Supporting Information

Mechanistic Insights into the Catalytic Carbonyl Hydrosilylation by Cationic [CpM(CO)$_2$(IMes)]+ (M = Mo, W) Complexes: The Intermediacy of η^1-H(Si) Metal Complexes

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Figure S1. The Optimized geometries of catalyst [CpM(CO)$_2$(IMes)]$^+$ (M = Mo,W) with IMes = imidazol-2-ylidene: **1Mo, 1W.** The Optimized geometries of catalyst [CpM(CO)$_2$(IMes)]$^+$ (M = Mo,W) with IMes = 1,3-bis(2,4,6-trimethylphenyl)-imidazol-2-ylidene: **S-1Mo, S-1W.**

Figure S2. The Optimized geometries of **TS2W**, **2W**, **TS3W, 3W, TS7W-II**，**4W**，**TS5W**，**5W**. Bond distances are shown in Å.

Figure S3. The Optimized geometries of **S-TS2W**, **S-2W**, **S-TS3W, S-3W, S-6W, S-TS7W**. [CpM(CO)$_2$(IMes)]$^+$ (M = W) with IMes = 1,3-bis(2,4,6-trimethylphenyl)-imidazol-2-ylidene in the reaction pathway mediated the hydrosilylation. Bond distances are shown in Å. (The gas-phase Gibbs energy are given in the bracket).

Figure S4. The Optimized geometries of **R-1Mo**, **R-3Mo**, **R-4Mo, R-TS5Mo, R-5Mo, R-6Mo**, **R-TS7Mo, R-TS7Mo-II**. [CpM(CO)(IMes)]$^+$ (M = Mo) with IMes = imidazol-2-ylidene in the reaction pathway mediated the hydrosilylation. Bond distances are shown in Å.

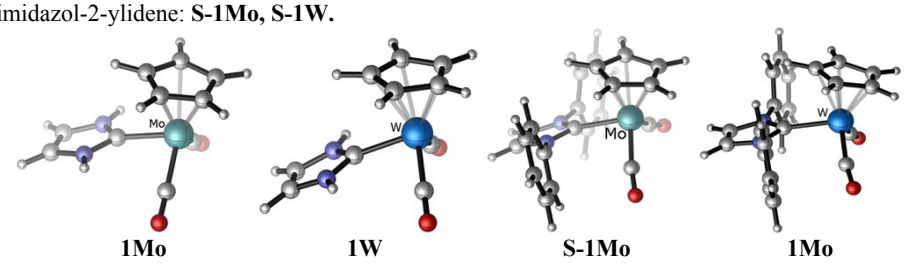
Figure S5. The Optimized geometries of **R-1W**, **R-3W**, **R-4W, R-TS5W, R-5W, R-6W**, **R-TS7Mo, R-TS7Mo-II**. [CpM(CO)(IMes)]$^+$ (M = Mo) with IMes = imidazol-2-ylidene in the reaction pathway mediated the hydrosilylation. Bond distances are shown in Å.

2. **Table S1** Cartesian coordinates for all optimized structures in XYZ format.

Complete refrence of 37

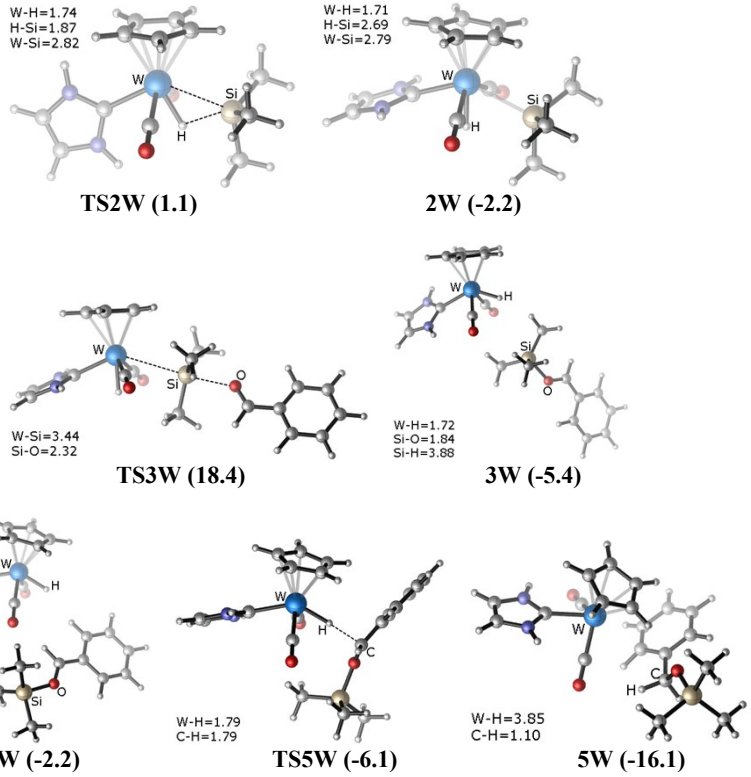
Frisch, M. J. et al. *Gaussian 09*; Gaussian, Inc. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, 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 geometries of catalyst $[CpM(CO)_2(IMes)]^+$ (M = Mo,W) with IMes = imidazol-2-ylidene: **1Mo, 1W.** The Optimized geometries of catalyst $[CpM(CO)_2(IMes)]^+$ (M = Mo,W) with IMes = 1,3-diphenyl-imidazol-2-ylidene: **S-1Mo, S-1W.**



