H	2.060249	-2.164770	3.812001
H	3.129133	-2.119918	6.051872
H	3.871713	0.037362	7.037068
H	3.541149	2.144743	5.761504
H	2.470049	2.090168	3.521781

4syn (PhOH)

Re	-1.686417	-0.195569	-0.310322
O	-3.602726	-1.101920	-0.261880
N	-1.057154	-2.068612	0.363143
O	-0.993811	-0.293485	-1.834739
H	-0.311873	0.509335	0.287993
O	-2.076619	0.074711	1.769832
N	-2.660052	1.610831	-0.456263
C	-2.047035	2.931729	-0.194434
C	-3.140787	3.903231	-0.639331
O	-4.343609	3.073029	-0.655746
C	-3.960626	1.792456	-0.630183
C	-4.963972	0.805406	-0.749731
C	-4.725480	-0.531327	-0.540736
C	-1.432150	-0.442806	2.757721
C	-0.664690	-1.583849	2.720776
C	-0.658719	-2.407947	1.567281
O	-0.317086	-3.701089	1.703112
C	-0.380015	-4.310591	0.377547
C	-1.180066	-3.299014	-0.447492
H	-1.127857	3.045454	-0.767485
H	-1.815240	3.020397	0.870066
H	-2.990270	4.281278	-1.652091
H	-3.318198	4.729169	0.045858
H	-5.972969	1.138148	-0.947787
H	-1.557252	0.061573	3.720155
H	-5.579650	-1.211801	-0.598306
H	-0.227141	-1.969077	3.630953
H	-0.857630	-5.282239	0.481500
H	0.643704	-4.433699	0.019010
H	-2.234564	-3.568979	-0.545957
H	-0.762636	-3.145441	-1.442806
Si	4.146489	2.243505	0.932341
C	3.411846	3.855401	0.378519

C	5.951996	2.285915	1.346211
C	3.101436	1.227572	2.077148
O	4.094703	1.330583	-0.698414
H	3.536776	0.242288	2.262987
H	3.035592	1.745719	3.040988
H	2.083833	1.098439	1.699423
H	4.010717	4.321870	-0.408895
H	2.384216	3.740707	0.021366
H	3.387833	4.547405	1.227442
H	6.364367	1.286189	1.504148
H	6.535111	2.795861	0.575228
H	6.076558	2.843034	2.282155
C	4.506704	-0.028785	-0.974129
H	3.484459	1.672301	-1.379627
C	3.565256	-1.038714	-0.875000
C	3.983562	-2.339236	-1.155052
C	5.307897	-2.591533	-1.511451
C	6.226082	-1.546227	-1.598444
C	5.826786	-0.236765	-1.331403
H	2.541799	-0.821642	-0.594440
H	3.270493	-3.152191	-1.092912
H	5.624116	-3.605756	-1.724872
H	7.253608	-1.742267	-1.880099
H	6.517987	0.592869	-1.404960

TS5 (PhOH)

Re	-1.154119	-0.318727	-0.222818
O	-0.537402	-0.050074	-1.757971
O	-2.590984	-1.741419	-0.479476
N	-2.663355	1.071027	-0.162928
O	-1.406127	-0.234831	1.835317
N	-0.002056	-1.975555	0.274105
H	-0.027450	0.909736	0.353166
H	0.930929	0.942553	0.158847
O	2.128398	1.243158	-0.001225
C	2.972193	0.189143	-0.418817
Si	2.718632	2.907545	0.239356
C	-3.850856	-1.563850	-0.767354
C	-4.537839	-0.386028	-0.791367
C	-3.940862	0.846467	-0.426747
O	-4.733610	1.902701	-0.288597
H	-3.876237	3.691429	-0.876422
C	-3.897664	3.066846	0.017158
C	-2.538406	2.451597	0.356183
C	-0.594482	-0.618240	2.776766
C	0.406234	-1.539442	2.638656
C	0.550089	-2.271166	1.429500
O	1.222796	-3.423747	1.455152
C	1.226596	-3.967575	0.095549
C	0.167210	-3.134642	-0.632823
C	1.158493	3.859287	0.597081
C	3.544266	3.412175	-1.353829
H	4.403505	2.779235	-1.591164
C	3.897249	2.872707	1.684009
H	-0.783686	-0.184303	3.759558
H	0.985483	-1.843892	3.498534
H	2.229066	-3.829445	-0.309521
H	0.991055	-5.026965	0.165898
H	0.501294	-2.800989	-1.615015
H	-0.786707	-3.653948	-0.739754
H	-4.385279	-2.487419	-0.992036
H	-5.592712	-0.386474	-1.025248
H	-4.369440	3.601287	0.838313
H	-2.346721	2.413641	1.430928
H	-1.715560	2.967113	-0.134739
H	0.648121	3.492652	1.491863
H	0.462058	3.835084	-0.244791
H	1.419767	4.908104	0.776430
H	2.849283	3.385639	-2.197913
H	3.911026	4.440444	-1.258617
H	4.228578	3.895930	1.894791
H	4.789245	2.275534	1.477619
H	3.420365	2.487211	2.589631
C	3.708457	-0.507854	0.532726
C	4.545280	-1.540087	0.109208
C	4.631830	-1.865319	-1.244175
C	3.876415	-1.159540	-2.180974
C	3.038435	-0.123118	-1.771947
H	3.630184	-0.245935	1.580418
H	5.127358	-2.088429	0.840793
H	5.286097	-2.666355	-1.568232
H	3.939715	-1.410283	-3.233582
H	2.446193	0.434951	-2.486039

5 (PhOH)

Re	1.822180	0.143125	-0.099104
O	0.472401	-0.216218	-0.994885
N	1.530268	1.963606	0.741544
O	3.005415	1.193768	-1.342524
N	3.115961	-1.404526	-0.286335
O	1.472353	-0.690207	1.707203
C	0.913835	-0.115035	2.745158
C	0.640484	1.208199	2.908148
C	0.983163	2.180978	1.937526
Si	-4.428170	-2.052533	0.688309
C	-3.202992	-1.100371	1.745624
C	-3.799798	-3.765090	0.274443
C	-6.097465	-2.115938	1.543252
O	-4.573370	-1.296297	-0.825511
C	-4.938956	-0.011230	-1.119517
C	-6.289816	0.333443	-1.233877
C	-6.647661	1.634179	-1.584622
C	-5.668802	2.598479	-1.824629
C	-4.322725	2.248863	-1.716101
C	-3.954282	0.951269	-1.365515
O	0.773982	3.450542	2.224711
C	1.094302	4.254980	1.036709
C	1.862599	3.285835	0.139238
C	3.937206	0.728807	-2.140256
C	4.464770	-0.524857	-2.145333
C	4.068701	-1.513275	-1.211837
O	4.705538	-2.667011	-1.215061
C	4.056133	-3.562500	-0.246856
C	3.155205	-2.629760	0.562433
H	4.843775	-4.038041	0.331821
H	3.506680	-4.305939	-0.823930
H	3.575412	-2.383197	1.537467
H	2.154165	-3.030553	0.698194
H	0.670167	-0.812355	3.545192
H	0.180080	1.550914	3.823480
H	0.145144	4.580103	0.611021
H	1.672322	5.112016	1.372306
H	1.535306	3.327434	-0.896038
H	2.940705	3.442305	0.178312

