Electronic Supplementary Information for Dalton Transactions

Metal Fragment Isomerization upon Grafting a d^2 ML_4 perhydrocarbyl Os Complex on a Silica Surface: Origin and Consequence

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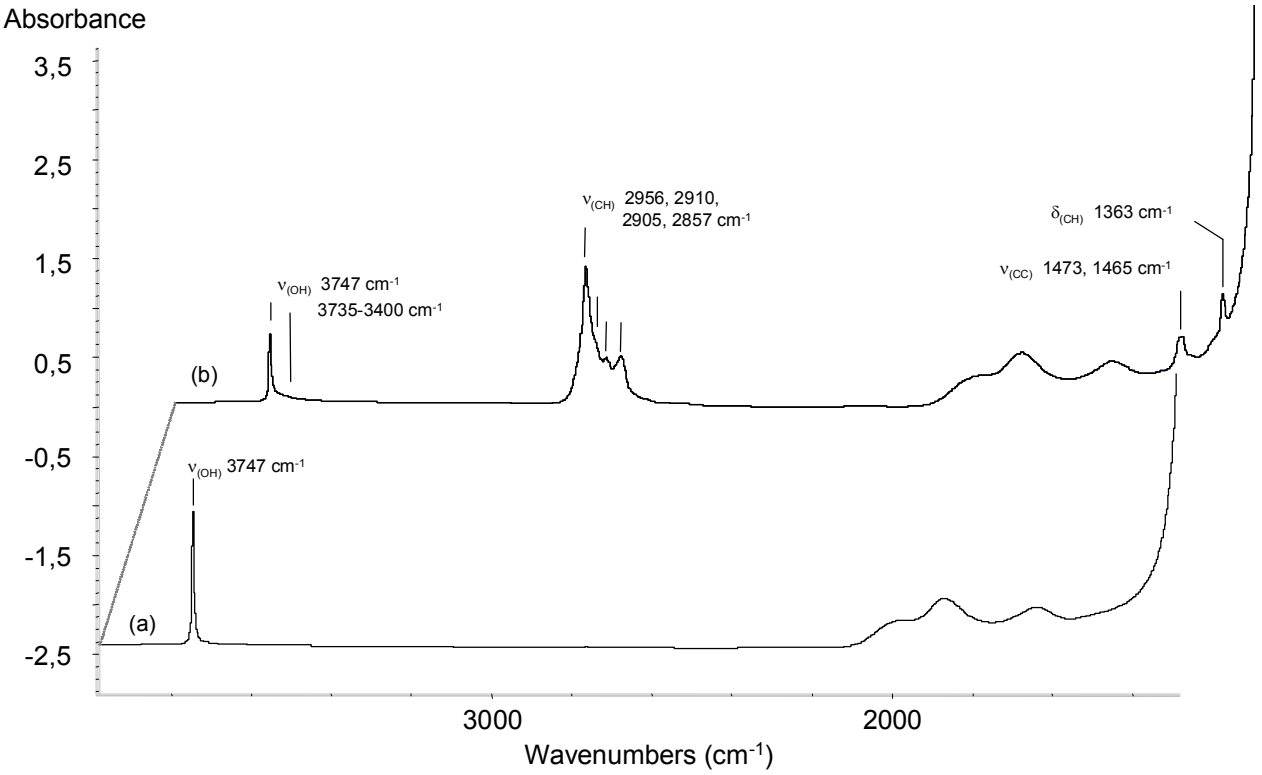

Figure S1. In situ IR spectroscopy. (a) $SiO_{2-(700)}$ pellet (25 mg, 6.7 μmol OH). (b) After impregnation of **1** [Os(=CH*t*Bu)$_2$(CH$_2$*t*Bu)$_2$] (3 equiv. per SiOH) in pentane (10 mL) during 3 h followed by three washings (10 min, 25 °C) in pentane and a drying step under vacuum (10^{-5} mmHg, 1 h, 25 °C).

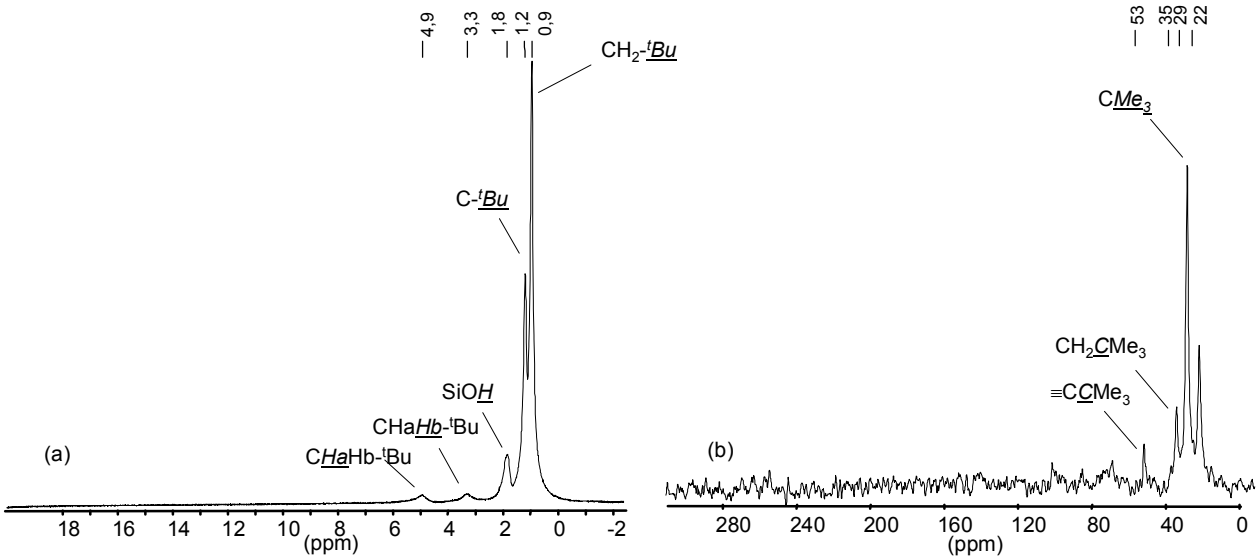

Figure S2. Solid-state NMR of [**1**/$SiO_{2-(700)}$]. (a) ^{1}H MAS 10 kHz. (b) ^{13}C CPMAS 10 kHz, NS = 20 000.

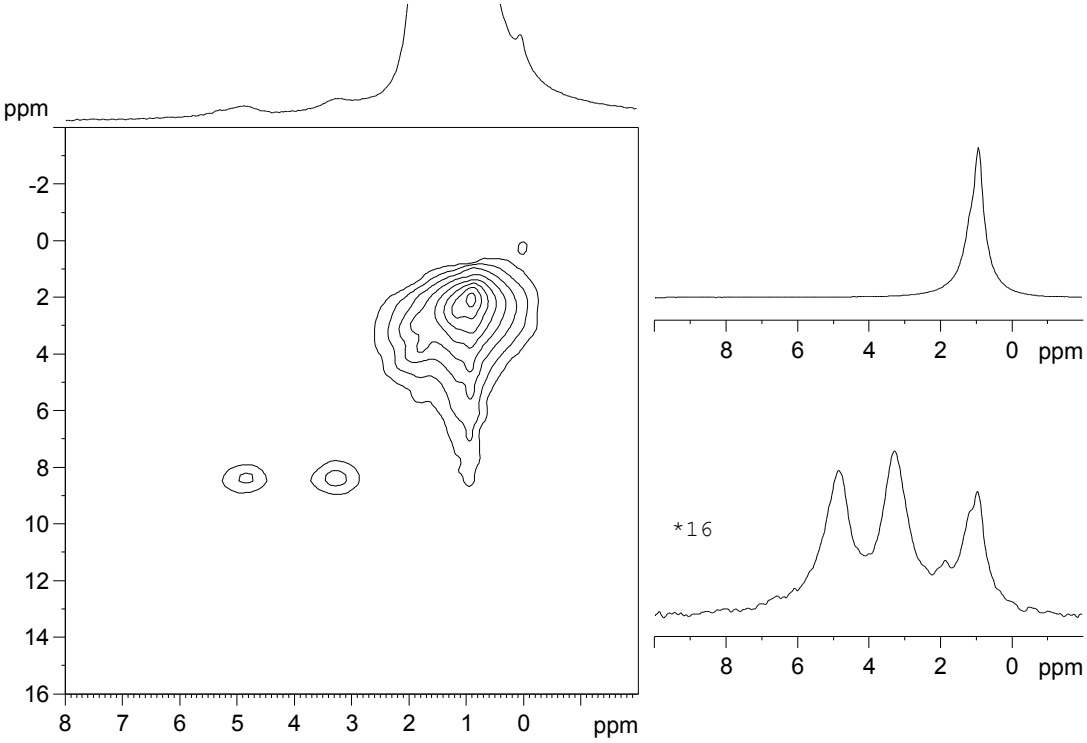

Figure S3. ^{1}H DQ pC7, wr = 10 KHz 3 basic 28 ms pC7 elements for excitation and reconversion, 512 increments of 16 scans, RD = 4s, experimental time = 9h, 1 zero filling in F1 dimension and LB = 50 Hz.

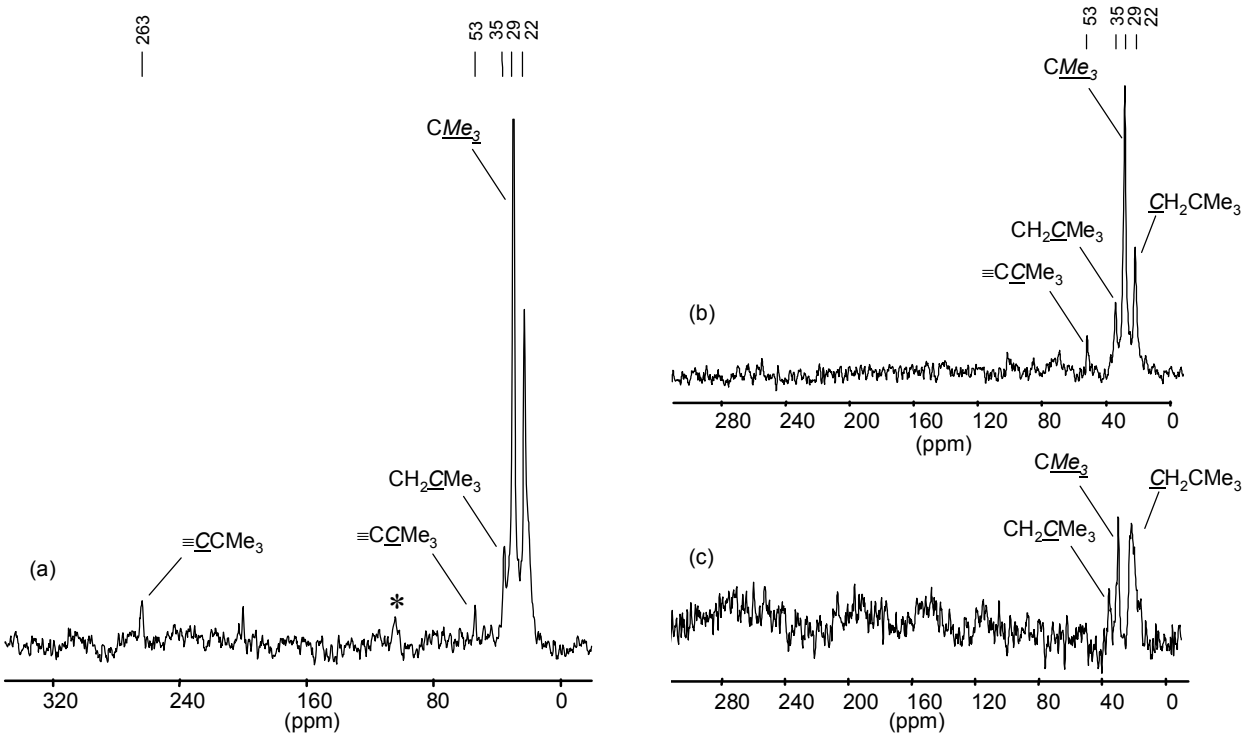

Figure S4. Solid-state NMR of [**1***/$SiO_{2-(700)}$]. (a) ^{13}C HPDEC of 5% labelled surface complex. (b) ^{13}C CPMAS of unlabelled surface complex. (c) ^{13}C CPMAS of 5% labelled surface complex. * corresponds to a spinning side band.