1Mo **1W** **S-1Mo** **1Mo**

Figure S2. The Optimized geometries of **TS2W**, **2W**, **TS3W, 3W, TS7W-II，4W，TS5W，5W**. Bond distances are shown in Å.

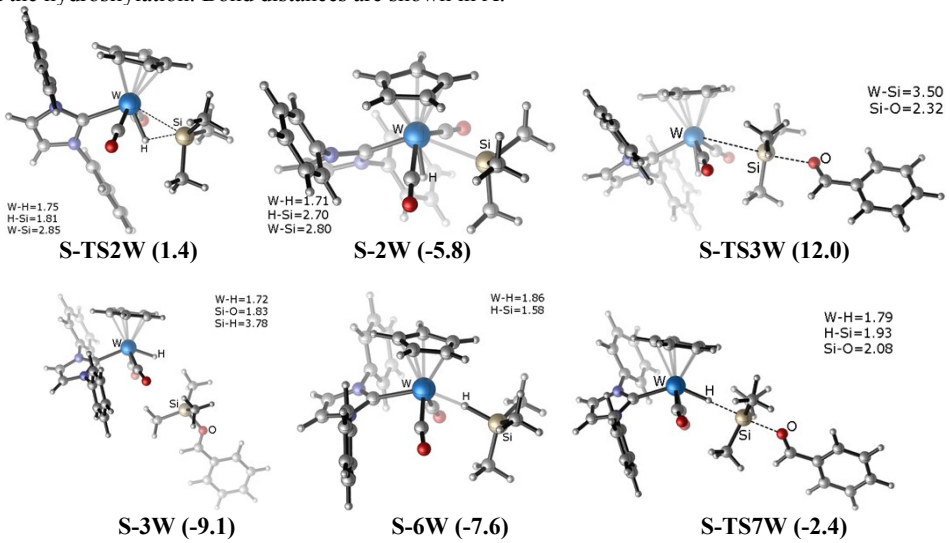


TS2W (1.1) **2W (-2.2)**

TS3W (18.4) **3W (-5.4)**

4W (-2.2) **TS5W (-6.1)** **5W (-16.1)**

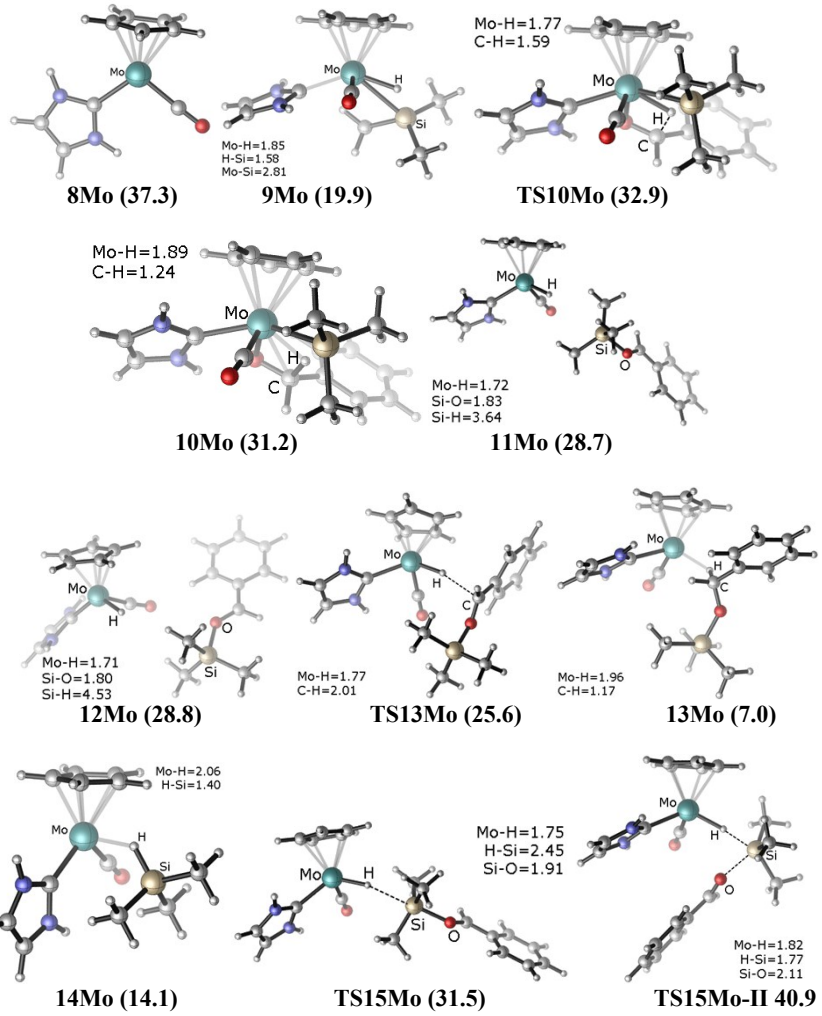
Figure S3. The Optimized geometries of **S-TS2W**, **S-2W**, **S-TS3W, S-3W, S-6W, S-TS7W**. $[CpM(CO)_2(IMes)]^+$ (M = W) with IMes = 1,3-diphenyl-imidazol-2-ylidene in the reaction pathway mediated the hydrosilylation. Bond distances are shown in Å.