H	4.306530	1.468715	-2.848855
H	5.241219	-0.778331	-2.852323
H	-2.216990	-1.044489	1.273976
H	-3.544493	-0.078219	1.937664
H	-3.081003	-1.593027	2.716849
H	-2.837731	-3.720533	-0.245240
H	-3.661048	-4.356144	1.186057
H	-4.504475	-4.303917	-0.366545
H	-6.002814	-2.624659	2.509315
H	-6.836624	-2.665125	0.951914
H	-6.494101	-1.114804	1.738300
H	-7.046998	-0.421453	-1.055640
H	-7.697631	1.892181	-1.672113
H	-5.951678	3.608254	-2.099450
H	-3.552384	2.988344	-1.907449
H	-2.910206	0.669550	-1.289689

TS4anti (CH_3OH)

Re	-0.038956	-0.020121	-0.001021
O	-0.033041	-0.058987	1.676390
N	2.033745	-0.046363	-0.251006
O	0.141649	1.956871	-0.748983
N	-2.056952	0.139197	-0.367031
O	0.018501	-0.503177	-2.081318
H	-0.084868	-1.673059	-0.059288
C	0.918042	-1.191599	-2.693816
C	2.215571	-1.387275	-2.280357
C	2.731777	-0.672878	-1.170788
O	4.063151	-0.511006	-1.072135
C	4.320700	0.228372	0.160716
C	2.954125	0.817172	0.518943
C	-0.826456	2.781068	-0.968466
C	-2.175594	2.522190	-0.955205
C	-2.708142	1.232595	-0.733188
O	-4.015854	1.054547	-0.945247
C	-4.356275	-0.308098	-0.538785
C	-2.996125	-1.001032	-0.452542
Si	0.946611	-4.313132	2.835901
O	1.261601	-5.760898	3.984703
H	1.375308	-5.631921	4.945336
H	1.766508	-6.545399	3.697538
C	2.627083	-3.592386	2.524570
C	-0.172731	-3.304975	3.915143
C	0.189678	-5.185771	1.374879
H	4.681422	-0.483312	0.906129
H	5.088255	0.969520	-0.050464
H	2.736208	0.754130	1.585136
H	2.840551	1.855519	0.196922
H	-0.510975	3.800485	-1.208197
H	-2.869274	3.316510	-1.191395
H	-4.864943	-0.244245	0.424878
H	-5.027597	-0.718651	-1.289715
H	-2.768373	-1.592393	-1.343143
H	-2.904515	-1.636565	0.426983
H	0.615938	-1.615193	-3.655929
H	2.906973	-1.926033	-2.912773
H	3.285859	-4.301127	2.014692
H	3.108526	-3.265685	3.450584
H	2.517418	-2.714901	1.877729
H	0.343414	-2.955091	4.814351
H	-0.497445	-2.417788	3.360882
H	-1.064266	-3.860733	4.216465
H	0.134688	-4.432741	0.577453
C	-1.190406	-5.827281	1.595778
H	0.909963	-5.931587	1.015401
H	-1.542381	-6.301151	0.675573
H	-1.162149	-6.597241	2.371818
H	-1.936453	-5.084274	1.888797

4anti (CH_3OH)

Re	-0.021712	0.049161	-0.014258
O	-0.069294	0.051692	1.662959
O	1.961959	-0.002061	-0.762917
N	0.007161	2.073577	-0.380211
O	-0.491862	-0.043812	-2.097403
H	-1.672757	-0.012611	-0.083188
N	0.084626	-2.022224	-0.254925
Si	-4.286203	-1.218285	2.753147
C	-3.476020	-2.866423	2.483510
C	-3.379749	-0.065974	3.890222
C	-5.034460	-0.447399	1.242282
C	-0.494399	-2.760104	-1.174723
C	2.721611	1.017027	-0.984582
C	2.376793	2.346834	-0.970712
C	1.056336	2.794818	-0.744652
O	0.794908	4.089875	-0.950249
C	-0.583558	4.339967	-0.532969
C	-1.190508	2.938993	-0.465182
C	-1.122676	-0.987186	-2.705964
C	-1.237344	-2.292699	-2.287008
O	-0.249686	-4.078510	-1.073603
C	0.506105	-4.287520	0.158275
C	1.001307	-2.885020	0.520478
O	-5.765605	-1.599482	3.792455
H	-0.177891	-4.699629	0.902871
H	1.298017	-5.001935	-0.055188
H	0.916953	-2.673407	1.586636
H	2.032088	-2.702527	0.205826
H	3.758675	0.767327	-1.226173
H	3.124900	3.090042	-1.207551
H	-0.546514	4.834762	0.439227
H	-1.038607	4.996584	-1.270923
H	-1.759676	2.683812	-1.362917
H	-1.825891	2.799900	0.408243
H	-1.563699	-0.716797	-3.669772
H	-1.730326	-3.019057	-2.917455
H	-3.125220	-0.546844	4.839667
H	-2.439389	0.233719	3.414940
H	-3.953764	0.841835	4.096438
H	-2.564441	-2.716514	1.894694
H	-4.116657	-3.556197	1.926977
H	-3.190329	-3.335691	3.429217
H	-4.231061	-0.158579	0.555814
H	-5.605188	0.450780	1.493519
H	-5.688637	-1.140607	0.705939
H	-5.728130	-1.351619	4.733367
C	-6.764499	-2.662539	3.549681
H	-7.682494	-2.355922	4.044436
H	-6.910640	-2.711737	2.474753
H	-6.383989	-3.601347	3.946027

TS4anti (CH_3CH_2OH)

C	1.112139	3.150295	-1.085107
N	0.626412	2.158691	-0.097263

C	0.110478	2.811200	0.919661
O	0.016421	4.132667	0.754019
C	0.426252	4.437437	-0.618245
Re	0.987872	0.118197	-0.290793
O	0.813751	0.178245	1.760563
C	0.164982	1.005578	2.530521
C	-0.252647	2.256472	2.176144
O	0.574764	-0.008219	-1.909934
O	2.930150	0.715750	-0.330258
C	3.996440	-0.036200	-0.379710
C	4.063979	-1.389932	-0.235374
C	2.925543	-2.177981	0.067526
N	1.662761	-1.780017	0.111521
C	0.859809	-2.888706	0.678472
C	1.810446	-4.080825	0.570203
O	3.121438	-3.451856	0.385224
C	-2.217738	-1.909714	-1.535840
Si	-2.355584	-0.538834	-0.261498
O	-4.754916	-1.028899	-0.535904
C	-5.863389	-0.312516	0.057829
C	-2.792061	1.176494	-0.882883
C	-2.679547	-1.008078	1.526430
H	-0.735741	-0.286283	0.016284
H	-0.475809	4.670221	-1.185570
H	1.080622	5.305055	-0.581028
H	0.816187	2.858667	-2.092773
H	2.201373	3.205699	-1.038402
H	4.918624	0.522213	-0.541752
H	5.023384	-1.884844	-0.277944
H	1.623385	-4.699275	-0.308424
H	1.866425	-4.699124	1.462669
H	0.602062	-2.647833	1.712374
H	-0.052254	-3.036872	0.104702
H	-0.003200	0.654758	3.548875
H	-0.732403	2.895549	2.903518
H	-2.719744	-1.618042	-2.463281
H	-1.179277	-2.131843	-1.785608
H	-2.690709	-2.824320	-1.168789
H	-1.918934	1.676647	-1.305669
H	-3.180587	1.799491	-0.072540
H	-3.556251	1.118592	-1.661070
H	-1.835304	-1.567726	1.936274
H	-3.571173	-1.632297	1.604990
H	-2.820990	-0.118493	2.145712
H	-4.990792	-1.256477	-1.445966
C	-7.096494	-1.190016	0.169991
H	-5.512971	-0.003937	1.043590
H	-6.072993	0.589573	-0.526141
H	-7.909116	-0.633513	0.646619
H	-7.443324	-1.510303	-0.817565
H	-6.888918	-2.079657	0.770152