Relative Stabilities

(a,a)-1_Q-bis-ene

Os	-0.010705	-0.099512	-0.034503
C	-0.918593	1.147203	1.360935
H	-0.068866	1.625843	1.881220
H	-1.369982	0.450441	2.090812
C	-1.343162	-0.905518	-0.999713
C	-2.327434	-1.914251	-0.468341
H	-1.465792	-0.651464	-2.064683
C	0.725604	0.966595	-1.331472
C	1.873500	1.923888	-1.144808
C	-1.941209	2.208846	0.955292
H	-2.809808	1.755304	0.468307
H	-2.303408	2.775831	1.823972
H	-1.508879	2.922876	0.247625
H	-2.185934	-2.130843	0.596341
H	-3.358488	-1.560388	-0.603322
H	2.703245	1.673419	-1.819620
H	2.265621	1.929717	-0.121810
H	1.562187	2.949086	-1.387340
H	0.314145	0.929384	-2.352868
H	-2.239658	-2.862935	-1.015481
C	1.360876	-1.592970	0.453556
H	1.669587	-2.204379	-0.401376
H	0.793014	-2.259824	1.126915
C	2.584322	-1.024112	1.179843
H	3.234155	-0.468881	0.495495
H	2.307578	-0.346449	1.998451
H	3.191443	-1.821914	1.627802

E = -406.321218207 a.u.
G = -406.128023 a.u.

(s,a)-1_Q-bis-ene

Os	-0.081208	-0.031848	0.024515
C	1.233289	-0.212726	1.631103
H	1.293177	-1.304601	1.790433
H	0.687411	0.190446	2.500627
C	-0.321078	1.756913	-0.268897
C	0.037778	2.662343	-1.410563
H	-0.844673	2.259665	0.570666
C	0.815034	-0.740953	-1.410583
C	1.185377	-2.196247	-1.548301
C	2.641341	0.381835	1.577741
H	2.608913	1.469710	1.462479
H	3.206664	0.161943	2.494083
H	3.209048	-0.017384	0.731571
H	0.552582	2.132751	-2.215381
H	-0.863792	3.127869	-1.831309
H	0.686633	3.479563	-1.067999
H	0.714810	-2.632366	-2.440253
H	0.878527	-2.799804	-0.686404
H	2.271139	-2.314278	-1.665941
H	1.124756	-0.098345	-2.246041
C	-1.980984	-0.889719	-0.048351
H	-2.467360	-0.764596	-1.022715
H	-1.791237	-1.970879	0.070181
C	-2.891816	-0.384567	1.074960
H	-3.182090	0.658857	0.911324
H	-3.815250	-0.975672	1.139014
H	-2.411103	-0.443682	2.059837

E = -406.320013804 a.u.
G = -406.126847 a.u.

(s,s)-1_Q-bis-ene

Os	0.121893	0.069947	-0.119532
C	-0.645078	2.008502	-0.007715
H	-0.479976	2.431513	-1.012531
H	0.049396	2.542210	0.662125
C	0.023204	-0.567177	1.591458
C	-0.725501	-1.668187	2.274014
H	0.694748	0.014303	2.258934
C	-0.936999	-0.761603	-1.357549
C	-1.918833	-1.890723	-1.324980
C	-2.088114	2.255008	0.433223
H	-2.270764	1.858497	1.436615
H	-2.322940	3.328471	0.451300
H	-2.800469	1.771666	-0.242519
H	-1.372701	-2.217227	1.585868
H	-0.029373	-2.385482	2.729897
H	-1.350208	-1.270499	3.085288
H	-2.040233	-2.307996	-0.322410
H	-1.597158	-2.701333	-1.993148
H	-2.905265	-1.560026	-1.677230
H	-0.803092	-0.302987	-2.360389
C	2.061989	-0.403625	-0.732527
H	2.234564	-1.486516	-0.754415
H	2.126025	-0.054044	-1.775344
C	3.125061	0.293685	0.121272
H	4.125561	0.178889	-0.317255
H	2.942006	1.371703	0.212724
H	3.161681	-0.122429	1.133736

E = -406.318887853 a.u.
G = -406.125330 a.u.

1_Q-yne

Os	-0.010125	0.045712	-0.180593
C	-0.496012	-0.195560	1.811751
H	-0.958721	0.674495	2.295132
H	0.536931	-0.251966	2.215693
C	-1.584043	0.045890	-0.817992
C	-2.986033	0.163969	-1.226096
C	1.279087	-1.327600	-1.139810
C	2.543378	-1.684370	-0.344399
C	-1.260969	-1.468303	2.147597
H	-0.808578	-2.350357	1.682450
H	-1.290845	-1.640369	3.233123

H	-2.297339	-1.406166	1.798294
H	-3.641840	0.036080	-0.356400
H	-3.167762	1.165304	-1.635414
H	-3.260913	-0.577688	-1.984478
C	0.326029	2.033531	0.385754
H	3.231377	-2.308763	-0.930754
H	2.299746	-2.243079	0.566167
H	3.113093	-0.797766	-0.038593
H	0.726733	-2.234123	-1.413069
H	1.554047	-0.843697	-2.094785
C	1.857259	2.082330	0.497930
H	-0.125737	2.366268	1.329384
H	-0.013057	2.710695	-0.406986
H	2.230874	1.522620	1.364537
H	2.211883	3.115065	0.612526
H	2.357451	1.690007	-0.400137

E = -406.297756069 a.u.
G = -406.105963 a.u.

(a,a)-1_L-bis-ene

Os	0.043508	-0.083722	-0.177054
C	-0.737266	0.922028	1.466242
H	0.187229	1.150618	2.034341
H	-1.229750	0.090887	2.009559
C	-1.295972	-0.539359	-1.346556
C	-2.389457	-1.581357	-1.240243
H	-1.292172	-0.048264	-2.337925
C	0.841851	1.093155	-1.342942
C	2.109625	1.919913	-1.268423
C	-1.660380	2.145469	1.541876
H	0.365752	1.184815	-2.338342
C	1.280571	-1.828213	-0.120197
H	2.118383	-1.701754	-0.817960
H	0.691177	-2.659025	-0.532668
C	1.838771	-2.297236	1.238953
C	-1.011336	3.378381	0.894204
H	-0.068373	3.628168	1.397640
H	-0.799956	3.177085	-0.161554
H	-1.681767	4.244610	0.968281
C	-3.005864	1.872005	0.851230
H	-3.498310	0.998830	1.298908
H	-3.671672	2.738119	0.960401
H	-2.848479	1.674475	-0.214483
C	-1.929606	2.458007	3.032514
H	-2.415845	1.604103	3.522212
H	-0.988380	2.669995	3.556386
H	-2.585268	3.333299	3.128920
C	-3.725553	-0.978777	-1.728762
H	-4.502917	-1.754070	-1.730476
H	-4.044602	-0.162438	-1.072286
H	-3.621336	-0.589264	-2.749391
C	-1.998456	-2.741685	-2.188776
H	-2.780087	-3.512729	-2.173560
H	-1.884644	-2.377423	-3.217111
H	-1.050790	-3.190243	-1.870352
C	-2.563398	-2.127641	0.185251
H	-1.629284	-2.576342	0.543905
H	-2.855523	-1.324228	0.870911
H	-3.342217	-2.900742	0.200603
C	2.648969	2.092728	0.158402
H	1.906697	2.591745	0.790578
H	2.892851	1.120603	0.598822
H	3.563162	2.699941	0.144062
C	1.837560	3.310702	-1.885324
H	1.093488	3.855936	-1.294732
H	2.766323	3.895393	-1.908050
H	1.465734	3.209381	-2.912762
C	3.172044	1.199513	-2.134741
H	2.812490	1.076781	-3.163899
H	4.098821	1.788416	-2.154610
H	3.388333	0.208438	-1.720262
C	2.717782	-3.544214	0.992377
H	2.128344	-4.339559	0.518269
H	3.558630	-3.295589	0.332173
H	3.119876	-3.926004	1.940609
C	2.707549	-1.224380	1.917505
H	2.109190	-0.337567	2.163100
H	3.133057	-1.614312	2.851505
H	3.533826	-0.922168	1.261949
C	0.707755	-2.691494	2.206966
H	0.056765	-1.832701	2.414664
H	0.098127	-3.498675	1.781316
H	1.125359	-3.040956	3.160083

E = -877.931427035 a.u.

(s,a)-1_L-bis-ene

Os	0.092056	-0.079793	-0.054617
C	-1.253554	0.012157	-1.644232
H	-1.437596	-1.058235	-1.852389
H	-0.606602	0.363565	-2.469085
C	0.688129	1.617489	0.277670
C	0.828196	2.621709	1.397431
H	1.151048	1.993890	-0.664786
C	-0.815535	-0.766347	1.394262
C	-1.342939	-2.169913	1.648875
C	-2.586536	0.768531	-1.736921
H	-0.959677	-0.113458	2.265448
C	1.808074	-1.282693	-0.120301
H	2.281991	-1.355256	0.868591
H	1.353074	-2.272562	-0.307914
C	2.906622	-1.062547	-1.174850
C	-0.351131	-2.862578	2.614997
H	-0.716599	-3.865921	2.871917
H	0.635037	-2.952334	2.145742
H	-0.246204	-2.281296	3.539597
C	-2.717835	-2.065041	2.346597
H	-3.083323	-3.068256	2.601909
H	-2.635448	-1.479845	3.271359
H	-3.447618	-1.580516	1.688853
C	-1.496094	-3.027706	0.380106
H	-2.212577	-2.568269	-0.309365
H	-0.536091	-3.147311	-0.136089
H	-1.861581	-4.026925	0.648839
C	-2.367344	2.285006	-1.614822

H	-1.940545	2.523611	-0.635384
H	-1.673085	2.638970	-2.388665
H	-3.319553	2.819170	-1.730680
C	-3.207396	0.474293	-3.122784
H	-4.160531	1.006923	-3.237903
H	-2.529644	0.797637	-3.923649
H	-3.394267	-0.601317	-3.238828
C	-3.577349	0.316817	-0.653094
H	-3.772069	-0.760731	-0.732763
H	-3.165597	0.519936	0.341462
H	-4.531044	0.849468	-0.764154
C	3.832226	0.098528	-0.775214
H	3.263414	1.029902	-0.681725
H	4.309775	-0.109533	0.190977
H	4.617988	0.238267	-1.529011
C	2.319240	-0.783671	-2.571217
H	1.600930	-1.563879	-2.854776
H	1.802813	0.185017	-2.595529
H	3.119822	-0.756945	-3.322273
C	3.756595	-2.351900	-1.255514
H	4.581985	-2.224449	-1.968509
H	4.179745	-2.591605	-0.271531
H	3.139886	-3.198527	-1.584838
C	0.262725	3.980970	0.922061
H	-0.812615	3.904094	0.729481
H	0.429537	4.741252	1.695933
H	0.761555	4.306431	0.000653
C	2.339019	2.798077	1.687700
H	2.871621	3.131729	0.788699
H	2.478087	3.552010	2.473667
H	2.774021	1.849491	2.020868
C	0.118172	2.208162	2.693009
H	-0.955482	2.077144	2.515896
H	0.534099	1.269344	3.075197
H	0.255324	2.987537	3.453136

E = -877.933775687 a.u.

1_L-yne

Os	-0.111087	0.069778	-0.178507
C	0.069130	-1.934828	0.348064
H	0.427329	-2.441774	-0.562494
H	-0.978456	-2.246213	0.464732
C	-0.116302	1.182059	1.571245
C	0.097011	2.693395	1.390801
H	-1.162669	0.994875	1.894687
C	1.519070	0.203954	-0.717716
C	2.614097	0.139507	-1.721535
C	0.851922	-2.472667	1.555101
H	0.527776	0.814091	2.377275
C	-1.803149	-0.410011	-1.421991
H	-1.580276	-1.376413	-1.904361
H	-1.785945	0.333379	-2.239757
C	-3.260398	-0.461229	-0.911493
C	-0.501464	3.161958	0.048844
H	0.013609	2.662870	-0.789985
H	-1.575380	2.945473	-0.006907
H	-0.363733	4.244199	-0.082317
C	-0.591917	3.453912	2.543274
H	-0.197188	3.119149	3.511052
H	-0.416020	4.533901	2.450267
H	-1.675345	3.275895	2.528838
C	1.600403	3.018333	1.406804
H	2.038271	2.746525	2.376036
H	2.110953	2.444127	0.625421
H	1.765135	4.090288	1.237184
C	-4.188696	-0.835470	-2.089356
H	-4.087222	-0.104547	-2.901868
H	-3.926444	-1.826939	-2.480113
H	-5.238589	-0.853921	-1.765506
C	-3.465391	-1.499624	0.206874
H	-2.883505	-1.236985	1.099445
H	-4.525165	-1.541996	0.491236
H	-3.159065	-2.498749	-0.128240
C	-3.698138	0.916874	-0.378632
H	-3.099663	1.202754	0.496341
H	-3.572626	1.685383	-1.152480
H	-4.753677	0.896438	-0.076836
C	0.881482	-4.014636	1.420709
H	1.416926	-4.311440	0.509451
H	1.390132	-4.462205	2.284702
H	-0.138821	-4.417335	1.371163
C	0.139210	-2.130160	2.876750
H	0.101036	-1.048052	3.030079
H	-0.888414	-2.517946	2.868632
H	0.671417	-2.582814	3.723605
C	2.298558	-1.960775	1.607626
H	2.836309	-2.233946	0.690125
H	2.311257	-0.870248	1.697089
H	2.826272	-2.404793	2.462175
C	2.623077	-1.251464	-2.394902
H	3.438924	-1.291971	-3.127714
H	2.779306	-2.039032	-1.650341
H	1.672109	-1.433332	-2.907948
C	2.341452	1.224620	-2.792184
H	2.317132	2.220373	-2.334864
H	3.143877	1.200544	-3.540397
H	1.382431	1.037937	-3.287991
C	3.979787	0.405675	-1.050547
H	4.773456	0.372823	-1.807910
H	3.985151	1.392036	-0.574144
H	4.183555	-0.352093	-0.287240

E = -877.908072208 a.u.