S-TS2W (1.4) **S-2W (-5.8)** **S-TS3W (12.0)**

S-3W (-9.1) **S-6W (-7.6)** **S-TS7W (-2.4)**

Figure S4. The Optimized geometries of **8Mo**, **9Mo, TS10Mo, 10Mo**, **11Mo, 12Mo, TS13Mo, 13Mo**, **14Mo, TS15Mo, TS15Mo-II**. $[CpM(CO)(IMes)]^+$ (M = Mo) with IMes = imidazol-2-ylidene in the reaction pathway mediated the hydrosilylation. Bond distances are shown in Å.



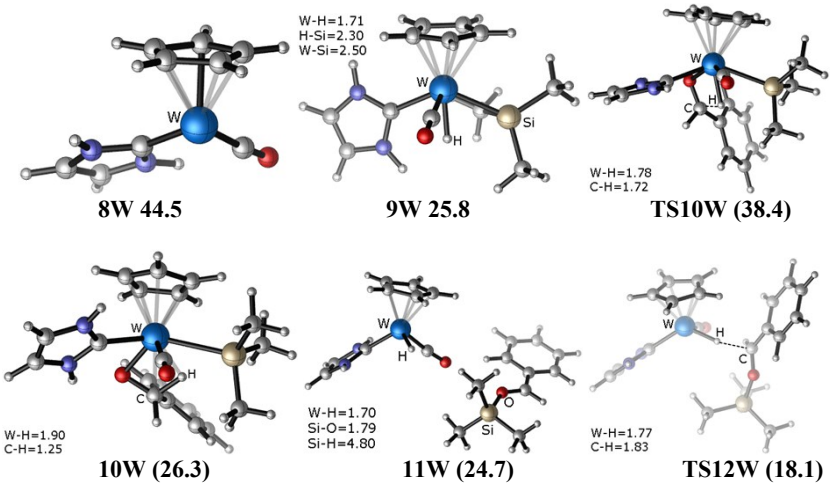
8Mo (37.3) **9Mo (19.9)** **TS10Mo (32.9)**

10Mo (31.2) **11Mo (28.7)**

12Mo (28.8) **TS13Mo (25.6)** **13Mo (7.0)**

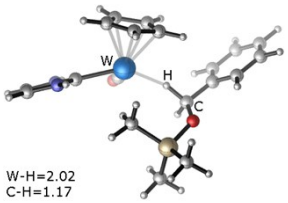
14Mo (14.1) **TS15Mo (31.5)** **TS15Mo-II 40.9**

Figure S5. The Optimized geometries of **8W**, **9W**, **TS10W, 10W, 11W, TS12W, 12W**, **13W, TS-14W TS14W-II**. $[CpM(CO)(IMes)]^+$ (M = Mo) with IMes = imidazol-2-ylidene in the reaction pathway mediated the hydrosilylation. Bond distances are shown in Å.

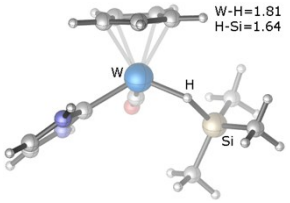


8W 44.5 **9W 25.8** **TS10W (38.4)**

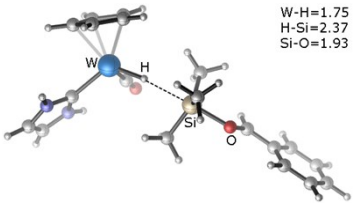
10W (26.3) **11W (24.7)** **TS12W (18.1)**



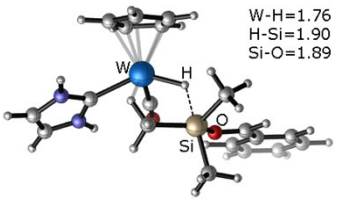
12W (8.5)



13W (26.0)



TS14W (26. 5)



TS14W-II (42.6)

Table S1 Cartesian coordinates for all optimized structures in XYZ format.