4anti (CH_3CH_2OH)

C	0.559112	2.852057	-1.400303
N	0.743941	2.061150	-0.165202
C	0.687246	2.881160	0.859539
O	0.323979	4.139027	0.552668
C	-0.041236	4.152914	-0.861224
Re	1.237100	0.032388	-0.165123
O	2.233347	0.595163	1.636211
C	1.873691	1.510059	2.468692
C	1.069787	2.591567	2.192628
O	0.117322	-0.437866	-1.324213
O	3.045046	0.715027	-1.041403
C	4.055078	-0.015075	-1.375025
C	4.275017	-1.338503	-1.079139
C	3.395661	-2.102701	-0.280097
N	2.199977	-1.754112	0.169996
C	1.746810	-2.796455	1.117655
C	2.702576	-3.953953	0.825516
O	3.807333	-3.311123	0.116163
C	-3.309670	-1.601776	-1.597986
Si	-3.985985	-0.645190	-0.159519
O	-5.794880	-0.876554	-0.430878
C	-6.900184	-0.235205	0.359268
C	-3.724861	1.191717	-0.238308
C	-3.718107	-1.406779	1.510997
H	0.137598	-0.248546	1.038690
H	-1.131293	4.171379	-0.923334
H	0.373380	5.056221	-1.303083
H	-0.109274	2.335204	-2.089155
H	1.524613	2.999838	-1.891110
H	4.825218	0.507819	-1.949180
H	5.191892	-1.808432	-1.405373
H	2.274927	-4.701629	0.155366
H	3.113795	-4.435779	1.709808
H	1.839738	-2.422008	2.140168
H	0.705805	-3.055303	0.929437
H	2.295605	1.426881	3.474306
H	0.890878	3.337799	2.953585
H	-3.693901	-1.230396	-2.553245
H	-2.220850	-1.482957	-1.620012
H	-3.533912	-2.669268	-1.519870
H	-2.657415	1.401887	-0.110822
H	-4.261032	1.717402	0.556764
H	-4.034612	1.602966	-1.203386
H	-2.645799	-1.395282	1.735555
H	-4.054144	-2.446948	1.533416
H	-4.223487	-0.854813	2.307938
H	-6.074863	-1.030298	-1.352084
C	-8.165776	-1.029860	0.178412
H	-6.537086	-0.251099	1.384232
H	-6.981107	0.790582	0.002952
H	-8.953385	-0.553845	0.768978
H	-8.490089	-1.034248	-0.865980
H	-8.045378	-2.057201	0.527278

TS4anti (t-BuOH)

Re	1.334223	0.091971	-0.316545
O	1.050383	0.034562	-1.967481
N	1.086894	2.157767	-0.115921
C	1.648817	3.119970	-1.091070
C	1.033203	4.444886	-0.631973
O	0.590922	4.164887	0.734258
C	0.596777	2.836031	0.893596
C	0.170686	2.302649	2.140362
C	0.496113	1.024883	2.497513
O	1.103028	0.158491	1.740033
C	0.930870	-2.934991	0.502015
N	1.851941	-1.858440	0.070781
O	3.338424	0.567133	-0.140834
C	4.342098	-0.256661	-0.115439
C	4.298843	-1.620106	-0.019731
C	3.087648	-2.335350	0.133622

O	3.168751	-3.634178	0.411172
C	1.811318	-4.181486	0.422790
H	-0.370887	-0.192285	-0.119455
Si	-2.165759	-0.391524	-0.346856
O	-4.300246	-0.749565	-0.585692
C	-5.616369	-0.447550	0.052540
C	-5.953013	-1.586947	1.012616
C	-5.470957	0.883045	0.777774
C	-6.632368	-0.352122	-1.084057
C	-1.957414	-1.579488	-1.787250
C	-2.239743	-1.053703	1.408096
C	-2.354578	1.426094	-0.753093
H	1.732813	-4.847908	1.278232
H	-3.283585	1.599987	-1.298307
H	-4.418968	-1.542228	-1.129438
H	-1.243417	-1.200686	1.825204
H	-2.763843	-2.012400	1.423878
H	-2.780213	-0.362485	2.059347
H	-2.358652	2.041336	0.149639
H	-1.524272	1.752795	-1.381802
H	-2.665397	-1.336811	-2.585671
H	-0.956594	-1.513706	-2.214945
H	-2.132166	-2.614921	-1.479840
H	-0.279239	2.971114	2.860331
H	0.152800	4.727907	-1.210834
H	1.736426	5.273330	-0.588477
H	1.354478	2.848717	-2.104930
H	2.738946	3.110627	-1.025038
H	5.318403	0.228795	-0.163803
H	5.221453	-2.181750	0.011705
H	1.679575	-4.740546	-0.504850
H	0.586709	-2.727551	1.518030
H	0.070711	-2.992932	-0.160610
H	0.281218	0.686172	3.511880
H	-6.421330	1.128538	1.257316
H	-4.707163	0.838053	1.556293
H	-5.225339	1.687536	0.082604
H	-7.622398	-0.123009	-0.682102
H	-6.353427	0.435849	-1.787051
H	-6.704717	-1.299083	-1.628428
H	-6.938675	-1.421548	1.455211
H	-5.980075	-2.545650	0.485966
H	-5.222827	-1.652579	1.821301

4anti (t-BuOH)

Re	1.765510	0.046795	-0.242061
N	2.797191	-1.695528	0.119616
C	4.082034	-1.914123	-0.115686
C	5.027716	-1.014106	-0.655211
C	4.753971	0.314125	-0.876357
O	3.640291	0.936933	-0.687430
O	2.360563	0.495033	1.758972
N	1.107707	2.028097	-0.166903
C	0.288953	4.119650	-0.823341
C	0.800188	2.740317	0.892645
C	1.782292	1.301535	2.580037
O	0.393859	3.994833	0.627822
C	0.957810	2.350667	2.246009
C	2.267444	-2.858017	0.866847
H	3.623550	-4.475278	1.539758
O	4.513187	-3.127579	0.243920
C	3.349815	-3.914929	0.648651
O	0.932919	-0.380305	-1.634237
H	0.489941	-0.428073	0.698767
Si	-3.774111	-0.755887	-0.337707
C	-3.222676	-1.806810	-1.772086
H	-3.655082	1.479264	-1.401687
C	-3.460217	-1.521316	1.326031
C	-3.269507	1.025898	-0.484201
O	-5.584600	-0.798666	-0.618800
H	-5.848600	-1.392602	-1.343936
C	-6.863654	-0.386802	0.183912
C	-6.475135	0.827560	1.002039
C	1.080642	2.918676	-1.346497
H	-2.376444	-1.543855	1.489977
H	-3.824841	-2.550575	1.375364
H	-3.900596	-0.948708	2.145621
H	-3.585598	1.629585	0.368973
H	-2.175048	1.063637	-0.527524
H	-3.521757	-1.379907	-2.733991
H	-2.128717	-1.861221	-1.767113
H	-3.602911	-2.830625	-1.706784
H	0.583235	3.008557	3.017331
H	-0.769977	4.073525	-1.085657
H	0.700876	5.086254	-1.104410
H	0.590261	2.426837	-2.186791
H	2.102764	3.175642	-1.636695
H	5.570707	0.942607	-1.242900
H	6.026644	-1.385545	-0.834668
H	3.117088	-4.599178	-0.169266
H	2.148752	-2.589005	1.919699
H	1.300375	-3.160533	0.467916
H	2.017995	1.149632	3.637314
H	-7.362521	1.160394	1.545528
H	-5.707559	0.592350	1.741103
H	-6.139323	1.648010	0.366559
C	-7.885419	-0.070105	-0.893609
H	-8.824656	0.211400	-0.412020
H	-7.556456	0.760186	-1.521217
H	-8.084015	-0.942307	-1.523396
C	-7.236472	-1.591820	1.027978
H	-8.148512	-1.360926	1.584313
H	-7.435098	-2.465607	0.402951
H	-6.450932	-1.833523	1.745424