(a,a)-2_Q-bis-ene

Os	0.114382	-0.000272	-0.089993
C	1.867079	0.001787	-1.194641
H	1.756357	0.886363	-1.847294
H	1.758453	-0.883069	-1.847265
C	0.450060	-1.347218	1.110286
C	0.497272	-2.816439	0.792299
H	0.550061	-1.118710	2.185685
C	0.447238	1.347135	1.110531
C	0.491298	2.816529	0.792891
C	3.248870	0.003435	-0.548811

H	3.386178	-0.877867	0.084984
H	4.046121	0.004090	-1.304123
H	3.384296	0.885379	0.084493
H	0.379982	-3.029082	-0.275341
H	1.456552	-3.241155	1.119346
H	-0.289404	-3.356772	1.335663
O	-1.665854	-0.002122	-0.855429
Si	-3.202374	-0.000606	-0.186679
H	-4.196023	0.000804	-1.305196
H	-3.426839	-1.215752	0.660905
H	-3.424188	1.214503	0.661648
H	-0.296515	3.355025	1.336430
H	0.373495	3.029172	-0.274694
H	1.449671	3.243231	1.120003
H	0.547914	1.118568	2.185858

E = -408.069927343 a.u.
G = -407.913156 a.u.

(s,a)-2_Q-bis-ene

Os	-0.103783	-0.012590	-0.199708
C	-1.849911	-0.526401	-1.195316
H	-1.752976	-1.619356	-1.321739
H	-1.717032	-0.086339	-2.198692
C	-0.419520	1.769168	0.109564
C	-0.556203	2.588596	1.359596
H	-0.414508	2.392248	-0.808229
C	-0.468496	-0.739421	1.446551
C	-0.564256	-2.216402	1.723432
C	-3.235683	-0.183824	-0.659410
H	-3.360964	0.899272	-0.565266
H	-4.025967	-0.558174	-1.324003
H	-3.395774	-0.618241	0.332061
H	-0.582111	1.988900	2.271658
H	0.273751	3.303120	1.441580
H	-1.477135	3.185511	1.313450
O	1.693867	-0.397219	-0.821354
Si	3.192782	-0.074271	-0.145746
H	4.239597	-0.704713	-1.009194
H	3.447845	1.400990	-0.075002
H	3.302908	-0.636735	1.239424
H	0.208516	-2.529532	2.438090
H	-0.460607	-2.830975	0.822717
H	-1.535490	-2.451448	2.180714
H	-0.548004	-0.110466	2.345019

E = -408.066207235 a.u.
G = -407.909787 a.u.

(s,s)-2_Q-bis-ene

Os	-0.093013	-0.271787	-0.007692
C	-1.789539	-1.473648	0.023240
H	-1.605672	-2.123611	0.896232
H	-1.688827	-2.117482	-0.865534
C	-0.503585	0.733912	-1.485333
C	-0.820911	2.166507	-1.776568
H	-0.421378	0.124660	-2.411444
C	-0.448968	0.709239	1.500621
C	-3.197345	-0.892787	0.089374
H	-3.400569	-0.254770	-0.776390
H	-3.955603	-1.687372	0.107192
H	-3.332089	-0.279679	0.985806
H	-0.951135	2.770331	-0.877419
H	-0.033475	2.619849	-2.393788
H	-1.748733	2.225884	-2.361739
O	1.734902	-0.926361	-0.009219
Si	3.205888	-0.127196	-0.045507
H	4.292785	-1.155550	-0.034171
H	3.347254	0.708782	-1.282086
H	3.374612	0.767521	1.145254
C	-0.491743	2.173470	1.814718
H	-1.492614	2.454723	2.170669
H	0.208803	2.410374	2.626211
H	-0.243722	2.802491	0.957719
H	-0.529761	0.081129	2.412626

E = -408.062245513 a.u.
G = -407.906098 a.u.

2_Q-yne

Os	-0.092248	-0.027303	0.105310
C	-0.748693	-1.878611	-0.540873
H	-0.665497	-2.569355	0.313740
H	0.054311	-2.147777	-1.245832
C	-0.672709	1.171901	-1.481308
C	-0.523392	2.665736	-1.209471
H	0.038892	0.854077	-2.260365
C	-1.471673	0.299061	1.079378
C	-2.462273	0.602704	2.116851
C	-2.105767	-2.027736	-1.208137
H	-2.207000	-1.364276	-2.072140
H	-2.256734	-3.056723	-1.562991
H	-2.916075	-1.791616	-0.511116
H	-1.260812	3.015849	-0.479546
H	0.472548	2.918270	-0.826722
H	-0.669184	3.245886	-2.131186
H	-3.252100	1.249712	1.716012
H	-2.008752	1.101989	2.981224
H	-2.935015	-0.323621	2.466202
O	1.832617	-0.195221	-0.177883
Si	3.414412	-0.201377	0.344575
H	4.003240	-1.568797	0.185288
H	4.221905	0.765066	-0.464850
H	3.513645	0.191233	1.788319
H	-1.678187	0.937811	-1.839190

E = -408.068810317 a.u.
G = -407.915055 a.u.

(a,a)-2_L-bis-ene

Os	-0.940498	0.000906	-0.177164
C	-2.943155	-0.026158	0.533116

H	-3.495819	-0.867908	0.099410
H	-3.467028	0.878088	0.201260
C	-0.992001	-1.247868	-1.520733
C	-0.975356	-2.756611	-1.473492
H	-0.914585	-0.888787	-2.564780
C	-1.018480	1.352026	-1.418799
C	-1.067133	2.853124	-1.265823
C	-3.054350	-0.110060	2.072275
O	0.704070	-0.040500	0.870814
Si	2.287287	-0.031386	0.447960
H	-0.911298	1.073680	-2.485523
C	-2.243736	-3.251851	-2.207611
H	-2.248611	-4.349072	-2.243306
H	-3.143531	-2.910206	-1.682300
H	-2.270695	-2.867745	-3.234978
C	-0.949988	-3.319727	-0.047096
H	-0.067821	-2.958617	0.496562
H	-1.846329	-3.013759	0.500083
H	-0.917579	-4.416386	-0.074944
C	0.278218	-3.241984	-2.237346
H	0.296677	-4.339230	-2.267001
H	0.274532	-2.863996	-3.267444
H	1.185360	-2.884292	-1.736696
C	0.226054	3.436500	-1.880850
H	0.193856	4.533373	-1.846174
H	1.101485	3.090832	-1.318299
H	0.335015	3.122697	-2.926586
C	-1.190988	3.315529	0.191044
H	-2.123871	2.948585	0.629606
H	-0.350916	2.943707	0.790639
H	-1.191961	4.411965	0.240283
C	-2.286002	3.356148	-2.075404
H	-2.336398	4.451820	-2.030174
H	-2.204108	3.052533	-3.126536
H	-3.213859	2.941944	-1.662929
C	-2.461769	-1.418308	2.626887
H	-2.965482	-2.288823	2.189292
H	-1.386570	-1.484762	2.415970
H	-2.595098	-1.456172	3.715996
C	-2.350593	1.067410	2.773634
H	-1.273201	1.066470	2.560914
H	-2.775555	2.024438	2.450429
H	-2.479263	0.984259	3.860845
C	-4.554883	-0.066256	2.436261
H	-4.684164	-0.131326	3.525052
H	-5.007685	0.870434	2.086515
H	-5.087603	-0.905381	1.970595
O	2.456856	-0.156171	-1.177001
O	3.027894	-1.295989	1.175311
O	2.965589	1.370664	0.955909
Si	3.027202	-0.051248	-2.744063
H	3.793847	1.235530	-2.964256
H	3.947138	-1.211127	-3.057126
H	1.867781	-0.087088	-3.711200
Si	3.629125	-2.563689	2.073677
H	4.678330	-2.078381	3.050065
H	2.529980	-3.240163	2.864326
H	4.265797	-3.596305	1.169975
Si	3.556265	2.718145	1.739795
H	2.427354	3.624227	2.180818
H	4.350515	2.330268	2.968297
H	4.460636	3.504837	0.817946

E = -1002.89239764 a.u.

(s,a)-2$_L$-bis-ene

Os	-0.915688	-0.065536	0.019674
C	-2.835192	0.015177	-0.838887
H	-3.521591	0.623727	-0.239287
H	-3.244156	-1.004412	-0.820569
C	-0.883453	1.608796	0.757376
C	-0.793475	2.305812	2.092820
H	-0.824792	2.367676	-0.053659
C	-1.259322	-1.249030	1.381385
C	-1.507582	-2.739045	1.250638
C	-2.848228	0.506114	-2.299857
O	0.779897	-0.462686	-0.880830
Si	2.308847	-0.068551	-0.459007
H	-1.171605	-0.941494	2.430071
C	0.558716	3.056946	2.135487
H	0.633615	3.634852	3.065951
H	1.386714	2.341233	2.089292
H	0.645056	3.748455	1.287884
C	-0.901396	1.395552	3.320834
H	-1.862227	0.869320	3.325107
H	-0.087513	0.662803	3.328644
H	-0.831825	2.002220	4.232747
C	-1.944973	3.341409	2.132095
H	-1.887876	3.921420	3.062210
H	-1.875146	4.034835	1.284716
H	-2.915134	2.832046	2.091599
C	-0.466248	-3.475316	2.123585
H	-0.651495	-4.557129	2.096422
H	0.546062	-3.281592	1.748941
H	-0.525405	-3.136504	3.165643
C	-1.397068	-3.255187	-0.196158
H	-2.156227	-2.795484	-0.838241
H	-0.406308	-3.033824	-0.611983
H	-1.548236	-4.342074	-0.216227
C	-2.925678	-3.020873	1.799220
H	-3.128340	-4.099748	1.773861
H	-3.014895	-2.672393	2.835959
H	-3.677850	-2.504234	1.191354
C	-2.200061	1.894911	-2.453426
H	-2.654356	2.613678	-1.759703
H	-1.119851	1.852008	-2.256610
H	-2.335572	2.261911	-3.478906
C	-2.113486	-0.489577	-3.218821
H	-1.060779	-0.587770	-2.924674
H	-2.584036	-1.480357	-3.164080
H	-2.152663	-0.146232	-4.260902
C	-4.321874	0.599679	-2.752044
H	-4.380847	0.908593	-3.804233
H	-4.815494	-0.375444	-2.648379
H	-4.865986	1.331504	-2.141162
O	2.538621	-0.280626	1.156276
O	2.614389	1.488897	-0.854480
O	3.333891	-1.053246	-1.282488

Si	3.401055	-0.624584	2.551788
H	4.528396	0.363762	2.762059
H	2.472738	-0.544785	3.740190
H	3.992821	-2.016770	2.503740
Si	2.870342	3.043081	-1.394772
H	3.644356	3.042919	-2.694444
H	1.550583	3.745027	-1.636663
H	3.647658	3.844340	-0.374571
Si	3.886341	-2.167090	-2.400572
H	3.817444	-1.614073	-3.807887
H	5.325383	-2.516213	-2.098489
H	3.071010	-3.441974	-2.358352

E = -1002.89167621 a.u.