1Mo $[CpMo(CO)_2(IMes)]^+$

1Mo

Mo	-3.032043	-0.861282	0.241623
C	-3.231486	-2.349645	-1.509713
C	-4.184765	-1.284543	-1.714303
C	-3.465201	-0.098605	-1.994061
C	-2.080523	-0.418951	-1.933604
C	-1.932386	-1.809221	-1.663159
C	-1.446912	0.579649	0.634916
N	-0.142950	0.337543	0.918973
C	0.567224	1.498363	1.162644
C	-0.317214	2.517402	1.018760
N	-1.526641	1.932170	0.693090
C	-2.105088	-1.920790	1.698467
C	-4.183000	0.470809	1.243463
H	-3.467641	-3.388925	-1.330406
H	-5.261023	-1.384858	-1.710460
H	-3.888891	0.864536	-2.233358
H	-1.271501	0.272716	-2.113183
H	-1.003444	-2.356160	-1.616372
H	0.248550	-0.591585	0.959836
H	1.613500	1.501582	1.414721
H	-0.191670	3.581284	1.121800
H	-2.381972	2.441818	0.529159
O	-1.540672	-2.570551	2.451588
O	-4.863579	1.255132	1.723291

TS2Mo

N	-0.743591	1.646707	-0.097317
C	-1.452412	0.829002	0.720463
N	-1.094177	1.252538	1.957238
C	-0.187908	2.304187	1.917489
C	0.035676	2.555503	0.608526
Mo	-2.847928	-0.783893	0.164961
C	-4.156366	0.591230	0.906824
O	-4.879562	1.346037	1.360705
C	-3.877121	-2.183809	-1.526637
C	-4.288014	-0.841772	-1.719794
C	-3.131687	-0.057470	-2.049051
C	-2.007183	-0.924618	-2.036807
C	-2.471619	-2.235084	-1.701789
C	-1.373283	-1.879065	1.052966
O	-0.566564	-2.478711	1.589656
H	-4.519847	-3.023462	-1.320156
H	-5.305759	-0.482477	-1.690522
H	-3.143021	0.985922	-2.325867
H	-0.989366	-0.673632	-2.294641
H	-1.860570	-3.123833	-1.645781
H	-1.457557	0.840311	2.802489
H	0.206978	2.767401	2.804545
H	0.664596	3.281750	0.124198
H	-0.785397	1.597471	-1.101802
Si	-4.417873	-2.417853	1.739513
C	-4.370670	-2.045151	3.595828
C	-6.210471	-2.208389	1.178153
C	-3.844879	-4.202493	1.505669
H	-6.838505	-2.868581	1.786825
H	-6.573637	-1.189110	1.331012
H	-6.377459	-2.475265	0.132749
H	-4.492481	-4.854623	2.102283
H	-3.900305	-4.546464	0.470675
H	-2.821828	-4.355689	1.857747
H	-5.041222	-2.737950	4.115095
H	-3.372935	-2.177898	4.023769
H	-4.709714	-1.031305	3.826600
H	-3.049145	-0.919014	1.862994

2Mo

N	-0.743591	1.646707	-0.097317
C	-1.452412	0.829002	0.720463
N	-1.094177	1.252538	1.957238
C	-0.187908	2.304187	1.917489
C	0.035676	2.555503	0.608526
Mo	-2.847928	-0.783893	0.164961
C	-4.156366	0.591230	0.906824
O	-4.879562	1.346037	1.360705
C	-3.877121	-2.183809	-1.526637
C	-4.288014	-0.841772	-1.719794
C	-3.131687	-0.057470	-2.049051
C	-2.007183	-0.924618	-2.036807
C	-2.471619	-2.235084	-1.701789
C	-1.373283	-1.879065	1.052966
O	-0.566564	-2.478711	1.589656
H	-4.519847	-3.023462	-1.320156
H	-5.305759	-0.482477	-1.690522
H	-3.143021	0.985922	-2.325867
H	-0.989366	-0.673632	-2.294641
H	-1.860570	-3.123833	-1.645781
H	-1.457557	0.840311	2.802489
H	0.206978	2.767401	2.804545
H	0.664596	3.281750	0.124198
H	-0.785397	1.597471	-1.101802
Si	-4.417873	-2.417853	1.739513
C	-4.370670	-2.045151	3.595828
C	-6.210471	-2.208389	1.178153
C	-3.844879	-4.202493	1.505669
H	-6.838505	-2.868581	1.786825
H	-6.573637	-1.189110	1.331012
H	-6.377459	-2.475265	0.132749
H	-4.492481	-4.854623	2.102283
H	-3.900305	-4.546464	0.470675
H	-2.821828	-4.355689	1.857747
H	-5.041222	-2.737950	4.115095
H	-3.372935	-2.177898	4.023769
H	-4.709714	-1.031305	3.826600
H	-3.049145	-0.919014	1.862994