TS4anti ($EtMe_2SiH$)

Re	-0.024831	0.017964	-0.020650
O	-0.040434	-0.006465	1.655063
O	1.988818	-0.002409	-0.589501
N	-0.011250	2.039082	-0.380405
O	-0.526433	-0.066833	-2.046824
N	0.151372	-2.050092	-0.284103
H	-1.729084	-0.074805	0.022475
Si	-3.647022	-0.395551	0.665949
O	-5.603386	-0.590713	1.162594
C	-3.241465	-2.195724	0.969655
C	-3.383742	0.801782	2.077532
C	-4.155080	0.179999	-1.055065
H	-6.172084	-1.153331	0.609933
H	-5.839204	-0.754071	2.091261
C	-0.316641	-2.804656	-1.249474
C	-1.025855	-1.037640	-2.747325
C	-1.020463	-2.361716	-2.400527
O	-0.005400	-4.104973	-1.152331

C	0.685050	-4.296895	0.122264
C	1.053754	-2.873776	0.551375
C	2.759098	1.025494	-0.753075
C	2.398887	2.347418	-0.767332
C	1.056603	2.776593	-0.653377
O	0.799252	4.065241	-0.874731
C	-0.617495	4.300598	-0.596220
C	-1.208549	2.890985	-0.557642
H	3.811709	0.779349	-0.910529
H	3.152861	3.101868	-0.940378
H	-0.678567	4.817304	0.362786
H	-1.008993	4.934280	-1.388828
H	-1.900359	2.752155	0.270677
H	-1.707504	2.621115	-1.491511
H	-1.443942	-0.749587	-3.713758
H	-1.410410	-3.102716	-3.083530
H	-0.014449	-4.778262	0.807845
H	1.539018	-4.945560	-0.058322
H	0.865349	-2.691235	1.609429
H	2.091799	-2.616184	0.329272
H	-3.709098	-2.529330	1.901543
H	-2.167567	-2.358774	1.055808
H	-2.326274	0.924454	2.310143
H	-3.875034	0.426169	2.981707
H	-3.812467	1.781344	1.850672
H	-3.620793	-2.822856	0.157314
H	-3.266308	0.233840	-1.685456
C	-4.923313	1.512439	-1.111301
H	-4.770053	-0.623088	-1.482168
H	-5.202334	1.746235	-2.142866
H	-5.841746	1.479490	-0.520411
H	-4.320863	2.344910	-0.739287

4anti ($EtMe_2SiH$)

Re	-0.038956	-0.020121	-0.001021
O	-0.033041	-0.058987	1.676390
N	2.033745	-0.046363	-0.251006
O	0.141649	1.956871	-0.748983
N	-2.056952	0.139197	-0.367031
O	0.018501	-0.503177	-2.081318
H	-0.084868	-1.673059	-0.059288
C	0.918042	-1.191599	-2.693816
C	2.215571	-1.387275	-2.280357
C	2.731777	-0.672878	-1.170788
O	4.063151	-0.511006	-1.072135
C	4.320700	0.228372	0.160716
C	2.954125	0.817172	0.518943
C	-0.826456	2.781068	-0.968466
C	-2.175594	2.522190	-0.955205
C	-2.708142	1.232595	-0.733188
O	-4.015854	1.054547	-0.945247
C	-4.356275	-0.308098	-0.538785
C	-2.996125	-1.001032	-0.452542
Si	0.946611	-4.313132	2.835901
O	1.261601	-5.760898	3.984703
H	1.375308	-5.631921	4.945336
H	1.766508	-6.545399	3.697538
C	2.627083	-3.592386	2.524570
C	-0.172731	-3.304975	3.915143
C	0.189678	-5.185771	1.374879
H	4.681422	-0.483312	0.906129
H	5.088255	0.969520	-0.050464
H	2.736208	0.754130	1.585136
H	2.840551	1.855519	0.196922
H	-0.510975	3.800485	-1.208197
H	-2.869274	3.316510	-1.191395
H	-4.864943	-0.244245	0.424878
H	-5.027597	-0.718651	-1.289715
H	-2.768373	-1.592393	-1.343143
H	-2.904515	-1.636565	0.426983
H	0.615938	-1.615193	-3.655929
H	2.906973	-1.926033	-2.912773
H	3.285859	-4.301127	2.014692
H	3.108526	-3.265685	3.450584
H	2.517418	-2.714901	1.877729
H	0.343414	-2.955091	4.814351
H	-0.497445	-2.417788	3.360882
H	-1.064266	-3.860733	4.216465
H	0.134688	-4.432741	0.577453
C	-1.190406	-5.827281	1.595778
H	0.909963	-5.931587	1.015401
H	-1.542381	-6.301151	0.675573
H	-1.162149	-6.597241	2.371818
H	-1.936453	-5.084274	1.888797

TS4anti (Et_2MeSiH)

C	1.555749	-2.598979	0.440869
N	1.970776	-1.245500	0.006437
C	3.296965	-1.203843	0.030327
O	3.883930	-2.374439	0.274642
C	2.846016	-3.405413	0.303753
Re	0.722783	0.350448	-0.324764
N	-0.293660	2.163092	-0.071230
C	-0.946223	2.608985	0.975241
O	-1.464199	3.837486	0.838738
C	-1.231956	4.259521	-0.542034
C	-0.183522	3.267109	-1.051770
C	-1.066787	1.960681	2.233489
C	-0.261061	0.902394	2.552188
O	0.581902	0.323141	1.752879
C	4.131677	-0.074455	-0.129296
C	3.644578	1.205056	-0.179292
O	2.405461	1.580123	-0.155838
O	0.436500	0.216492	-1.970805
C	-1.677946	-2.442879	-1.854624
Si	-2.456899	-1.479615	-0.450731
C	-2.375639	-2.085772	1.335183
O	-4.187807	-2.555241	-0.698864
C	-3.271498	0.161964	-0.885639
H	-0.707176	-0.568205	-0.073212
H	-4.920957	-2.413758	-0.077162
H	-4.569506	-2.618207	-1.590150
H	-1.607937	-1.518987	1.864519
C	-2.127705	-3.595632	1.502830
H	-3.325335	-1.810821	1.811333
C	-4.301817	0.696769	0.123649
H	-3.749289	0.014333	-1.862426
H	-2.487754	0.903928	-1.046221
H	-2.382191	-2.516939	-2.690062
H	-0.777696	-1.956909	-2.228835
H	-1.428476	-3.460191	-1.542158
H	-1.692565	2.413889	2.988687
H	-2.181464	4.183826	-1.074407
H	-0.896343	5.293700	-0.520177

H	-0.399138	2.906293	-2.057544
H	0.831498	3.669933	-1.032430
H	4.363795	2.025747	-0.229580
H	5.199791	-0.237659	-0.134455
H	2.909123	-3.956285	-0.636055
H	3.061300	-4.064652	1.141215
H	1.200699	-2.550870	1.473260
H	0.758620	-2.977498	-0.194733
H	-0.275987	0.517609	3.573357
H	-4.721020	1.645105	-0.224719
H	-5.140674	0.007892	0.261984
H	-3.855273	0.877399	1.104745
H	-2.107105	-3.862236	2.563575
H	-2.910606	-4.191718	1.027797
H	-1.171551	-3.900359	1.069715