2_L-yne

Os	-0.740537	0.016439	-0.381984
C	-1.399458	-1.503585	-1.619622
H	-0.623526	-1.383847	-2.401098
H	-2.361302	-1.265432	-2.094013
C	-1.731364	1.317317	-1.646890
C	-2.018927	2.763463	-1.233708
H	-0.974115	1.327858	-2.454481
C	-1.891371	-0.099407	0.886170
C	-2.509292	-0.145533	2.234736
C	-1.406922	-2.964706	-1.162072
O	1.160408	0.304341	-0.827648
Si	2.485816	0.168089	0.112031
H	-2.640082	0.870001	-2.071189
C	-3.317719	2.842553	-0.416262
H	-4.165214	2.470836	-1.007091
H	-3.230384	2.226506	0.484096
H	-3.525627	3.878688	-0.119161
C	-2.199992	3.598907	-2.521520
H	-3.006972	3.183403	-3.138877
H	-2.453669	4.637053	-2.269538
H	-1.274234	3.600334	-3.111522
C	-0.857918	3.356964	-0.416960
H	-0.743013	2.810383	0.529195
H	0.083659	3.284970	-0.975491
H	-1.051892	4.412974	-0.185976
C	-4.047568	-0.226762	2.114151
H	-4.489763	-0.269999	3.117581
H	-4.438639	0.651633	1.591089
H	-4.339630	-1.123922	1.558192
C	-1.981137	-1.385367	2.994613
H	-2.416621	-1.399439	4.001868
H	-2.259199	-2.308196	2.476854
H	-0.890396	-1.343042	3.080565
C	-2.103378	1.124070	3.020619
H	-2.550763	1.086969	4.022022
H	-1.013160	1.174651	3.119426
H	-2.455081	2.026068	2.510313
C	-2.721956	-3.286016	-0.434036
H	-2.850858	-2.609805	0.416630
H	-3.575286	-3.152568	-1.111752
H	-2.722506	-4.322143	-0.071382
C	-0.214027	-3.270407	-0.240161
H	0.733426	-3.022450	-0.736126
H	-0.287059	-2.680603	0.683009
H	-0.198212	-4.335574	0.027512
C	-1.310706	-3.862232	-2.416490
H	-0.359295	-3.693370	-2.937580
H	-1.369204	-4.921458	-2.133004
H	-2.132358	-3.641636	-3.110153
O	2.006852	-0.414669	1.586100
O	3.549540	-0.878649	-0.562442
O	3.199219	1.625667	0.309018
Si	2.426021	-1.045079	3.091707
H	3.920754	-0.979614	3.321554
H	1.741534	-0.255186	4.183093
H	1.987266	-2.487051	3.197269
Si	4.464295	-1.798800	-1.614482
H	5.340060	-0.923705	-2.484525
H	5.354010	-2.737473	-0.832565
H	3.578946	-2.626487	-2.520342
Si	3.823692	3.172015	0.312651
H	3.216300	4.011419	-0.789340
H	3.545924	3.848351	1.636790
H	5.321754	3.135318	0.106638

E = -1002.90020927 a.u.

(a,a)-2_S-bis-ene

Cell parameters
a = 13.188734Å, b = 12.375218Å, c = 25.181828Å
α = 91.025532, β = 89.600938, γ = 92.576393

Fractional coordinates

H	2.235795E-01	8.554608E-01	4.502830E-01
H	1.003866E-01	7.947630E-01	4.526707E-01
H	3.361068E-01	5.940217E-01	4.135896E-01
H	1.979016E-01	5.263780E-01	4.191419E-01
H	9.599755E-01	3.839676E-01	3.788125E-01
H	5.917478E-02	4.266945E-01	3.344749E-01
H	8.921301E-02	3.714267E-01	3.970094E-01
H	3.330172E-03	6.072116E-01	4.810876E-01
H	9.271761E-01	4.891712E-01	4.639165E-01
H	5.590788E-02	4.771903E-01	4.830945E-01
H	9.565991E-01	6.863449E-01	3.915525E-01
H	-1.530633E-02	6.164808E-01	3.310955E-01
H	8.852581E-01	5.664961E-01	3.733610E-01
H	2.638969E-01	1.367502E-02	3.868106E-01
H	2.226139E-01	9.346848E-01	3.303768E-01
H	1.664764E-01	5.879262E-02	3.452183E-01
H	3.892125E-02	8.399823E-01	3.321337E-01
H	9.602419E-01	8.633992E-01	3.885901E-01
H	9.943763E-01	9.707635E-01	3.451309E-01
H	5.373232E-02	8.100092E-02	4.253716E-01
H	2.524668E-02	9.705076E-01	4.682310E-01
H	1.493584E-01	3.364437E-02	4.676715E-01
H	5.539222E-01	7.930806E-01	4.384690E-01
H	4.295864E-01	8.154910E-01	4.634334E-01
H	4.793753E-01	6.842203E-01	4.662565E-01
H	4.708808E-01	6.242756E-01	3.188448E-01
H	5.784152E-01	6.849748E-01	3.526655E-01

H	5.073296E-01	5.745408E-01	3.814000E-01
H	3.987021E-01	8.156436E-01	3.140052E-01
H	3.848348E-01	8.940785E-01	3.734606E-01
H	5.077969E-01	8.686949E-01	3.482803E-01
H	8.065722E-01	3.026036E-01	2.851279E-01
H	4.313800E-01	3.054500E-01	2.068999E-02
H	3.233500E-01	7.541300E-01	9.873300E-01
H	8.273800E-01	2.350200E-01	5.481999E-02
H	7.707600E-01	7.306900E-01	1.011000E-01
H	5.616100E-01	1.082300E-01	1.965000E-02
H	5.165300E-01	6.355900E-01	3.138999E-02
H	4.924000E-02	8.231000E-02	2.582000E-02
H	9.076000E-01	5.760800E-01	1.754999E-02
H	3.244998E-02	4.845500E-01	4.715999E-02
H	9.904400E-01	7.721600E-01	2.134998E-02
H	5.168600E-01	4.565100E-01	3.623999E-02
H	4.958300E-01	9.469400E-01	2.009986E-03
H	2.645700E-01	3.190200E-01	6.002999E-02
H	1.824200E-01	7.526600E-01	5.720999E-02
H	7.165000E-01	3.188700E-01	9.757200E-01
H	6.762900E-01	6.834200E-01	4.565999E-02
C	1.587048E-01	8.284860E-01	4.253435E-01
C	3.289448E-01	6.737276E-01	3.942663E-01
C	4.328855E-01	7.298515E-01	3.864026E-01
C	1.452427E-01	5.837463E-01	4.014925E-01
C	3.649888E-02	5.372666E-01	4.023359E-01
C	1.162559E-01	9.289501E-01	3.981601E-01
C	3.658711E-02	4.230888E-01	3.765697E-01
C	4.119432E-03	5.273754E-01	4.611915E-01
C	9.618276E-01	6.058745E-01	3.728621E-01
C	1.970544E-01	9.867592E-01	3.632956E-01
C	2.249231E-02	8.985582E-01	3.641722E-01
C	8.435322E-02	7.978511E-03	4.425381E-01
C	4.762355E-01	7.571894E-01	4.420524E-01
C	5.013607E-01	6.483968E-01	3.581021E-01
C	4.305270E-01	8.329331E-01	3.537102E-01
O	3.754900E-01	2.524300E-01	2.553999E-02
O	2.893300E-01	7.025900E-01	9.989990E-03
O	8.540000E-01	2.138000E-01	8.850999E-02
O	7.774100E-01	6.592300E-01	8.371999E-02
O	4.931900E-01	8.275000E-02	1.219000E-02
O	4.543800E-01	5.909800E-01	3.908999E-02
O	2.569995E-03	1.380900E-01	3.371000E-02
O	9.481500E-01	5.865200E-01	4.880999E-02
O	7.793999E-02	4.250100E-01	4.719999E-02
O	9.924000E-01	8.465300E-01	3.207998E-02
O	5.430000E-01	3.862000E-01	2.680999E-02
O	5.126500E-01	8.710400E-01	2.429987E-03
O	2.394000E-01	3.506200E-01	9.247999E-02
O	1.411300E-01	7.705700E-01	8.787999E-02
O	7.125600E-01	2.841200E-01	9.329992E-03
O	6.171900E-01	7.155600E-01	2.958999E-02
O	5.392688E-02	3.088220E-01	1.356800E-01
O	6.877373E-03	8.783723E-01	1.428005E-01
O	6.079033E-01	2.260440E-01	9.067180E-02
O	5.600116E-01	8.572373E-01	1.088919E-01
O	3.113610E-01	6.936845E-02	2.180998E-01
O	5.056030E-01	5.022754E-01	2.211694E-01
O	3.358837E-01	4.843538E-01	1.766124E-01
O	2.706493E-01	9.419172E-01	1.347013E-01
O	7.624510E-01	3.426280E-01	1.902941E-01
O	7.603441E-01	8.409902E-01	1.346710E-01
O	1.390522E-01	4.925019E-01	1.486079E-01
O	1.217052E-01	9.886645E-01	7.440103E-02
O	6.970466E-01	4.185223E-01	9.372866E-02
O	7.018078E-01	9.170869E-01	4.312208E-02
O	3.386067E-01	2.894759E-01	2.106931E-01
O	2.388579E-01	8.654826E-01	2.320462E-01
O	7.673857E-01	1.406224E-01	2.244621E-01
O	6.640009E-01	7.196341E-01	2.177947E-01
O	5.021389E-01	3.290190E-01	1.615203E-01
O	4.231012E-01	8.807396E-01	1.880668E-01
O	9.448704E-01	2.562339E-01	2.212960E-01
O	8.600501E-01	8.122765E-01	2.180588E-01
O	1.415819E-01	2.022299E-01	2.158555E-01
O	5.724522E-02	7.604681E-01	2.246440E-01
O	5.785706E-01	1.323724E-01	1.888516E-01
O	5.042511E-01	6.806172E-01	1.659901E-01
O	3.034272E-01	5.577406E-02	4.532910E-02
O	2.798585E-01	5.829795E-01	9.303714E-02
O	8.766282E-01	9.971488E-01	8.112956E-02
O	8.608715E-01	4.928808E-01	1.355488E-01
O	4.367331E-01	1.394033E-01	1.128315E-01
O	3.858504E-01	7.638660E-01	9.690752E-02
O	9.909821E-01	1.146530E-01	1.458890E-01
O	9.437732E-01	6.803316E-01	1.460059E-01
O	6.879884E-01	9.405882E-01	2.195823E-01
O	2.330548E-01	1.485765E-01	1.324824E-01
O	2.333783E-01	6.659526E-01	1.915658E-01
O	7.109608E-01	4.550175E-02	1.304815E-01
O	6.774338E-01	5.360655E-01	1.763040E-01
O	1.896835E-01	6.962686E-01	2.932123E-01
Si	3.638404E-02	2.195511E-01	1.808062E-01
Si	9.661383E-01	7.856382E-01	1.842929E-01
Si	5.314006E-01	2.059048E-01	1.417728E-01
Si	4.674874E-01	7.972200E-01	1.426038E-01
Si	2.304154E-01	3.601624E-02	9.756196E-02
Si	2.468592E-01	5.593457E-01	1.542101E-01
Si	7.649381E-01	9.511938E-01	9.689185E-02
Si	7.487224E-01	4.433935E-01	1.512672E-01
Si	1.268093E-01	3.939167E-01	1.033735E-01
Si	6.421108E-02	8.691507E-01	8.462148E-02
Si	6.385757E-01	3.321290E-01	5.578342E-02
Si	5.961396E-01	8.418458E-01	4.589104E-02
Si	2.603905E-01	1.822411E-01	1.952834E-01
Si	1.791436E-01	7.453645E-01	2.352641E-01
Si	6.842860E-01	6.352661E-02	1.928276E-01
Si	5.842690E-01	6.071266E-01	1.976889E-01
Si	4.038938E-01	1.363899E-01	4.929476E-02
Si	3.563823E-01	6.587209E-01	5.918690E-02
Si	9.348336E-01	1.180191E-01	8.737596E-02
Si	8.822128E-01	6.051300E-01	1.041523E-01
Si	4.189567E-01	4.016294E-01	1.945536E-01
Si	3.128545E-01	9.416983E-01	1.950602E-01
Si	8.221092E-01	2.623474E-01	2.303549E-01
Si	7.393984E-01	8.247883E-01	2.004158E-01
Os	2.019213E-01	7.063514E-01	3.703900E-01