TS3Mo

C	-6.344152	0.771890	0.320989
C	-5.815189	-0.488542	-0.008792
C	-6.676521	-1.560051	-0.293734
C	-8.052421	-1.375890	-0.249370
C	-8.569430	-0.122907	0.078956
C	-7.717081	0.949528	0.363526
C	-4.379363	-0.712391	-0.058718
O	-3.528591	0.144534	0.175624
C	-1.162906	-1.592360	0.766029
Si	-1.151910	0.151545	0.072451
C	-1.284894	1.623007	1.222140
Mo	2.231677	0.307535	-0.049707
C	1.343662	-0.902873	-1.344898
O	0.898089	-1.616007	-2.140287
C	2.798230	1.873691	-1.813951
C	1.685204	2.397959	-1.083498
C	2.122008	2.661229	0.241843
C	3.500095	2.296587	0.340707
C	3.905775	1.816116	-0.937956
C	3.972063	-0.988121	0.166362
N	4.842386	-1.059901	1.203887

C	5.863332	-1.972362	0.978969
C	5.631927	-2.498161	-0.246712
N	4.480329	-1.883513	-0.716910
C	1.584407	0.114253	1.802975
O	1.238700	0.027129	2.903062
C	-1.489408	0.465879	-1.749719
H	0.712235	2.622381	-1.489877
H	1.530798	3.103550	1.028428
H	4.134594	2.440437	1.201058
H	4.896610	1.477752	-1.199525
H	2.799677	1.602430	-2.858834
H	4.040844	-2.077863	-1.603191
H	6.171478	-3.238586	-0.810764
H	6.644363	-2.164061	1.693637
H	4.721085	-0.521521	2.047161
H	-2.341308	1.839047	1.392554
H	-0.811357	1.431774	2.184721
H	-0.829085	2.509300	0.777650
H	-2.307150	1.185183	-1.831703
H	-0.627239	0.860586	-2.283532
H	-1.792294	-0.456642	-2.249461
H	-2.171525	-1.903197	1.043630
H	-0.774342	-2.304694	0.036103
H	-0.548328	-1.650571	1.664923
H	1.821560	-1.233823	0.514527
H	-4.064320	-1.736609	-0.326147
H	-6.263414	-2.530884	-0.547181
H	-8.720401	-2.199843	-0.467912
H	-9.643014	0.022013	0.114300
H	-8.132814	1.917070	0.617373
H	-5.666989	1.588449	0.538553

3Mo

Mo	-3.017568	-0.684387	0.145183
C	-3.127326	-2.465831	-1.394126
C	-4.179319	-1.571301	-1.747784
C	-5.124286	-1.577083	-0.678809
C	-4.675606	-2.477465	0.316248
C	-3.435608	-3.018860	-0.115200
H	-1.543607	-1.277406	0.775894
C	-2.726913	-0.311006	2.066880
C	-1.554177	0.332949	-0.636821
O	-0.639483	0.872338	-1.130207
O	-2.569387	-0.124010	3.198258
Si	2.525773	0.497506	-0.632404
O	4.362911	0.423283	-0.456225
C	5.096823	-0.286808	0.282333
C	6.517718	-0.195428	0.291048
C	7.233854	-1.042162	1.165854
C	8.616758	-0.980250	1.205497
C	9.289102	-0.078700	0.376932
C	7.208193	0.713130	-0.543579
C	8.587653	0.765390	-0.495167
C	-4.015210	1.273421	0.223657
N	-4.226310	2.131533	1.256779
C	-4.928641	3.265659	0.876774
C	-5.179638	3.127637	-0.445328
N	-4.614823	1.914670	-0.816491
H	-4.603296	1.541340	-1.751481
H	-5.698201	3.768300	-1.136657
H	-5.184881	4.051593	1.565274
H	-3.913908	1.933494	2.194515
C	1.909145	-0.798778	0.555855
C	2.342194	0.093723	-2.436043
C	2.218040	2.264515	-0.149582
H	-2.848957	-3.752690	0.415050
H	-2.283378	-2.729551	-2.012128
H	-4.281914	-1.058269	-2.692156
H	-6.043772	-1.011950	-0.641661
H	-5.182860	-2.707310	1.240749
H	2.789299	2.952810	-0.777321
H	1.155925	2.481113	-0.285834
H	2.474533	2.453323	0.895879
H	2.680812	-0.920055	-2.664206
H	1.284610	0.168820	-2.700567
H	2.899614	0.794891	-3.061896
H	2.270190	-1.801106	0.307038
H	2.167823	-0.576604	1.595169
H	0.817005	-0.834114	0.502548
H	4.621031	-1.010274	0.952554
H	6.698414	-1.737132	1.803557
H	9.173689	-1.625149	1.873236
H	10.371515	-0.030695	0.408376
H	9.129097	1.456625	-1.128785
H	6.647324	1.356353	-1.209640