4anti (Et_2MeSiH)

C	1.676368	-2.794735	0.803816
N	2.057257	-1.634754	-0.032073
C	3.268412	-1.860621	-0.516571
O	3.757643	-3.074676	-0.245705
C	2.698990	-3.854948	0.393003
Re	0.983708	0.115481	-0.177850
N	0.373454	2.098838	0.035312
C	0.269104	2.793615	1.146144
O	-0.166847	4.054413	0.980974
C	-0.519301	4.213597	-0.427013
C	0.149340	3.014138	-1.104094
C	0.671321	2.380394	2.440142
C	1.551517	1.334273	2.595358
O	1.969268	0.546611	1.665998
C	4.092768	-0.965902	-1.235091
C	3.788029	0.363719	-1.395151
O	2.736501	0.991154	-0.987545
O	-0.123715	-0.313244	-1.365190
C	-3.353189	-1.791851	-1.603233
Si	-4.038742	-0.913634	-0.121619
C	-3.666443	-1.613297	1.566245
O	-5.850662	-1.379063	-0.309952
C	-4.036603	0.950912	-0.181824
H	-0.081558	-0.345485	1.001218
H	-6.525785	-1.087670	0.331766
H	-6.260200	-1.487662	-1.188612
H	-2.695974	-1.189862	1.855851
C	-3.634453	-3.145587	1.691445
H	-4.388500	-1.183287	2.272155
H	-4.607695	1.318333	0.679283
C	-4.541970	1.600128	-1.481354
H	-2.997875	1.250671	0.010102
H	-3.831825	-1.461744	-2.530054
H	-2.285922	-1.559302	-1.685999
H	-3.462921	-2.876261	-1.523024
H	0.445899	3.023735	3.278905
H	-1.608280	4.189064	-0.502793
H	-0.144649	5.180587	-0.755320
H	-0.490813	2.546624	-1.852264
H	1.106481	3.266150	-1.567731
H	4.518836	0.990014	-1.914500
H	5.035066	-1.341867	-1.607706
H	2.314168	-4.554646	-0.351133
H	3.145303	-4.399275	1.222318
H	1.754469	-2.522939	1.859498
H	0.651622	-3.096357	0.591485
H	1.985903	1.170535	3.585737
H	-4.496157	2.690018	-1.408048
H	-3.939011	1.303616	-2.343435
H	-5.582209	1.334164	-1.691753
H	-3.413193	-3.438516	2.721238
H	-4.592408	-3.597527	1.419733
H	-2.864350	-3.584482	1.052242

TS4anti (Et_3SiH)

Re	0.813297	0.269507	-0.314039
O	0.422585	0.073268	-1.931402
N	0.064474	2.214745	-0.118992
O	2.644197	1.275535	-0.301665
N	1.864263	-1.452242	0.067704
O	0.791270	0.369312	1.770407
H	-0.707330	-0.433971	0.067780
C	0.095818	1.110443	2.577198
C	-0.563946	2.260013	2.238812
C	-0.437295	2.811388	0.936117
O	-0.775657	4.095099	0.753488
C	-0.574457	4.407676	-0.660247
C	0.262080	3.232664	-1.175981
C	3.823897	0.743201	-0.347227
C	4.147673	-0.582231	-0.227400
C	3.184566	-1.580944	0.043282
O	3.629343	-2.797060	0.355230
C	2.472862	-3.679810	0.509940
C	1.299523	-2.706156	0.615664
Si	-2.585824	-1.087493	-0.124948
O	-4.500459	-1.872456	-0.207607
H	-4.936608	-1.928697	-1.073694
H	-5.162939	-1.555961	0.428360
C	-3.197504	0.663838	-0.469735
C	-2.094850	-2.179148	-1.584025
C	-2.433915	-1.710860	1.649918
H	-1.557874	4.467019	-1.129012
H	-0.074093	5.371547	-0.718440
H	-0.090119	2.856608	-2.136663
H	1.325112	3.469182	-1.257817
H	4.636893	1.459922	-0.482140
H	5.185558	-0.881495	-0.259673
H	2.426378	-4.312883	-0.377455
H	2.639433	-4.287078	1.396586
H	0.985872	-2.536035	1.648431
H	0.441067	-3.026512	0.030161
H	0.089439	0.787237	3.619684
H	-1.065808	2.842244	2.998122
C	-4.005550	1.323842	0.660655
H	-3.808594	0.607217	-1.378115
H	-2.339157	1.286797	-0.725672
C	-2.515769	-1.649555	-2.967722
H	-1.013767	-2.323404	-1.568653
H	-2.537216	-3.166073	-1.407940
H	-1.532848	-1.282729	2.093607
C	-2.432345	-3.240573	1.818652
H	-3.271780	-1.279183	2.211705
H	-2.340247	-3.505925	2.876063
H	-3.355284	-3.690742	1.445734
H	-1.598360	-3.709239	1.290311
H	-4.325486	2.327617	0.365997
H	-4.910863	0.760413	0.908071

H	-3.416994	1.423533	1.575814
H	-2.215851	-2.352920	-3.749915
H	-3.598510	-1.513610	-3.056185
H	-2.041902	-0.690790	-3.188869

4anti (Et_3SiH)

Re	1.145524	0.097651	-0.218957
O	0.143859	-0.370159	-1.481519
N	0.564598	2.101668	-0.177344
O	2.986312	0.893855	-0.909753
N	2.158773	-1.660396	0.121892
O	1.965514	0.619955	1.685358
H	-0.029929	-0.282665	0.880915
C	1.488176	1.475344	2.521211
C	0.655258	2.529086	2.222178
C	0.380120	2.867375	0.874160
O	-0.010047	4.122957	0.592871
C	-0.239046	4.195461	-0.847672
C	0.460126	2.945029	-1.387175
C	4.053390	0.223249	-1.186206
C	4.308973	-1.101706	-0.928175
C	3.401569	-1.938613	-0.241367
O	3.831620	-3.147829	0.133127
C	2.697411	-3.869607	0.707623
C	1.679583	-2.763271	0.984517
Si	-3.987183	-0.758451	-0.033120
O	-5.843205	-1.067840	0.028985
H	-6.390108	-1.035145	-0.778675
H	-6.380369	-0.796127	0.796863
C	-3.840604	1.097158	-0.180579
C	-3.532282	-1.733550	-1.557345
C	-3.485569	-1.480294	1.612220
H	-1.317918	4.181014	-1.014729
H	0.180763	5.133726	-1.203455
H	-0.121238	2.438855	-2.158108
H	1.459461	3.151469	-1.778889
H	4.843159	0.803816	-1.671303
H	5.269947	-1.517117	-1.196221
H	2.354187	-4.587774	-0.039397
H	3.052383	-4.391257	1.593524
H	1.687019	-2.437132	2.027708
H	0.665245	-3.049150	0.710129
H	1.826087	1.365869	3.555732
H	0.373935	3.229186	2.995929
C	-4.350613	1.918967	1.016644
H	-4.344646	1.409722	-1.102414
H	-2.773599	1.297370	-0.345375
C	-4.112978	-1.244173	-2.897192
H	-2.435587	-1.707864	-1.601341
H	-3.797519	-2.782352	-1.384992
H	-2.446377	-1.164470	1.771761
C	-3.604979	-3.007711	1.755579
H	-4.061087	-0.975294	2.397657
H	-3.292132	-3.321814	2.754995
H	-4.632593	-3.352458	1.610052
H	-2.972283	-3.530042	1.033614
H	-4.209401	2.987695	0.835092
H	-5.418172	1.759648	1.196252
H	-3.814313	1.668697	1.935062
H	-3.758265	-1.875024	-3.716241
H	-5.207003	-1.281990	-2.915116
H	-3.810623	-0.217758	-3.118509