E = -936.85389 eV

(s,a)-2$_S$-bis-ene

Cell parameters

a = 13.188734Å, b = 12.375218Å, c= 25.181828Å

α = 91.025532, β = 89.600938, γ = 92.576393

Fractional coordinates

H	1.080294E-01	6.971349E-01	4.597600E-01
H	1.058824E-01	5.595059E-01	4.408073E-01
H	2.143678E-01	8.643975E-01	3.964967E-01
H	3.813706E-01	5.957698E-01	4.008808E-01
H	9.239877E-01	7.006526E-01	4.774428E-01
H	8.359932E-01	6.376675E-01	4.318738E-01
H	9.219120E-01	5.578694E-01	4.666760E-01
H	9.945744E-01	8.281216E-01	4.063431E-01
H	3.006564E-02	7.755583E-01	3.426324E-01
H	9.012640E-01	7.694916E-01	3.624247E-01
H	2.330080E-02	5.674143E-01	3.256846E-01
H	9.724211E-01	4.809212E-01	3.761302E-01
H	8.926580E-01	5.692454E-01	3.426873E-01
H	1.317644E-01	4.217779E-01	3.761226E-01
H	1.922211E-01	4.369250E-01	3.130161E-01
H	2.000892E-01	3.143555E-01	3.480080E-01
H	3.029995E-01	3.112304E-01	4.344925E-01
H	3.717485E-01	4.301889E-01	4.572654E-01
H	2.367086E-01	4.226268E-01	4.611392E-01
H	4.613875E-01	4.377983E-01	3.681250E-01
H	3.886532E-01	3.231496E-01	3.430798E-01
H	3.914045E-01	4.484782E-01	3.086634E-01
H	4.191700E-01	9.575347E-01	4.830020E-01
H	2.921929E-01	9.747416E-01	4.621299E-01
H	3.214330E-01	8.595596E-01	4.997142E-01
H	4.323090E-01	7.139244E-01	4.580886E-01
H	4.791347E-01	7.288593E-01	3.916794E-01
H	5.240918E-01	8.186056E-01	4.429206E-01
H	3.542176E-01	-9.080896E-03	3.650782E-01
H	4.802652E-01	9.766690E-01	3.883117E-01
H	4.304156E-01	8.891207E-01	3.368681E-01
H	8.062331E-01	3.030654E-01	2.850325E-01
H	4.313800E-01	3.054500E-01	2.068999E-02
H	3.233500E-01	7.541300E-01	9.873300E-01
H	8.273800E-01	2.350200E-01	5.481999E-02
H	7.707600E-01	7.306900E-01	1.011000E-01
H	5.616100E-01	1.082300E-01	1.965000E-02
H	5.165300E-01	6.355900E-01	3.138999E-02
H	4.924000E-02	8.231000E-02	2.582000E-02
H	9.076000E-01	5.760800E-01	1.754999E-02
H	3.244998E-02	4.845500E-01	4.715999E-02
H	9.904400E-01	7.721600E-01	2.134998E-02
H	5.168600E-01	4.565100E-01	3.623999E-02
H	4.958300E-01	9.469400E-01	2.009986E-03
H	2.645700E-01	3.190200E-01	6.002999E-02
H	1.824200E-01	7.526600E-01	5.720999E-02
H	7.165000E-01	3.188700E-01	9.757200E-01
H	6.762900E-01	6.834200E-01	4.565999E-02
C	9.928097E-02	6.415790E-01	4.253144E-01
C	2.718589E-01	8.003169E-01	3.975418E-01
C	3.727719E-01	8.512688E-01	4.166206E-01
C	3.050654E-01	5.696012E-01	3.866333E-01
C	2.967715E-01	4.466561E-01	3.803496E-01
C	9.916477E-01	6.508327E-01	4.015113E-01
C	9.140563E-01	6.359148E-01	4.471108E-01
C	9.791940E-01	7.623734E-01	3.770328E-01
C	9.692032E-01	5.620719E-01	3.591453E-01
C	1.996542E-01	4.029456E-01	3.528348E-01
C	3.022982E-01	4.002326E-01	4.367599E-01
C	3.901349E-01	4.118154E-01	3.481900E-01
C	3.495866E-01	9.144988E-01	4.684899E-01
C	4.563835E-01	7.728715E-01	4.278416E-01
C	4.113508E-01	9.318551E-01	3.740348E-01
O	3.754900E-01	2.524300E-01	2.553999E-02
O	2.893300E-01	7.025900E-01	9.989990E-03
O	8.540000E-01	2.138000E-01	8.850999E-02
O	7.774100E-01	6.592300E-01	8.371999E-02
O	4.931900E-01	8.275000E-02	1.219000E-02
O	4.543800E-01	5.909800E-01	3.908999E-02
O	2.569995E-03	1.380900E-01	3.371000E-02
O	9.481500E-01	5.865200E-01	4.880999E-02
O	7.793999E-02	4.250100E-01	4.719999E-02
O	9.924000E-01	8.465300E-01	3.207998E-02
O	5.430000E-01	3.862000E-01	2.680999E-02
O	5.126500E-01	8.710400E-01	2.429987E-03
O	2.394000E-01	3.506200E-01	9.247999E-02
O	1.411300E-01	7.705700E-01	8.787999E-02
O	7.125600E-01	2.841200E-01	9.329992E-03
O	6.171900E-01	7.155600E-01	2.958999E-02
O	5.400255E-02	3.094704E-01	1.359684E-01
O	7.746704E-03	8.779010E-01	1.432705E-01
O	6.081565E-01	2.263722E-01	9.068646E-02
O	5.599001E-01	8.574316E-01	1.088670E-01
O	3.111104E-01	6.908974E-02	2.187985E-01
O	5.060128E-01	5.026807E-01	2.209673E-01
O	3.359299E-01	4.840893E-01	1.766942E-01
O	2.688395E-01	9.413084E-01	1.359993E-01
O	7.625516E-01	3.429439E-01	1.901414E-01
O	7.609737E-01	8.409717E-01	1.347365E-01
O	1.392627E-01	4.928992E-01	1.485605E-01
O	1.216797E-01	9.884549E-01	7.455860E-02
O	6.973914E-01	4.190532E-01	9.358016E-02
O	7.020503E-01	9.169178E-01	4.323083E-02
O	3.388857E-01	2.890740E-01	2.105515E-01
O	2.408767E-01	8.644075E-01	2.340748E-01
O	7.674234E-01	1.408894E-01	2.244110E-01
O	6.644894E-01	7.198502E-01	2.177899E-01
O	5.025666E-01	3.289776E-01	1.616351E-01
O	4.232537E-01	8.809304E-01	1.881511E-01
O	9.448712E-01	2.565830E-01	2.214636E-01
O	8.611577E-01	8.117046E-01	2.182673E-01
O	1.417698E-01	2.025131E-01	2.160179E-01
O	5.967181E-02	7.598790E-01	2.252942E-01
O	5.787158E-01	1.320631E-01	1.887896E-01
O	5.044484E-01	6.810760E-01	1.659903E-01
O	3.036861E-01	5.487147E-02	4.596487E-02
O	2.802592E-01	5.821474E-01	9.263441E-02
O	8.770647E-01	9.971901E-01	8.126094E-02
O	8.612891E-01	4.932394E-01	1.356185E-01
O	4.368893E-01	1.395349E-01	1.128621E-01
O	3.856513E-01	7.639183E-01	9.692911E-02
O	9.912237E-01	1.153026E-01	1.459429E-01

O	9.447361E-01	6.802426E-01	1.463061E-01
O	6.889588E-01	9.405080E-01	2.195990E-01
O	2.333380E-01	1.482491E-01	1.327512E-01
O	2.349409E-01	6.672646E-01	1.902791E-01
O	7.112117E-01	4.544418E-02	1.304694E-01
O	6.777302E-01	5.365660E-01	1.761330E-01
O	1.941301E-01	6.878506E-01	2.920934E-01
Si	3.652735E-02	2.200916E-01	1.810588E-01
Si	9.681027E-01	7.850206E-01	1.850430E-01
Si	5.316602E-01	2.058126E-01	1.417369E-01
Si	4.673202E-01	7.974766E-01	1.426052E-01
Si	2.302488E-01	3.531911E-02	9.814095E-02
Si	2.473110E-01	5.592933E-01	1.538538E-01
Si	7.653772E-01	9.511695E-01	9.695261E-02
Si	7.490452E-01	4.439213E-01	1.511649E-01
Si	1.268567E-01	3.941140E-01	1.034055E-01
Si	6.406972E-02	8.689201E-01	8.477628E-02
Si	6.387266E-01	3.324985E-01	5.578537E-02
Si	5.961941E-01	8.418968E-01	4.592785E-02
Si	2.605524E-01	1.818749E-01	1.955071E-01
Si	1.820282E-01	7.437636E-01	2.356927E-01
Si	6.845926E-01	6.335540E-02	1.928404E-01
Si	5.845314E-01	6.075594E-01	1.975642E-01
Si	4.037610E-01	1.362000E-01	4.937243E-02
Si	3.564816E-01	6.587682E-01	5.911353E-02
Si	9.350239E-01	1.182512E-01	8.743147E-02
Si	8.827166E-01	6.055758E-01	1.043410E-01
Si	4.191997E-01	4.013681E-01	1.945534E-01
Si	3.127924E-01	9.409750E-01	1.961352E-01
Si	8.220428E-01	2.626403E-01	2.303218E-01
Si	7.404763E-01	8.246888E-01	2.004417E-01
Os	2.155907E-01	6.740328E-01	3.684698E-01

E = -936.71547 eV

2_S-yne

Cell parameters

a = 13.188734Å, b = 12.375218Å, c= 25.181828Å

α = 91.025532, β = 89.600938, γ = 92.576393

Fractional coordinates

H	1.240014E-01	5.122692E-01	3.660268E-01
H	1.775802E-01	5.163426E-01	4.304767E-01
H	2.250943E-02	6.772355E-01	3.785505E-01
H	6.134997E-02	7.016915E-01	4.451740E-01
H	3.205582E-01	8.245078E-01	5.587715E-01
H	2.293206E-01	8.718136E-01	5.138988E-01
H	2.208363E-01	7.348814E-01	5.348425E-01
H	4.532820E-01	7.063891E-01	5.312282E-01
H	3.621985E-01	6.062661E-01	5.078641E-01
H	4.630092E-01	6.523717E-01	4.653718E-01
H	4.595953E-01	8.957274E-01	4.946742E-01
H	4.640106E-01	8.442920E-01	4.280921E-01
H	3.680090E-01	9.340819E-01	4.475774E-01
H	9.173858E-02	9.076914E-01	4.773698E-01
H	1.747896E-01	9.336839E-01	4.223488E-01
H	6.512347E-02	1.063075E-02	4.317568E-01
H	1.081673E-01	8.978669E-01	3.271623E-01
H	9.878391E-01	8.298697E-01	3.175988E-01
H	9.956183E-01	9.658321E-01	3.420204E-01
H	9.186996E-01	8.151224E-01	4.637997E-01
H	8.893889E-01	9.222636E-01	4.208878E-01
H	8.734740E-01	7.854148E-01	3.983715E-01
H	2.240617E-01	4.486598E-01	2.858272E-01
H	3.245861E-01	5.467683E-01	2.978973E-01
H	3.498274E-01	4.063410E-01	2.952741E-01
H	4.101486E-01	5.570486E-01	3.892500E-01
H	3.698298E-01	4.661294E-01	4.400029E-01
H	4.338009E-01	4.170254E-01	3.825743E-01
H	1.648781E-01	3.188149E-01	3.584144E-01
H	2.922285E-01	2.795715E-01	3.650638E-01
H	2.242311E-01	3.255078E-01	4.219066E-01
H	8.066093E-01	3.018331E-01	2.851542E-01
H	4.313800E-01	3.054500E-01	2.068999E-02
H	3.233500E-01	7.541300E-01	9.873300E-01
H	8.273800E-01	2.350200E-01	5.481999E-02
H	7.707600E-01	7.306900E-01	1.011000E-01
H	5.616100E-01	1.082300E-01	1.965000E-02
H	5.165300E-01	6.355900E-01	3.138999E-02
H	4.924000E-02	8.231000E-02	2.582000E-02
H	9.076000E-01	5.760800E-01	1.754999E-02
H	3.244998E-02	4.845500E-01	4.715999E-02
H	9.904400E-01	7.721600E-01	2.134998E-02
H	5.168600E-01	4.565100E-01	3.623999E-02
H	4.958300E-01	9.469400E-01	2.009986E-03
H	2.645700E-01	3.190200E-01	6.002999E-02
H	1.824200E-01	7.526600E-01	5.720999E-02
H	7.165000E-01	3.188700E-01	9.757200E-01
H	6.762900E-01	6.834200E-01	4.565999E-02
C	1.947931E-01	5.317322E-01	3.884316E-01
C	7.092899E-02	7.311905E-01	4.044164E-01
C	3.207074E-02	8.472551E-01	4.010516E-01
C	2.801633E-01	7.302597E-01	4.320009E-01
C	3.437283E-01	7.694000E-01	4.774099E-01
C	2.766153E-01	4.546612E-01	3.683200E-01
C	2.736647E-01	8.022464E-01	5.239107E-01
C	4.094960E-01	6.774628E-01	4.962973E-01
C	4.129336E-01	8.669152E-01	4.607209E-01
C	9.473447E-02	9.292004E-01	4.351688E-01
C	3.099520E-02	8.870032E-01	3.436828E-01
C	9.219839E-01	8.419209E-01	4.223337E-01
C	2.943227E-01	4.656258E-01	3.083576E-01
C	3.782388E-01	4.750067E-01	3.967961E-01
C	2.368591E-01	3.379301E-01	3.791376E-01
O	5.374832E-02	3.092959E-01	1.357144E-01
O	7.591665E-03	8.782231E-01	1.431450E-01
O	6.079682E-01	2.257324E-01	9.050922E-02
O	5.604375E-01	8.578067E-01	1.088791E-01
O	3.113809E-01	6.900082E-02	2.177567E-01
O	5.066435E-01	5.030367E-01	2.208593E-01
O	3.372101E-01	4.841486E-01	1.758061E-01
O	2.710610E-01	9.413812E-01	1.344100E-01
O	7.628358E-01	3.431007E-01	1.904352E-01
O	7.607548E-01	8.409851E-01	1.344880E-01
O	1.394243E-01	4.924467E-01	1.488037E-01
O	1.218566E-01	9.882126E-01	7.412042E-02
O	6.972673E-01	4.183226E-01	9.371894E-02
O	7.021051E-01	9.167528E-01	4.280597E-02