4Mo

Mo	-3.017568	-0.684387	0.145183
C	-3.127326	-2.465831	-1.394126
C	-4.178770	-1.566321	-1.743235
C	-3.594524	-0.359675	-2.211757
C	-2.188769	-0.500767	-2.133743
C	-1.888327	-1.805347	-1.640277
C	-1.395163	0.684384	0.718532
C	-2.465790	-1.660962	1.735736
H	-4.415731	-1.250394	0.949425
C	-4.134862	0.729941	0.962583
H	-5.235292	-1.779753	-1.698078
H	-4.127441	0.511841	-2.560033
H	-1.468183	0.248398	-2.426518
H	-0.907787	-2.248961	-1.554754
H	-3.248757	-3.486636	-1.067118
H	0.292357	-0.356272	0.095551
N	-0.064583	0.490209	0.507591
C	0.710871	1.548589	0.962093
C	-0.155426	2.447249	1.483575
N	-1.420696	1.902387	1.321921
O	-2.180031	-2.312644	2.665622
O	-4.808148	1.557120	1.412316
H	1.782941	1.568935	0.875240
H	0.013157	3.405773	1.942045
H	-2.281209	2.350617	1.595362
Si	-4.052863	-3.811084	4.823011
C	-3.075487	-5.207955	4.085894
C	-3.099317	-2.592219	5.850268
H	-3.721139	-5.959110	3.623979
H	-2.418777	-4.799826	3.313716
H	-2.432266	-2.030932	5.191810
H	-2.488992	-3.098458	6.602178
H	-3.757123	-1.881878	6.357350
O	-5.384582	-3.109098	3.752794
C	-4.976533	-4.709634	6.150392
H	-2.452361	-5.700220	4.836517
H	-6.042846	-4.685611	5.930572
H	-4.637699	-5.743740	6.192072
H	-4.792772	-4.228481	7.109894
C	-5.780412	-3.465904	2.458186
C	-6.879416	-2.618489	2.037973
H	-5.538052	-4.167740	1.661563
C	-7.448666	-2.787659	0.770166
C	-8.509773	-1.969465	0.364443
C	-9.001629	-0.982101	1.226528
C	-8.432379	-0.812931	2.494335

C	-7.371272	-1.631125	2.900058
H	-7.066072	-3.555688	0.099588
H	-8.952569	-2.101056	-0.621730
H	-9.827019	-0.345663	0.910933
H	-8.814973	-0.044903	3.164913
H	-6.928476	-1.499534	3.886231

TS5Mo

Mo	1.200089	-0.676599	0.140712
C	0.746561	-2.622330	1.353859
C	0.381046	-2.875733	-0.008614
C	1.567648	-2.893036	-0.787649
C	2.656148	-2.626492	0.079647
C	2.161038	-2.474722	1.404962
C	3.075083	0.391548	-0.329014
C	1.090521	0.718693	1.535580
H	-0.507548	-0.218133	0.279906
C	0.562547	0.229686	-1.500336
H	-0.615406	-3.073468	-0.371595
H	1.631666	-3.079212	-1.848697
H	3.693186	-2.573709	-0.216236
H	2.752577	-2.332470	2.296429
H	0.082132	-2.622792	2.203748
H	4.112945	0.290344	1.468907
N	4.125085	0.594741	0.508183
C	5.166887	1.280256	-0.097370
C	4.764468	1.522758	-1.367371
N	3.498333	0.971018	-1.481359
O	0.997610	1.483620	2.399698
O	0.161244	0.692529	-2.481850
H	6.080137	1.529211	0.414022
H	5.257918	2.026228	-2.180156
H	2.936990	0.988917	-2.318595
Si	-2.175782	3.085630	0.187284
C	-2.122408	3.226921	2.047835
C	-0.607662	3.618818	-0.662133
H	-3.019769	2.820562	2.523130
H	-1.240868	2.750725	2.483246
H	0.272000	3.149437	-0.217461
H	-0.495835	4.703744	-0.568258
H	-0.629686	3.373272	-1.726171
O	-2.366918	1.354184	-0.199767
C	-3.716634	3.806365	-0.571819
H	-2.075245	4.287989	2.314491
H	-4.622328	3.404286	-0.110829
H	-3.729305	4.892110	-0.434754
H	-3.761868	3.608109	-1.645613
C	-2.275387	0.289953	0.508843
C	-2.914233	-0.932175	0.070203
H	-2.001411	0.382362	1.559402
C	-3.099732	-1.968506	1.002686
C	-3.780859	-3.119136	0.632400
C	-4.266263	-3.247199	-0.670659
C	-4.077734	-2.223201	-1.604051
C	-3.408602	-1.065478	-1.239321
H	-2.720774	-1.859692	2.013168
H	-3.938092	-3.913327	1.351729
H	-4.796716	-4.146874	-0.960018
H	-4.460628	-2.332637	-2.611307
H	-3.260863	-0.261544	-1.948832