TS4anti ($PhMe_2SiH$)

Re	-0.884210	0.353219	-0.292105
O	-0.145372	0.257152	-1.791494
N	-0.190181	2.161341	0.381706
C	1.034745	2.373311	1.184848
C	1.173452	3.894985	1.189359
O	-0.163962	4.356019	0.815019
C	-0.828339	3.321241	0.300978
C	-2.118187	3.565193	-0.222706
C	-2.966499	2.559286	-0.606716
O	-2.733481	1.286346	-0.612444
N	-2.026604	-1.394216	-0.508226
C	-2.697487	-1.740368	-1.781751
C	-3.218858	-3.152757	-1.501584
O	-3.189643	-3.247656	-0.043325
C	-2.433387	-2.236895	0.409887
C	-2.225862	-2.125498	1.810576
O	-1.460487	0.118747	1.705807
H	0.435467	-0.502092	0.367555
Si	2.028774	-1.770562	0.765848
C	3.150697	-0.709476	-0.284561
C	1.096767	-3.149201	-0.081527
H	1.361021	-2.183750	3.102833
O	3.567700	-2.960323	1.313915
C	-1.810652	-0.943502	2.361718
C	1.736206	-1.315128	2.552287
C	3.097353	-0.769494	-1.687004
C	3.973508	-0.017205	-2.466805
C	4.918642	0.807311	-1.857986
C	4.986304	0.878974	-0.466830
C	4.109686	0.127468	0.313176
H	4.215517	-3.201464	0.629719
H	3.385874	-3.754598	1.845876
H	1.760635	-3.685660	-0.766021
H	0.240868	-2.785113	-0.646983
H	2.675138	-1.001888	3.016959
H	1.012594	-0.508768	2.658622
H	0.732658	-3.864643	0.662463
H	-2.556691	-2.934038	2.446638
H	-2.565243	-3.932388	-1.896801
H	-4.243239	-3.324754	-1.824133
H	-1.986571	-1.711677	-2.607557
H	-3.496398	-1.021781	-1.979239
H	-3.969759	2.836363	-0.938803
H	-2.460660	4.589589	-0.252758
H	1.868263	4.263632	0.433055
H	1.410270	4.326223	2.159077
H	0.882724	1.965287	2.187653
H	1.884003	1.876562	0.721486
H	-1.803595	-0.845326	3.448994
H	2.363961	-1.398015	-2.179207
H	3.916751	-0.073196	-3.548186
H	5.600426	1.392293	-2.465386
H	5.721001	1.518478	0.009876
H	4.178837	0.195541	1.393951

4anti ($PhMe_2SiH$)

Re	-1.290970	0.107102	-0.253133
O	-0.370365	0.224805	-1.649553
H	0.043680	-0.320936	0.625202
O	-3.350772	0.438486	-0.637632

C	-3.951158	1.580232	-0.643733
C	-3.459600	2.796124	-0.234459
C	-2.171495	2.956229	0.322934
O	-1.871745	4.140731	0.865912
C	-0.461976	4.113055	1.252004
C	-0.121080	2.622987	1.237026
N	-1.208430	2.051772	0.411317
O	-2.024460	-0.257695	1.719220
C	-1.833014	-2.622840	1.846570
C	-1.965753	-1.361834	2.379680
N	-1.807704	-1.905497	-0.484451
C	-2.268270	-2.483856	-1.764519
C	-2.245275	-3.985417	-1.466589
C	-1.920657	-2.824551	0.446000
Si	3.782980	-1.395453	0.646754
O	5.522755	-2.106924	0.653827
C	3.508949	-1.236882	2.470652
H	6.076379	-2.069113	-0.149590
H	5.756711	-2.896785	1.178282
C	4.079220	0.178878	-0.289106
C	2.777738	-2.680458	-0.229610
H	3.159440	-2.889432	-1.232274
H	1.744522	-2.331178	-0.323904
H	4.207236	-0.531596	2.928018
H	3.606944	-2.203457	2.974229
H	2.491656	-0.874231	2.650388
O	-2.252271	-4.046479	-0.007386
H	2.762951	-3.614827	0.339238
H	-1.865716	-3.487596	2.494127
H	-1.332173	-4.471611	-1.815917
H	-3.117454	-4.527285	-1.825625
H	-1.593893	-2.206370	-2.574911
H	-3.269772	-2.112660	-1.997349
H	-4.981472	1.550860	-1.009286
H	-4.100088	3.665760	-0.273465
H	0.092674	4.683800	0.504993
H	-0.377016	4.589531	2.226127
H	-0.148988	2.176056	2.234156
H	0.847918	2.419194	0.784050
H	-2.079976	-1.271171	3.463741
C	3.680816	0.305803	-1.631798
C	3.896753	1.493141	-2.327519
C	4.513389	2.570437	-1.693193
C	4.911490	2.463861	-0.360135
C	4.693415	1.279551	0.337792
H	3.191955	-0.518972	-2.138386
H	3.581206	1.577944	-3.361173
H	4.681309	3.494272	-2.235667
H	5.387536	3.303124	0.134209
H	5.002300	1.216267	1.376042

TS4anti (Ph_2MeSiH)

Re	-1.273344	0.333814	-0.240342
O	-0.990458	0.915197	-1.786891
N	-1.961234	-1.549732	-0.877942
C	-2.834112	-1.698797	-2.064381
C	-2.922367	-3.219680	-2.213018
O	-2.514554	-3.717322	-0.900916
O	-3.319628	0.670668	0.077449
C	-1.922853	-2.701479	-0.253984
H	-3.803846	3.637847	1.516540
C	-1.404840	-2.940747	1.046554
C	-1.129471	-1.900234	1.889086
O	-1.218542	-0.640045	1.587702
C	-3.218079	2.814743	1.132873
C	-1.819094	2.861219	1.328399
O	-1.333039	3.864594	2.058450
C	0.127219	3.774409	2.040077
C	0.385255	2.358465	1.527773
N	-0.906356	1.997965	0.900065
H	0.368232	-0.181886	-0.185111
Si	2.215205	-0.841456	-0.898622
C	2.404956	-1.671907	0.767831
C	1.375648	-1.751375	-2.293983
C	2.736227	0.935822	-1.165598
O	4.070931	-1.466025	-1.431321
C	3.810493	1.497254	-0.450884
C	4.232824	2.800466	-0.705670
C	3.596048	3.563195	-1.684254
C	2.537837	3.017838	-2.409670
C	2.111304	1.716319	-2.152823
C	2.631716	-0.943923	1.947002
C	2.833391	-1.596502	3.161377
C	2.811839	-2.989544	3.219877
C	2.583694	-3.728115	2.060215
C	2.379855	-3.075278	0.845911
C	-3.855528	1.742894	0.563682
H	4.477572	-1.103723	-2.237040
H	4.313554	-2.404857	-1.358161
H	1.764976	-1.399077	-3.253775
H	0.295770	-1.618125	-2.288226
H	1.587651	-2.822389	-2.221933
H	-1.360525	-3.958444	1.406337
H	-2.220601	-3.614594	-2.949908
H	-3.923745	-3.593429	-2.413220
H	-2.385230	-1.216209	-2.932669
H	-3.801572	-1.232415	-1.863975
H	-4.946805	1.764882	0.514871
H	0.492104	4.547965	1.362646
H	0.480960	3.962794	3.051077
H	0.599435	1.654071	2.335631
H	1.188021	2.318723	0.795460
H	-0.851772	-2.114718	2.921974
H	1.277900	1.316320	-2.717306
H	2.042969	3.604498	-3.175616
H	3.925929	4.576835	-1.883554
H	5.060848	3.217849	-0.143487
H	4.328899	0.918122	0.305279
H	2.190156	-3.673308	-0.039912
H	2.559960	-4.811496	2.099942
H	2.970326	-3.496846	4.165066
H	3.008224	-1.017704	4.061579
H	2.652212	0.139259	1.924824