O	3.397402E-01	2.882670E-01	2.090031E-01
O	2.383987E-01	8.655810E-01	2.318480E-01
O	7.674813E-01	1.405734E-01	2.239218E-01
O	6.640205E-01	7.199189E-01	2.175962E-01
O	5.040426E-01	3.294353E-01	1.617230E-01
O	4.230378E-01	8.804050E-01	1.880597E-01
O	9.451383E-01	2.561947E-01	2.213647E-01
O	8.602785E-01	8.120761E-01	2.180840E-01
O	1.421983E-01	2.025366E-01	2.155309E-01
O	5.748596E-02	7.585986E-01	2.248863E-01
O	5.785688E-01	1.318074E-01	1.886686E-01
O	5.045776E-01	6.808772E-01	1.655425E-01
O	3.038538E-01	5.536154E-02	4.504092E-02
O	2.794189E-01	5.852883E-01	9.380378E-02
O	8.768450E-01	9.971753E-01	8.109574E-02
O	8.613408E-01	4.927384E-01	1.353887E-01
O	4.366441E-01	1.398823E-01	1.128309E-01
O	3.865197E-01	7.648436E-01	9.647109E-02
O	9.912148E-01	1.149114E-01	1.458303E-01
O	9.437751E-01	6.805536E-01	1.459793E-01
O	6.882410E-01	9.404385E-01	2.192812E-01
O	2.327956E-01	1.478338E-01	1.319900E-01
O	2.334847E-01	6.630878E-01	1.944027E-01
O	7.107506E-01	4.529565E-02	1.300446E-01
O	6.782224E-01	5.368378E-01	1.759313E-01
O	1.905336E-01	7.037833E-01	2.965638E-01
O	3.754900E-01	2.524300E-01	2.553999E-02
O	2.893300E-01	7.025900E-01	9.989990E-03
O	8.540000E-01	2.138000E-01	8.850999E-02
O	7.774100E-01	6.592300E-01	8.371999E-02
O	4.931900E-01	8.275000E-02	1.219000E-02
O	4.543800E-01	5.909800E-01	3.908999E-02
O	2.569995E-03	1.380900E-01	3.371000E-02
O	9.481500E-01	5.865200E-01	4.880999E-02
O	7.793999E-02	4.250100E-01	4.719999E-02
O	9.924000E-01	8.465300E-01	3.207998E-02
O	5.430000E-01	3.862000E-01	2.680999E-02
O	5.126500E-01	8.710400E-01	2.429987E-03
O	2.394000E-01	3.506200E-01	9.247999E-02
O	1.411300E-01	7.705700E-01	8.787999E-02
O	7.125600E-01	2.841200E-01	9.329992E-03
O	6.171900E-01	7.155600E-01	2.958999E-02
Si	3.664477E-02	2.197963E-01	1.807831E-01
Si	9.667783E-01	7.853351E-01	1.846220E-01
Si	5.316100E-01	2.058418E-01	1.417499E-01
Si	4.677184E-01	7.975588E-01	1.424428E-01
Si	2.307536E-01	3.524356E-02	9.717931E-02
Si	2.470969E-01	5.594127E-01	1.548626E-01
Si	7.650736E-01	9.510875E-01	9.659355E-02
Si	7.491226E-01	4.435567E-01	1.512021E-01
Si	1.268941E-01	3.941262E-01	1.034187E-01
Si	6.410680E-02	8.689902E-01	8.471313E-02
Si	6.385703E-01	3.320583E-01	5.581310E-02
Si	5.961739E-01	8.418728E-01	4.586794E-02
Si	2.608111E-01	1.817318E-01	1.946535E-01
Si	1.791991E-01	7.457185E-01	2.368186E-01
Si	6.843675E-01	6.309046E-02	1.924297E-01
Si	5.846686E-01	6.075417E-01	1.972854E-01
Si	4.039739E-01	1.364588E-01	4.928883E-02
Si	3.564581E-01	6.591436E-01	5.927035E-02
Si	9.349281E-01	1.181335E-01	8.739291E-02
Si	8.822736E-01	6.051412E-01	1.041697E-01
Si	4.200757E-01	4.017931E-01	1.944027E-01
Si	3.126691E-01	9.412220E-01	1.949269E-01
Si	8.222773E-01	2.622215E-01	2.302880E-01
Si	7.396870E-01	8.247365E-01	2.001915E-01
Os	2.143252E-01	6.973526E-01	3.739987E-01

E = 936.87030 eV

Grafting reaction pathways

TS(1-1)(ene-ap)

Os	-0.449328	-0.098508	0.112498
C	-0.607130	-0.724613	1.830541
H	-1.552844	-1.210693	2.133859
C	-0.629078	1.950078	0.446310
C	-0.706537	2.638366	-0.919547
C	0.415667	-0.660106	2.920697
H	1.348351	-0.205654	2.585792
H	0.006158	-0.088576	3.766301
H	0.623195	-1.669506	3.302626
O	1.862303	0.101657	0.270872
Si	2.955115	1.160681	-0.391311
H	2.877204	2.517090	0.245896
H	4.356430	0.654372	-0.217108
H	2.728194	1.351159	-1.868780
H	-1.687423	2.508029	-1.387589
H	0.053669	2.271451	-1.624121
H	-0.530981	3.717655	-0.822910
H	0.291084	2.232379	0.973623
C	0.644699	-1.683341	-1.266278
H	-0.160608	-2.363932	-0.969097
H	1.283167	-0.792486	-0.506217
C	1.945228	-2.510702	-1.345943
H	1.823090	-3.345747	-2.044466
H	2.792508	-1.909114	-1.687875
H	2.207684	-2.920394	-0.366525
C	-2.227174	-0.480649	-0.251455
H	-2.855981	-1.018223	0.484973
C	-2.997136	-0.182384	-1.507470
H	-3.873723	0.440087	-1.277848
H	-2.406960	0.329210	-2.275088
H	-3.389511	-1.113091	-1.941396
H	0.391645	-1.279827	-2.255290
H	-1.476671	2.239733	1.071662

E = -487.805559378 a.u.
G = -487.581832 a.u.

TS(1-1)(alk-ap)

Os	-0.377321	0.010620	-0.068515
C	-0.996242	-1.354698	-1.140703
H	-1.391240	-0.935251	-2.090682
C	-0.039177	-0.915243	1.483349
C	-0.412854	-0.571089	2.894217

C	-0.956464	-2.844383	-1.133282
H	-0.539228	-3.245860	-0.208060
H	-1.973574	-3.242139	-1.257495
H	-0.369824	-3.219491	-1.982612
O	1.822545	-0.187196	-0.823384
Si	3.129375	-0.853383	-0.032272
H	3.022833	-2.349102	0.019912
H	4.402959	-0.502864	-0.739978
H	3.242228	-0.366084	1.385948
H	-1.005641	-1.390175	3.326464
H	-0.991124	0.351626	2.978268
H	0.488677	-0.480731	3.514941
H	0.579711	-1.826558	1.411932
C	0.699983	2.122696	-0.273040
H	0.074469	2.512129	-1.087673
H	1.358804	0.931470	-0.546650
C	2.053691	2.861383	-0.274773
H	1.914412	3.942373	-0.157884
H	2.693803	2.520195	0.545677
H	2.600035	2.694805	-1.208299
C	-2.213867	0.808897	0.503871
H	-2.820789	0.111191	1.093526
H	-1.963466	1.648123	1.176088
C	-3.041595	1.340162	-0.669891
H	-3.935395	1.877491	-0.326530
H	-2.474004	2.038987	-1.298090
H	-3.381771	0.520733	-1.314589
H	0.192064	2.360571	0.673309

E = -487.793415318 a.u.
G = -487.571379 a.u.

TS(1-2)

Os	0.266362	0.060909	-0.103260
C	0.677972	-1.002211	1.705715
H	1.756847	-1.159252	1.814533
H	0.196419	-1.985301	1.603751
C	0.576406	1.749029	-0.277430
C	0.545485	3.213131	-0.220505
C	1.673245	-0.651514	-1.108404
C	1.723618	-2.134095	-1.325048
C	0.125746	-0.296047	2.943938
H	-0.949782	-0.120833	2.849726
H	0.285544	-0.898715	3.848257
H	0.616811	0.670495	3.110105
H	-0.483313	3.590094	-0.214818
H	1.053213	3.550356	0.689574
H	1.071398	3.638863	-1.083104
O	-1.560856	-0.576716	0.387024
Si	-2.897880	-0.362917	-0.592343
H	-4.093181	-0.939148	0.103274
H	-3.166153	1.089689	-0.866074
H	-2.745565	-1.053076	-1.916027
H	1.707503	-2.374799	-2.395409
H	0.912547	-2.678829	-0.831731
H	2.673168	-2.514863	-0.921984
H	2.423452	-0.089225	-1.664515
H	-0.380091	1.070268	-1.390747

E = -408.015158430 a.u.
G = -407.862951 a.u.

3_Q

Os	-0.236419	0.177216	-0.096502
C	-0.512108	-0.771446	1.832455
H	-1.453542	-0.429188	2.275999
H	0.316425	-0.401579	2.447093
C	-1.727440	-0.266255	-0.825731
C	-2.810669	-0.938851	-1.539845
C	-0.577521	1.985643	0.182671
C	0.466916	2.799935	0.891083
C	-0.468313	-2.295398	1.764986
H	0.452803	-2.639820	1.284765
H	-0.496990	-2.738247	2.769890
H	-1.318472	-2.708891	1.208211
H	-2.431424	-1.444830	-2.434685
H	-3.281434	-1.685014	-0.889004
H	-3.576060	-0.214972	-1.843726
O	1.608626	-0.534695	0.288200
Si	2.838415	-0.696378	-0.830488
H	4.063305	-1.186409	-0.118312
H	2.497508	-1.687548	-1.903965
H	3.174505	0.605624	-1.497763
H	0.772909	3.643733	0.259384
H	1.357652	2.225296	1.158714
H	0.038130	3.220678	1.810710
H	-1.470496	2.530414	-0.120335
H	0.490993	0.387424	-1.585307

E = -408.033651221 a.u.
G = -407.880452 a.u.

TS(1-3)

Os	-0.240301	0.198283	0.021828
C	-0.760864	-1.230517	1.527315
H	-1.670401	-0.916566	2.050591
H	0.075188	-1.186323	2.236089
C	-1.805207	0.254999	-0.693256
C	-3.018226	0.033619	-1.478403
C	0.063838	2.050877	0.223150
C	1.222787	2.565165	1.025510
C	-0.906683	-2.656402	0.994760
H	-0.015583	-2.967459	0.439975
H	-1.042288	-3.373691	1.815624
H	-1.772187	-2.761876	0.329360
H	-2.805482	-0.522097	-2.398782
H	-3.744255	-0.534601	-0.884501
H	-3.477760	0.993195	-1.745278
O	1.517214	-0.751478	0.206600
Si	2.711918	-0.930880	-0.940562
H	3.953060	-1.444442	-0.275899
H	2.320790	-1.907401	-2.010320
H	3.043291	0.372563	-1.613052
H	1.804696	3.281037	0.430624

H	1.885619	1.773243	1.379413
H	0.834513	3.109656	1.896027
H	-0.576342	2.827843	-0.192711
H	0.571563	1.125109	-1.195464

E = -408.022944376 a.u.
G = -407.870745 a.u.

TS(2-1)(alk-ap)

Os	-0.186533	0.185995	-0.089414
C	-0.870222	0.367229	1.864542
H	-1.874909	0.781289	2.013356
H	-0.137431	1.109734	2.231069
C	0.350724	1.727938	-0.922250
C	0.677555	2.997391	-0.195759
C	-0.699249	-0.947477	2.627658
H	0.302545	-1.370945	2.495929
H	-0.854206	-0.798219	3.704406
H	-1.429452	-1.698810	2.304664
O	1.747185	-1.049698	0.070229
Si	3.299529	-0.419881	0.150667
H	3.460026	0.379868	1.405846
H	4.313040	-1.521378	0.147675
H	3.575072	0.479341	-1.019328
H	1.682790	3.343295	-0.468836
H	0.627351	2.900275	0.891574
H	-0.027989	3.782128	-0.501521
H	0.409312	1.781785	-2.015795
C	-0.265072	-1.257130	-1.417067
H	-0.856868	-1.022786	-2.310600
H	1.142382	-1.134144	-0.968304
C	-0.405629	-2.720074	-1.028602
H	0.030684	-3.348829	-1.817266
H	0.115878	-2.964398	-0.098381
H	-1.456357	-3.023321	-0.929931
C	-2.203477	0.649867	-0.551831
H	-2.495657	1.576373	-0.038375
H	-2.272985	0.851161	-1.630261
C	-3.213882	-0.446036	-0.199414
H	-4.236489	-0.115629	-0.426155
H	-3.040477	-1.362860	-0.772112
H	-3.195104	-0.713895	0.862988

E = -487.780273466 a.u.
G = -487.554979 a.u.