5Mo

Mo	2.107881	0.395460	-0.124212
C	4.054143	1.561528	-1.005079
C	3.321059	2.483979	-0.223672
C	3.297193	2.034694	1.132223
C	4.005927	0.809529	1.182357
C	4.461427	0.509684	-0.147619
C	2.632241	-1.729419	0.158481
C	1.537814	-0.359489	-1.877575
C	0.734192	-0.191781	1.221947
N	2.850748	-2.707880	-0.755464
C	3.171050	-3.920514	-0.168919
C	3.163283	-3.705555	1.168118
N	2.837008	-2.370119	1.337595
Si	-5.758094	-0.630205	0.042886
C	-6.679357	0.078787	-1.433541
C	-5.480616	-2.477106	-0.178579
C	-6.632304	-0.252928	1.651800
O	-4.256597	0.144807	0.194013
C	-3.232035	0.149832	-0.765625
C	-2.109201	1.079219	-0.346103
C	-2.166271	1.784607	0.859625
C	-1.144810	2.659817	1.231268
C	-0.046646	2.844133	0.401060
C	0.039047	2.133081	-0.813669
C	-1.007419	1.261983	-1.177732
H	2.872871	3.394974	-0.593237
H	2.866872	2.558467	1.971357
H	4.243275	0.249317	2.073312
H	5.077866	-0.329385	-0.430532
H	4.266610	1.646393	-2.059797
H	2.768914	-2.562215	-1.750431
H	3.371608	-4.809396	-0.741182
H	3.356182	-4.369100	1.992846
H	2.729419	-1.917053	2.231818
H	-6.167443	-0.114903	-2.380955
H	-6.812644	1.160026	-1.337062
H	-7.675010	-0.369344	-1.510443
H	-4.929149	-2.706987	-1.095441
H	-6.438483	-3.002975	-0.240373
H	-4.927065	-2.900118	0.664694
H	-7.625401	-0.711685	1.672248
H	-6.761987	0.823849	1.789607
H	-6.071375	-0.638030	2.507622
H	-3.604370	0.478428	-1.747223
H	-0.971007	0.761944	-2.139690
H	0.767747	2.423076	-1.563183
H	0.712291	3.571026	0.661109
H	-1.220526	3.210776	2.161092
H	-3.032916	1.644096	1.492211
O	1.341011	-0.807215	-2.920718
O	0.012754	-0.512054	2.052212
H	-2.817875	-0.860424	-0.903451

6Mo

Mo	-3.163916	-0.952179	0.034686
C	-3.000340	-2.421354	-1.771641
C	-3.989009	-1.429870	-2.106846
C	-3.334002	-0.182526	-2.247011
C	-1.956871	-0.390145	-1.970620
C	-1.742350	-1.773052	-1.701013
C	-1.692753	0.526919	0.783861
C	-2.384161	-1.979388	1.568311
C	-4.420041	0.379474	0.846219
N	-1.819550	1.869748	0.922740
C	-0.666262	2.464222	1.406302
C	0.229675	1.462137	1.575438
N	-0.418209	0.301050	1.188528
O	-1.890744	-2.613123	2.389525
O	-5.151802	1.180121	1.227618
H	-3.172366	-3.481182	-1.663765
H	-5.037350	-1.612546	-2.287019
H	-3.794800	0.752682	-2.525635

H	-1.189467	0.367839	-2.010756
H	-0.790277	-2.246618	-1.517325
H	-2.670542	2.366921	0.708223
H	-0.585346	3.522321	1.584368
H	1.245718	1.474267	1.929419
H	-0.007942	-0.619735	1.216515
H	-4.584441	-2.036625	0.556636
Si	-5.782660	-2.819543	1.214056
C	-5.675165	-2.470690	3.045278
C	-7.305766	-2.107489	0.396831
C	-5.438023	-4.600960	0.761530
H	-8.195622	-2.598936	0.804535
H	-7.406323	-1.036402	0.586361
H	-7.308859	-2.271019	-0.683332
H	-6.220189	-5.238308	1.187640
H	-5.440900	-4.759579	-0.319456
H	-4.480960	-4.943368	1.161973
H	-6.487863	-2.995770	3.558367
H	-4.734018	-2.821221	3.474307
H	-5.780400	-1.405749	3.263951