4anti (Ph_2MeSiH)

C	5.119602	1.329371	-1.191429
C	3.924751	0.615320	-1.400114
C	2.930370	1.191501	-2.211488
C	3.122484	2.444655	-2.789537
C	4.312221	3.137416	-2.572911
C	5.311419	2.578203	-1.776167
Si	3.613665	-1.045466	-0.629145
C	2.388104	-2.117419	-1.510329
O	5.263796	-1.868379	-0.963066

C	3.573853	-1.162362	1.223903
O	-1.178148	0.687618	-1.784532
Re	-1.832970	0.222730	-0.311858
N	-2.429591	-1.686628	-0.919336
C	-3.123682	-1.957465	-2.196045
C	-3.066234	-3.485299	-2.275832
O	-2.811723	-3.891972	-0.896592
C	-2.382997	-2.804071	-0.232121
C	-2.035228	-2.940207	1.135295
C	-2.040970	-1.846940	1.969632
O	-2.200049	-0.618919	1.615080
O	-3.919915	0.601561	-0.221695
C	-4.478825	1.704049	0.146740
C	-3.887640	2.797023	0.733354
C	-2.517423	2.837943	1.074271
O	-2.091366	3.863490	1.818956
C	-0.637884	3.758101	1.939111
C	-0.351341	2.319209	1.509432
N	-1.581477	1.950521	0.774176
H	-0.371877	-0.377472	0.177238
H	5.634318	-1.940462	-1.864027
H	5.577252	-2.609021	-0.409295
H	2.565989	-2.121289	-2.588865
H	1.373231	-1.749929	-1.329836
H	2.435169	-3.148217	-1.148351
H	-1.962466	-3.935229	1.550770
H	-2.236019	-3.844552	-2.887462
H	-3.994723	-3.953989	-2.594176
H	-2.604069	-1.474974	-3.023990
H	-4.145857	-1.573063	-2.149417
H	-5.558337	1.746321	-0.024631
H	-4.499321	3.642931	1.013278
H	-0.199728	4.498872	1.267810
H	-0.374973	3.984122	2.970066
H	-0.221623	1.644886	2.359658
H	0.519010	2.240548	0.859832
H	-1.949034	-2.021132	3.045487
H	1.999567	0.666494	-2.397368
H	2.345471	2.875921	-3.410351
H	4.462812	4.110604	-3.026906
H	6.238856	3.114699	-1.610342
H	5.909274	0.910420	-0.576827
C	3.066223	-2.322841	1.838380
C	3.014257	-2.427609	3.225844
C	3.462345	-1.373829	4.021290
C	3.961187	-0.213866	3.429334
C	4.015380	-0.106957	2.042227
H	2.700464	-3.146753	1.235164
H	2.618622	-3.326401	3.684992
H	3.417993	-1.454283	5.101700
H	4.303219	0.608262	4.047782
H	4.395133	0.806483	1.599322

TS4anti (Ph_3SiH)

Re	-1.325199	-0.608064	-0.239763
O	-0.994192	-0.431648	-1.873076
N	-0.478456	-2.516903	-0.062561
O	-3.098483	-1.732850	-0.187413
N	-2.482931	1.049416	0.138071
O	-1.255030	-0.713304	1.833342
H	0.169303	0.194581	0.087161
C	-0.509694	-1.419094	2.628947
C	0.186405	-2.543071	2.281139
C	0.056033	-3.099448	0.979888
O	0.433934	-4.372170	0.791066
C	0.166354	-4.716158	-0.604315
C	-0.642865	-3.524240	-1.132723
C	-4.306571	-1.275704	-0.240740
C	-4.708821	0.031388	-0.153521
C	-3.809280	1.092087	0.096080
O	-4.334571	2.287396	0.366507
C	-3.236760	3.246221	0.488907
C	-2.012610	2.351867	0.663027
Si	2.111060	1.035572	-0.153324
O	3.946356	1.917286	-0.239320
H	4.347640	2.046859	-1.116427
H	4.638900	1.585229	0.358019
C	2.625880	-0.422540	-1.205954
C	1.340357	2.529831	-0.976388
C	2.238177	0.977075	1.714369
H	1.125895	-4.836541	-1.106853
H	-0.378417	-5.658167	-0.611357
H	-0.253255	-3.136181	-2.074383
H	-1.703247	-3.751377	-1.257534
H	-5.076811	-2.042495	-0.354404
H	-5.762466	0.267621	-0.194567
H	-3.211106	3.831521	-0.431765
H	-3.454937	3.889518	1.338165
H	-1.731166	2.231415	1.712111
H	-1.153314	2.702717	0.098531
H	-0.494633	-1.090072	3.668842
H	0.724608	-3.103331	3.032039
C	1.381804	1.757005	2.508294
C	1.520278	1.788009	3.894093
C	2.516967	1.036369	4.514611
C	3.377452	0.257103	3.743519
C	3.241820	0.228811	2.356874
H	0.600869	2.347347	2.045573
H	0.849920	2.398965	4.488327
H	2.624234	1.059509	5.593314
H	4.155637	-0.329004	4.219395
H	3.926318	-0.387960	1.783991
C	2.860713	-1.690830	-0.650794
C	3.354461	-2.732644	-1.433734
C	3.606161	-2.532025	-2.790237
C	3.366613	-1.283232	-3.361242
C	2.887279	-0.236857	-2.576018
H	2.660705	-1.875150	0.397781
H	3.541836	-3.700427	-0.982345
H	3.987231	-3.344328	-3.399133
H	3.556408	-1.120650	-4.416301
H	2.717229	0.727467	-3.042756
C	0.557244	2.427984	-2.138227
C	0.022918	3.565784	-2.740110
C	0.252406	4.824834	-2.187176
C	1.026529	4.944574	-1.033516
C	1.570505	3.809160	-0.437007
H	0.347353	1.458572	-2.571584
H	-0.575194	3.466268	-3.639031
H	-0.167921	5.708774	-2.654045
H	1.210704	5.921043	-0.599430
H	2.179855	3.926278	0.451757

4anti (Ph_3SiH)