$4a_Q$

Os	0.101139	-0.013488	0.161429
C	0.569938	1.985405	0.272831
H	1.592177	2.145717	0.630201
H	-0.146293	2.224351	1.079325
C	-0.155089	-0.903734	1.720906
C	-0.240652	-0.410244	3.127151
C	0.277531	2.814882	-0.968852
H	-0.761065	2.710660	-1.281586
H	0.488004	3.871695	-0.758599
H	0.924956	2.524594	-1.803757
O	-1.683972	0.657830	-0.580900
Si	-3.128800	-0.144400	-0.638739
H	-3.799806	-0.182698	0.708615
H	-4.061906	0.533699	-1.597140
H	-2.995208	-1.581862	-1.078559
H	-1.222565	-0.633000	3.561827
H	-0.061114	0.665171	3.201811
H	0.515201	-0.921466	3.738109
H	-0.379949	-1.965876	1.530211
C	0.257087	-1.170356	-1.540118
H	-0.761940	-1.211896	-1.944417
H	0.852078	-0.541569	-2.218198
C	0.855649	-2.561521	-1.402152
H	0.792293	-3.084299	-2.365996
H	1.904363	-2.541161	-1.098052
H	0.302610	-3.170649	-0.678682
C	2.250196	-0.223126	0.296810
H	2.573564	0.344335	1.182371
H	2.509914	-1.268286	0.501875
C	3.081738	0.255738	-0.898220
H	4.154602	0.211735	-0.669996
H	2.927678	-0.360628	-1.791020
H	2.862432	1.293211	-1.177581

E = -487.842076080 a.u.
G = -487.611475 a.u.

TS(2-1)(ene-ap)

Os	0.443519	0.170712	-0.043118
C	0.608428	0.159496	2.030320
H	0.915333	1.187690	2.277397
H	1.440645	-0.487791	2.334071
C	0.182260	-1.559611	-1.137026
C	0.282209	-2.704608	-0.128785
C	-0.684512	-0.227314	2.738953
H	-0.959688	-1.267892	2.540016
H	-0.558878	-0.126201	3.825427
H	-1.525263	0.397211	2.429457
O	-1.953827	0.177051	-0.091886
Si	-3.274368	-0.749008	-0.467269
H	-3.170701	-2.125567	0.127783
H	-4.541658	-0.130808	0.048458
H	-3.442745	-0.920206	-1.953018
H	0.324361	-3.666485	-0.656258
H	-0.584574	-2.733362	0.536921
H	1.188130	-2.649203	0.488823
H	0.962164	-1.632286	-1.904661
C	-0.226141	1.729190	-0.994698
H	0.421996	2.042619	-1.821804
H	-1.291468	0.881335	-0.949614
C	-0.920946	2.910533	-0.335297
H	-1.551409	3.426969	-1.071534
H	-1.562807	2.598023	0.491171
H	-0.191547	3.643544	0.032653
C	2.256815	0.386700	-0.344147
H	2.660674	1.416331	-0.386687
C	3.344938	-0.623916	-0.558294
H	3.871860	-0.429274	-1.503211

H	4.100399	-0.519904	0.234322
H	2.995000	-1.658984	-0.561037
H	-0.793777	-1.572975	-1.630975

E = -487.794946950 a.u.
G = -487.571703 a.u.

4b$_Q$

Os	-0.273385	0.020241	0.049917
C	-0.247199	2.009531	-0.501950
H	-1.155207	2.333073	-1.015988
H	0.593227	2.038811	-1.212869
C	-2.161662	0.059605	-0.114206
C	-3.000227	0.367011	-1.316600
C	0.044136	2.900499	0.704468
H	0.960821	2.602188	1.220510
H	0.169787	3.940036	0.374931
H	-0.782836	2.882562	1.421938
O	1.758267	0.024192	0.324213
Si	3.121538	0.357279	-0.543803
H	4.039838	-0.830506	-0.594870
H	2.817366	0.736909	-1.974203
H	3.894201	1.497915	0.054841
H	-2.419300	0.595456	-2.215342
H	-3.669357	1.214767	-1.106087
H	-3.668218	-0.479562	-1.537141
H	-2.826570	-0.139783	0.749600
C	-0.227426	-1.303286	-1.523947
H	-1.183430	-1.456636	-2.029273
H	0.433887	-0.721951	-2.192528
C	0.418025	-2.639868	-1.167548
H	0.571679	-3.232709	-2.078553
H	1.386138	-2.513312	-0.677257
H	-0.227753	-3.229024	-0.507513
C	-0.613767	-0.469229	1.997589
H	-0.061896	0.341906	2.502763
H	-1.666248	-0.428414	2.307296
C	0.008959	-1.820566	2.329890
H	-0.094044	-2.021661	3.404658
H	-0.499588	-2.638210	1.806129
H	1.072018	-1.847805	2.078631

E = -487.850108847 a.u.
G = -487.620153 a.u.

TS(2-2)

Os	-0.300400	0.061489	-0.101374
C	0.298128	2.047523	-0.853870
H	-0.603189	2.653001	-1.009119
H	0.719744	1.803490	-1.835423
C	-1.638192	-0.166106	-1.161826
C	-2.677367	-0.472337	-2.141353
C	1.326695	2.829135	-0.048442
H	2.212781	2.218108	0.146213
H	1.656686	3.720091	-0.599789
H	0.934412	3.185655	0.911197
O	1.647473	-0.107100	-0.418306
Si	2.888425	-1.197117	-0.583677
H	4.043552	-0.482188	-1.214572
H	3.361820	-1.752091	0.728610
H	2.526973	-2.356300	-1.466930
H	-2.823468	-1.552566	-2.250922
H	-2.371332	-0.065116	-3.111615
H	-3.628222	-0.005838	-1.859765
H	-1.776522	-0.520046	0.350559
C	0.063749	-1.901677	0.763355
H	0.487052	-2.523208	-0.037791
H	0.884366	-1.707397	1.466573
C	-1.048626	-2.668428	1.478272
H	-0.672816	-3.597896	1.928206
H	-1.497428	-2.078588	2.286460
H	-1.857476	-2.949044	0.793042
C	-1.092782	1.318437	1.428066
H	-1.100908	2.366170	1.122117
H	-2.109641	1.046630	1.720536
C	-0.142517	1.084694	2.602429
H	-0.390333	1.777935	3.417816
H	-0.222943	0.067896	2.997849
H	0.905008	1.267149	2.339293

E = -487.806583829 a.u.
G = -487.578466 a.u.

TS(2-3)(alk-ap)

Os	0.257837	0.026986	0.149802
C	-0.246321	2.137822	0.853798
H	0.372712	2.695691	1.566758
H	-1.163887	1.845453	1.366614
C	0.469500	-0.936096	1.704994
C	-0.605628	-1.664028	2.447131
C	-0.514587	2.965029	-0.399651
H	-1.135864	2.421540	-1.120498
H	-1.056631	3.885064	-0.148137
H	0.410071	3.264579	-0.906554
O	-1.806913	-0.123516	0.161161
Si	-3.033219	-0.128627	-0.934324
H	-4.221481	0.617367	-0.396640
H	-2.664084	0.526079	-2.244897
H	-3.507073	-1.516552	-1.274034
H	-0.368732	-2.737716	2.464575
H	-1.587426	-1.513331	2.000682
H	-0.616678	-1.334995	3.495994
H	1.468464	-1.027593	2.174229
C	0.115255	-1.455567	-1.361501
H	-0.793223	-2.035148	-1.171321
H	-0.095667	-0.836224	-2.254213
C	1.294075	-2.386479	-1.630422
H	1.084712	-3.066426	-2.467186
H	2.206873	-1.835124	-1.879849
H	1.515888	-3.003412	-0.753355
C	2.158706	0.293463	0.068503
H	1.180540	1.349313	0.659282
H	2.816575	-0.057278	0.889321
C	2.970517	0.988816	-0.985972

H	3.601011	1.782448	-0.562107
H	3.663616	0.252593	-1.416234
H	2.365947	1.403907	-1.797441

E = -487.788335191 a.u.
G = -487.563085 a.u.

TS(2-3)(ene-ap)

Os	0.350478	-0.092579	0.077882
C	0.422138	1.911060	1.126981
H	1.292745	2.171675	1.735560
H	-0.499941	2.087148	1.686311
C	0.540908	-1.108602	1.641965
C	-0.576143	-1.676449	2.463680
C	0.422563	2.764451	-0.148168
O	-1.708261	0.246823	0.341371
Si	-3.003859	0.810599	-0.492423
H	1.547919	-1.382238	2.008582
C	-0.110693	-1.037410	-1.746638
H	-0.589998	-0.213598	-2.306757
H	0.782839	-1.332367	-2.308207
C	-1.078459	-2.220695	-1.657300
C	2.213189	-0.167528	-0.178348
H	0.505541	0.511022	1.694495
H	2.899602	-0.545822	0.610039
C	3.007896	0.268384	-1.372490
H	-0.403452	2.504541	-0.820147
H	1.365116	2.686563	-0.696198
H	0.282436	3.818391	0.126607
H	3.571080	-0.589609	-1.770193
H	3.765236	1.013458	-1.088874
H	2.394953	0.677727	-2.181242
H	-0.598821	-3.082140	-1.178993
H	-1.970544	-1.972241	-1.076518
H	-1.404042	-2.543190	-2.655006
H	-3.702815	1.912042	0.259720
H	-4.035653	-0.254076	-0.750689
H	-2.641673	1.390164	-1.841589
H	-0.402067	-1.501222	3.533765
H	-1.543946	-1.276039	2.160248
H	-0.579144	-2.766453	2.324922

E = -487.786649420 a.u.
G = -487.561669 a.u.

TS(3-1)

Os	0.094839	-0.184360	0.037501
C	-0.594136	1.311596	1.429497
H	-0.517840	2.322423	1.011142
H	0.008159	1.285234	2.343454
C	1.759018	-0.574258	0.280295
C	3.196978	-0.586043	0.572612
C	-0.672513	-1.711748	-0.751137
C	-2.167206	-1.819267	-0.832295
C	-2.054572	1.006989	1.784437
H	-0.142823	-2.627266	-1.017615
C	-0.529850	1.302967	-1.384671
H	-1.462593	1.778009	-1.042811
H	-0.750132	0.818900	-2.342819
C	0.528549	2.385954	-1.618508
H	-2.171466	0.002547	2.208660
H	-2.439263	1.717795	2.528459
H	-2.716466	1.081103	0.912332
H	3.600436	-1.604607	0.532962
H	3.715299	0.011614	-0.185688
H	-2.690538	-0.917105	-0.497375
H	-2.545790	-2.672558	-0.254522
H	0.175416	3.147959	-2.326699
H	0.799604	2.907230	-0.693014
H	1.448026	1.958062	-2.033891
H	0.719493	-0.951358	1.450319
H	-2.449074	-1.987126	-1.881715
H	3.414181	-0.156629	1.557370

E = -406.263022742 a.u.
G = -406.073087 a.u.

5_Q

Os	0.175327	0.178861	-0.127717
C	-1.045840	-1.190634	-1.307380
H	-1.027323	-2.199124	-0.888450
H	-0.667563	-1.255413	-2.330920
C	1.775929	-0.379389	-0.224424
C	3.132933	-0.926232	-0.286789
C	0.258628	1.963995	0.538852
C	-0.963516	2.833809	0.620550
C	-2.478595	-0.647364	-1.324415
H	1.178512	2.503123	0.777417
C	-0.707396	-0.824588	1.587168
H	-1.648692	-0.268444	1.741884
H	-0.064731	-0.539844	2.428306
C	-0.982958	-2.322677	1.651438
H	-2.526092	0.376130	-1.720919
H	-3.131810	-1.257385	-1.963243
H	-2.931651	-0.638649	-0.325524
H	3.880537	-0.130250	-0.192928
H	3.285231	-1.642529	0.528379
H	-1.890901	2.323510	0.336962
H	-0.860024	3.725993	-0.011193
H	-1.329077	-2.613063	2.652889
H	-1.757980	-2.641242	0.948293
H	-0.083542	-2.910000	1.435645
H	0.105288	0.791611	-1.657417
H	-1.083289	3.187985	1.654485
H	3.293150	-1.447358	-1.237170

E = -406.276857562
G = -406.086910

TS(3-2)

Os	0.101222	-0.197903	-0.027523
C	-0.448209	1.315659	-1.431568
H	-1.478570	1.654703	-1.302349
H	-0.346887	0.940321	-2.453909
C	-1.051436	-1.399458	-0.364144
C	-1.985512	-2.512035	-0.556748
C	1.829292	-0.939832	0.483955
C	3.156988	-0.243738	0.641498
C	0.524162	2.476902	-1.204809
H	1.933914	-2.028878	0.506562
C	-0.914833	0.908618	1.482651
H	-0.111266	1.605472	1.790395
H	-1.043433	0.227440	2.332990
C	-2.207540	1.685078	1.255039
H	1.574024	2.163441	-1.291705
H	0.377687	3.267582	-1.953266
H	0.395105	2.943093	-0.220787
H	-1.467113	-3.477757	-0.543453
H	-2.729503	-2.509318	0.248145
H	3.093007	0.842952	0.530773
H	3.922325	-0.617787	-0.052006
H	-2.549018	2.162735	2.183655
H	-2.097562	2.480462	0.511785
H	-3.011908	1.025282	0.911750
H	1.424964	-0.528880	-1.089426
H	3.518675	-0.447275	1.658402
H	-2.514801	-2.410087	-1.511051

E = -406.265815625 a.u.
G = -406.076766 a.u.