Re	2.322470	0.074038	-0.224305
O	1.713778	-0.122921	-1.774451
N	1.971453	2.129922	-0.099511
O	4.366812	0.659856	-0.252262
N	2.985103	-1.833306	0.165077
O	2.590570	0.312312	1.879954
H	0.835403	-0.237047	0.427279
C	1.989995	1.152481	2.649693
C	1.402940	2.334632	2.262655
C	1.564981	2.819182	0.940259
O	1.394100	4.134350	0.712427
C	1.599727	4.358415	-0.716137
C	2.293150	3.077333	-1.187437
C	5.384431	-0.130464	-0.292181
C	5.400037	-1.496996	-0.145009
C	4.240802	-2.253069	0.137427
O	4.401490	-3.542714	0.453314
C	3.073637	-4.142755	0.575294
C	2.149391	-2.931752	0.699253
Si	-4.026910	-0.262412	-0.252355
O	-5.863802	-0.374805	-0.628797
H	-6.206873	-0.286486	-1.539068
H	-6.533937	-0.063370	0.010096
C	-3.626530	1.539831	-0.461396
C	-3.389266	-1.394307	-1.577340
C	-4.024895	-0.904300	1.489314
H	0.620044	4.500597	-1.175577
H	2.198603	5.259760	-0.827555
H	1.901129	2.715879	-2.138330
H	3.377475	3.187202	-1.271538
H	6.344623	0.369855	-0.448901
H	6.344372	-2.021563	-0.177091
H	2.893184	-4.724540	-0.330564
H	3.085339	-4.797025	1.444174
H	1.881381	-2.712276	1.736064
H	1.237845	-3.036560	0.113057
H	1.997314	0.906993	3.715679
H	0.987063	2.998544	3.007279
C	-3.389094	-2.119504	1.798621
C	-3.392097	-2.609346	3.102644
C	-4.035238	-1.898379	4.114138
C	-4.671423	-0.690977	3.824855
C	-4.661702	-0.193478	2.524940
H	-2.885808	-2.684734	1.022491
H	-2.892505	-3.544739	3.327807
H	-4.038409	-2.281875	5.128268
H	-5.168673	-0.135671	4.611958
H	-5.149309	0.755242	2.323777
C	-2.963566	2.257076	0.549530
C	-2.654824	3.605172	0.376861
C	-3.007228	4.256712	-0.803586
C	-3.660363	3.558245	-1.819982
C	-3.962923	2.210610	-1.652904
H	-2.680061	1.765489	1.472962
H	-2.138785	4.144243	1.162923
H	-2.770731	5.306890	-0.933924
H	-3.929329	4.062818	-2.741005
H	-4.461544	1.682861	-2.459940
C	-2.257925	-1.029020	-2.327901
C	-1.737689	-1.891188	-3.291006
C	-2.344221	-3.124116	-3.524117
C	-3.468961	-3.500991	-2.789319
C	-3.984774	-2.647291	-1.818861
H	-1.776346	-0.072164	-2.160182
H	-0.860583	-1.598887	-3.856741
H	-1.941107	-3.792675	-4.276641
H	-3.941358	-4.460019	-2.969561
H	-4.854667	-2.961316	-1.251652

TS4anti ($BuMe_2SiH$)

Re	0.875955	0.102959	-0.289778
O	0.516651	0.083347	-1.926387
N	0.662279	2.189276	-0.082620
O	2.908772	0.595068	-0.293392
N	1.424349	-1.842059	0.066836
C	0.579738	-2.911766	0.648481
H	-0.813449	-0.203004	0.013653
O	0.880091	0.210223	1.769050
C	0.462382	1.111670	2.608740
Si	-2.673561	-0.323518	-0.750597
O	-4.535106	-0.469854	-1.723353
C	-2.604225	1.498370	-1.191017
C	-2.100761	-1.650671	-1.951714
C	-3.456038	-0.829925	0.936421
C	0.163196	2.406000	2.295448
C	0.387016	2.901093	0.981098
O	0.395230	4.228691	0.795782
C	0.605039	4.472344	-0.630085
C	1.063972	3.113042	-1.167248
C	3.896694	-0.234970	-0.383754
C	3.851218	-1.602273	-0.297167
C	2.665761	-2.313010	-0.004888
O	2.782250	-3.609722	0.276235
C	1.436672	-4.157885	0.448816
C	-2.455397	-0.757553	2.105215
C	-3.993452	-2.273653	0.833093
C	-4.625229	0.129939	1.260301
H	0.393891	0.784725	3.647011
H	-0.124662	3.102767	3.069411
H	-0.346875	4.797242	-1.053021
H	1.345576	5.263428	-0.725224
H	2.144831	3.053557	-1.312342
H	0.569252	2.839927	-2.099237
H	4.870766	0.237159	-0.530606
H	4.768363	-2.169225	-0.369100
H	1.190530	-4.707714	-0.461347
H	1.462385	-4.833496	1.300510
H	-0.376200	-2.977384	0.135981
H	0.405584	-2.691844	1.704757
H	-2.088916	0.258795	2.260870
H	-1.592697	-1.407565	1.956710
H	-2.960188	-1.072461	3.026547
H	-3.190738	-2.998321	0.669014
H	-4.488485	-2.542959	1.773382
H	-4.726886	-2.388562	0.031526
H	-5.049142	-0.142075	2.233704
H	-5.434782	0.071383	0.529526
H	-4.558636	-0.969205	-2.555321
H	-5.058013	0.336772	-1.855947
H	-4.295301	1.170772	1.328931
H	-2.803979	-2.488859	-1.947225
H	-2.062371	-1.240368	-2.965412
H	-1.111954	-2.038579	-1.722096

H	-2.323866	1.620847	-2.241087
H	-3.580712	1.969900	-1.044542
H	-1.879132	2.034613	-0.580763

4anti ($BuMe_2SiH$)

Re	1.559087	0.122072	-0.369095
O	1.131728	0.041365	-1.988343
N	0.870913	2.066157	-0.039075
O	3.470161	1.006388	-0.108203
N	2.484045	-1.699111	-0.129203
C	1.789106	-2.967402	0.184703
H	0.088833	-0.489461	0.077643
O	1.596904	0.112275	1.768763
C	0.808451	0.747164	2.563799
Si	-4.792771	-0.214492	-0.718541
O	-6.498165	0.562041	-0.668865
C	-3.648302	1.246423	-0.639447
C	-4.893033	-1.031353	-2.382667
C	-4.826525	-1.343168	0.797491
C	0.077213	1.872348	2.258647
C	0.275748	2.546364	1.027645
O	-0.076789	3.841789	0.939453
C	0.203232	4.274974	-0.427053
C	1.135144	3.186889	-0.965880
C	4.603517	0.390761	-0.123465
C	4.829231	-0.964494	-0.121127
C	3.787850	-1.916746	-0.050484
O	4.126481	-3.193364	0.155250
C	2.910851	-4.001515	0.075220
C	-3.394844	-1.901612	0.979900
C	-5.812257	-2.508921	0.575793
C	-5.226496	-0.552638	2.061391
H	0.762953	0.367377	3.588626
H	-0.499099	2.365638	3.028479
H	-0.746768	4.319170	-0.963749
H	0.649761	5.265439	-0.376533
H	2.190860	3.465815	-0.914104
H	0.897253	2.900490	-1.990369
H	5.478062	1.047765	-0.122323
H	5.845485	-1.331635	-0.102931
H	2.924007	-4.517515	-0.886294
H	2.940379	-4.724607	0.887551
H	0.983868	-3.146301	-0.526467
H	1.367199	-2.910279	1.191213
H	-2.670325	-1.112746	1.200339
H	-3.044778	-2.448433	0.098476
H	-3.385785	-2.602660	1.822164
H	-5.529145	-3.127504	-0.280563
H	-5.818635	-3.155605	1.460579
H	-6.837420	-2.159810	0.418237
H	-5.177802	-1.213471	2.934030
H	-6.252103	-0.171833	2.008718
H	-6.995837	0.739741	-1.489150
H	-6.773062	1.189318	0.026166
H	-4.554892	0.288894	2.253320
H	-5.766274	-1.682143	-2.474115
H	-4.918545	-0.289662	-3.186463
H	-4.001300	-1.647706	-2.537037
H	-3.845619	1.936288	-1.465394
H	-3.731672	1.794488	0.302524
H	-2.612954	0.902714	-0.734197