1_Q-yne·SIOH-SBP

Os	0.359553	-0.042299	0.008864
C	2.130202	-0.665792	-0.892113
H	2.362897	-1.709625	-0.646893
H	2.985755	-0.050718	-0.585344
C	-0.547181	-1.879853	-0.622462
C	-1.457151	-2.631320	0.354584
H	-1.136194	-1.600447	-1.518715
C	0.938056	-0.309380	1.573987
C	1.462589	-0.558919	2.919186
C	1.936765	-0.537532	-2.409625
H	1.770140	0.499700	-2.721781
H	2.830824	-0.889714	-2.941756
H	1.096238	-1.140375	-2.773598
H	-0.873116	-3.040640	1.186129
H	-2.224375	-1.989897	0.807777
H	-1.985570	-3.471961	-0.119006
H	0.888028	-1.336321	3.435601
H	1.453013	0.351462	3.529402
H	2.501603	-0.901257	2.837781
H	0.217649	-2.580311	-0.988574
C	0.862062	1.990742	-0.507035
H	0.422138	2.132221	-1.514317
H	1.945816	2.086281	-0.655736
C	0.406818	3.144242	0.397369
H	0.601159	4.132805	-0.042143
H	-0.670051	3.140635	0.642786
H	0.921452	3.104434	1.362912
O	-1.751153	0.866287	-0.208643
H	-1.593480	1.813332	-0.091765
Si	-3.404934	0.396080	-0.181233
H	-3.799367	-0.007287	1.196682
H	-4.184932	1.598459	-0.600941
H	-3.570323	-0.714561	-1.149112

E = -487.831530952 a.u.
G = -487.603813 a.u.

TS(3-3)

Os	0.294159	0.019030	0.014025
C	2.279609	-0.500532	0.560735
H	2.305133	-1.584496	0.751699
H	2.506900	-0.007861	1.512888
C	0.527499	-1.503406	-1.372872
C	-0.130804	-2.766439	-0.808773
H	-0.035707	-1.128907	-2.248395
C	-0.361942	0.040301	1.646671
C	-0.892313	-0.703600	2.802699
C	3.403014	-0.155828	-0.425348
H	3.497912	0.922798	-0.585490
H	4.368808	-0.506247	-0.039013
H	3.267122	-0.620122	-1.407809
H	0.434345	-3.163992	0.041562
H	-1.162714	-2.595597	-0.482675
H	-0.164265	-3.555971	-1.570653
H	-0.826796	-0.099843	3.715362
H	-0.349857	-1.642408	2.958061
H	-1.950725	-0.940407	2.633353
H	1.548832	-1.722858	-1.696576
C	0.950370	1.941315	-0.388257
H	1.310545	1.754029	-1.418793
H	1.831263	2.149616	0.228438
C	-0.017775	3.112488	-0.364129
H	0.487505	4.015434	-0.733387
H	-0.903998	2.929121	-0.972423
H	-0.353110	3.320548	0.657369
O	-1.892822	0.810829	-0.347613
H	-1.150437	0.834516	0.901158
Si	-3.239024	-0.125650	-0.599821
H	-3.420022	-1.168502	0.476213
H	-4.479795	0.717431	-0.607255
H	-3.174056	-0.865906	-1.905462

E = -487.778644099 a.u.
G = -487.554523 a.u.

TS(4-1)

Os	0.365192	-0.012892	-0.102059
C	0.140380	-1.584600	1.431892
H	-0.475877	-1.185082	2.256954
H	1.135317	-1.689973	1.884737

C	0.782975	1.157933	1.658686
C	1.862781	2.228366	1.509350
H	-0.166709	1.629137	1.960242
C	1.604555	-0.775289	-1.021803
C	2.686191	-1.476729	-1.720576
C	-0.376081	-2.962438	1.015697
H	0.291492	-3.430752	0.284060
H	-0.458705	-3.649604	1.870457
H	-1.364962	-2.913846	0.544856
H	2.810676	1.791289	1.176191
H	1.585687	2.988787	0.770776
H	2.057937	2.745733	2.459952
H	3.650850	-1.127038	-1.337953
H	2.650877	-1.281880	-2.798965
H	2.620966	-2.559194	-1.560331
H	1.062198	0.488767	2.481650
C	-0.040450	1.594364	-1.088371
H	0.542287	1.821080	-1.988151
H	0.162937	-1.271158	-1.314874
C	-1.057016	2.661901	-0.846163
H	-0.525911	3.616858	-0.715781
H	-1.702505	2.801460	-1.724652
H	-1.678439	2.487311	0.033052
O	-2.047588	0.213617	0.661801
H	-1.930303	-0.350183	1.438421
Si	-3.191230	-0.369859	-0.468299
H	-3.231897	0.637174	-1.558180
H	-2.832829	-1.716637	-0.992070
H	-4.519745	-0.444430	0.215620

E = -487.786326506 a.u.
G = -487.562053 a.u.

5_Q·SiOH

Os	-0.468343	-0.001938	-0.191599
C	0.016358	2.028683	0.577650
H	0.962231	1.931683	1.127489
H	-0.734782	2.263264	1.340781
C	0.066263	-0.518543	1.847126
C	-0.479309	-1.841564	2.385728
H	1.166637	-0.548128	1.867803
C	-2.160236	0.112257	-0.095891
C	-3.613335	0.230279	-0.002602
C	0.103605	3.191341	-0.409012
H	-0.838663	3.327847	-0.950080
H	0.344803	4.142857	0.087627
H	0.874474	3.036706	-1.178890
H	-1.574890	-1.849478	2.395597
H	-0.159903	-2.689134	1.770298
H	-0.143894	-2.029811	3.416615
H	-3.932534	0.180546	1.044675
H	-4.104854	-0.580259	-0.554323
H	-3.946481	1.186272	-0.421625
H	-0.218549	0.300482	2.517683
C	-0.241340	-1.677211	-1.133449
H	-1.148820	-2.223850	-1.415660
H	-0.305444	0.868311	-1.600002
C	0.954291	-2.379226	-1.695842
H	1.002481	-3.392572	-1.270210
H	0.842340	-2.516528	-2.780858
H	1.897530	-1.869769	-1.503688
O	2.041352	0.250202	-0.589597
H	1.925191	1.090214	-1.051328
Si	3.428941	0.162647	0.401082
H	3.565625	-1.271309	0.765070
H	4.601306	0.620727	-0.404389
H	3.306487	1.014446	1.618307

E = -487.805471181 a.u.
G = -487.582069 a.u.

TS(4-2)

Os	0.409690	0.052201	0.155481
C	0.653413	1.427548	-1.522538
H	-0.179006	1.274120	-2.236667
H	1.534293	1.107439	-2.090652
C	0.083216	-1.366946	-1.441583
C	0.111321	-2.839175	-1.028821
H	-0.897963	-1.131381	-1.882054
C	2.039607	-0.380985	0.381897
C	3.446025	-0.760675	0.478080
C	0.780783	2.911320	-1.180611
H	1.654527	3.090749	-0.545439
H	0.888823	3.537836	-2.078268
H	-0.089612	3.282488	-0.625367
H	1.097352	-3.129772	-0.648759
H	-0.607744	-3.048600	-0.229490
H	-0.123005	-3.506490	-1.871777
H	3.608658	-1.708289	-0.048932
H	3.747741	-0.894557	1.523859
H	4.088274	0.002718	0.023034
H	0.803150	-1.197245	-2.252759
C	-0.307569	-0.051466	1.976154
H	0.425920	-0.294662	2.750419
H	0.295375	1.394880	1.224191
C	-1.592530	0.384826	2.623304
H	-2.044904	-0.495083	3.102304
H	-1.423684	1.119004	3.423177
H	-2.318267	0.807673	1.927318
O	-1.888169	0.696531	-0.372451
H	-1.692237	1.214256	-1.165186
Si	-3.233194	-0.357634	-0.514525
H	-2.896059	-1.602517	0.216610
H	-4.419708	0.313052	0.094556
H	-3.503927	-0.614917	-1.958991

E = -487.795433229 a.u.
G = -487.571375 a.u.

1_Q-yne·SiOH-TBP

Os	-0.297441	0.083381	-0.089998
C	-0.074607	2.207068	0.254425
H	0.607569	2.408229	1.105303
H	-1.030794	2.626447	0.588160

C	-0.698313	0.103108	1.949140
C	-1.486698	-1.089539	2.468775
H	0.330370	0.076840	2.348105
C	-1.932600	0.030805	-0.556306
C	-3.354291	0.141195	-0.884211
C	0.398050	2.957076	-0.993091
H	-0.326261	2.850726	-1.808581
H	0.533572	4.034036	-0.813770
H	1.355195	2.576173	-1.375654
H	-2.525575	-1.061912	2.121778
H	-1.053363	-2.036655	2.131827
H	-1.508795	-1.101510	3.568732
H	-3.945101	0.215032	0.037129
H	-3.707969	-0.728099	-1.450350
H	-3.541026	1.044041	-1.478505
H	-1.146122	1.042220	2.300174
C	0.539945	-1.711037	-0.901860
H	1.376732	-2.047132	-0.267440
H	1.012339	-1.356245	-1.842006
C	-0.344985	-2.918897	-1.218866
H	0.224787	-3.750500	-1.659445
H	-0.833076	-3.299142	-0.315677
H	-1.138327	-2.654268	-1.925244
O	2.033749	0.386853	0.308214
H	2.091813	1.306273	0.597966
Si	3.530786	-0.428937	0.113293
H	3.727182	-0.784532	-1.316766
H	4.582936	0.533625	0.557156
H	3.539401	-1.638972	0.977096

E = -487.828255540 a.u.
G = -487.602119 a.u.

TS(4-3)

Os	-0.315652	0.057481	-0.026500
C	-1.352266	0.506058	1.709414
H	-1.545672	1.585254	1.764726
H	-0.553334	0.289298	2.441823
C	-0.417308	-2.042478	0.138599
C	0.171591	-2.782245	-1.066522
H	0.185166	-2.259514	1.034920
C	-1.650921	0.252934	-1.061085
C	-2.724911	0.444731	-2.036790
C	-2.608501	-0.274291	2.054630
H	-2.434008	-1.353147	2.057927
H	-2.979070	0.006987	3.050314
H	-3.409184	-0.068515	1.335921
H	-0.463935	-2.674496	-1.952913
H	1.168392	-2.410709	-1.338374
H	0.281621	-3.858026	-0.871906
H	-3.256376	-0.496324	-2.220885
H	-2.324601	0.809512	-2.989885
H	-3.447394	1.182005	-1.666557
H	-1.426483	-2.413422	0.342662
C	0.693306	2.175270	0.243206
H	0.853030	2.541871	1.268266
H	-0.305722	2.541150	-0.023536
C	1.703169	2.790095	-0.737448
H	1.661422	3.886768	-0.740349
H	2.740037	2.517375	-0.502355
H	1.509122	2.453037	-1.762136
O	1.833017	-0.153958	0.547726
H	1.480804	0.921743	0.451334
Si	3.371821	-0.720631	0.165156
H	3.636784	-0.606129	-1.302856
H	4.387391	0.088595	0.905572
H	3.476982	-2.151820	0.574233

E = -487.814131416 a.u.
G = -487.592050 a.u.

$HOSiH_3$

Si	0.539877	-0.007946	-0.000006
H	1.038080	1.394872	-0.002340
H	1.050139	-0.731223	-1.209463
H	1.050571	-0.727306	1.211598
O	-1.135966	0.112364	0.000042
H	-1.609348	-0.724004	-0.000057

E = -81.5201824920 a.u.
G = -81.506357 a.u.

Ethane

C	0.000000	0.000000	0.762605
H	0.000000	1.019274	1.162653
H	0.882717	-0.509637	1.162653
H	-0.882717	-0.509637	1.162653
C	0.000000	0.000000	-0.762605
H	0.000000	-1.019274	-1.162653
H	-0.882717	0.509637	-1.162653
H	0.882717	0.509637	-1.162653

E = -79.8084443288 a.u.
G = -79.754795 a.u.