TS7Mo

Si	-1.525858	0.027048	-0.030532
C	-1.579156	1.189316	1.446589
C	-1.548298	0.707619	-1.779783
C	-1.237232	-1.797577	0.267794
O	-3.526797	-0.224917	-0.088748
C	-4.486052	0.320397	0.485520
C	-5.862279	-0.025873	0.244118
C	-6.862148	0.664339	0.955025
C	-8.198121	0.355767	0.744856
C	-8.538793	-0.639590	-0.172088
C	-7.550364	-1.331125	-0.883048
C	-6.215501	-1.029878	-0.679997
H	-0.578221	1.390935	1.822367
H	-2.036176	2.148387	1.184766
H	-2.150130	0.746385	2.268120
H	-1.532535	1.800672	-1.768306
H	-0.684799	0.361875	-2.346873
H	-2.452577	0.387887	-2.302130
H	-0.676064	-2.239108	-0.557313
H	-2.186345	-2.329608	0.358448
H	-0.665741	-1.952483	1.184455
H	-4.291461	1.111855	1.220956
H	-6.584669	1.435833	1.665387
H	-8.972107	0.883047	1.288263
H	-9.582593	-0.881116	-0.336293
H	-7.832925	-2.100856	-1.590543
H	-5.435715	-1.552899	-1.219131
C	1.751062	-0.408034	1.634946
C	1.762037	-0.952759	-1.443468
C	3.973262	-0.938738	0.179711
H	0.474617	0.255721	-0.076698
C	1.831578	2.502065	-1.121888
C	1.966680	2.711576	
0.290007			
C	3.314532	2.429599	
0.644112			
C	3.996751	2.036723	-0.541941
C	3.093380	2.100635	-1.631571
N	4.848847	-0.938017	1.218256
C	5.836497	-1.901843	1.085695
C	5.580090	-2.539051	-0.081109
N	4.451521	-1.933846	-0.609693
O	1.447156	-0.820667	2.669202
H	1.205733	3.094200	0.951996
H	0.944791	2.681138	-1.708980
H	3.751635	2.547635	1.623849
H	5.039081	1.763494	-0.609238
H	3.326371	1.887280	-2.663471
H	4.753962	-0.312807	2.002853
H	6.615110	-2.046703	1.813855
H	6.090691	-3.350440	-0.569444
H	4.012565	-2.196804	-1.478588
O	1.488301	-1.703025	-2.281109
Mo	2.244526	0.415674	-0.101106

TS7Mo-II

Mo	-1.585152	-0.093572	-0.001064
C	-3.406607	1.277933	0.631783
C	-3.477758	1.050697	-0.782280
C	-3.740620	-0.329828	-0.983567
C	-3.826799	-0.945103	0.301045
C	-3.643274	0.047713	1.293883
C	-1.193619	-2.269518	-0.092847
C	-0.354900	-0.263000	1.554191
H	-0.609391	1.463301	-0.010760
C	-0.400100	-0.146112	-1.589407
H	-3.412610	1.800824	-1.553526
H	-3.913915	-0.811309	-1.933586
H	-4.035665	-1.987559	0.488314
H	-3.678354	-0.104935	2.361790
H	-3.258966	2.229865	1.117648
H	-0.631526	-2.839498	1.829740
N	-0.821267	-3.134475	0.884233
C	-0.725453	-4.440349	0.431660
C	-1.053309	-4.407229	-0.882008
N	-1.331839	-3.081218	-1.172029
O	0.274108	-0.394640	2.513017
O	0.267864	-0.139460	-2.532253
H	-0.442175	-5.260148	1.068344
H	-1.112078	-5.191879	-1.615808
H	-1.596715	-2.731989	-2.079729
Si	0.274622	3.063378	0.055058
C	-1.169206	3.747820	-0.961870
C	0.130554	3.337653	1.897531
H	-1.172017	3.338862	-1.975605
H	-2.137958	3.545301	-0.507856
H	-0.818153	2.977054	2.297245
H	0.197339	4.413507	2.091910
H	0.941233	2.848507	2.439745
O	1.687380	1.447497	0.215361
C	1.726661	4.029099	-0.682126
H	-1.042571	4.832359	-1.047074
H	1.924011	3.774732	-1.728331
H	1.445905	5.087340	-0.675917
H	2.654883	3.924643	-0.118143
C	2.568807	1.064944	-0.565854
C	3.575203	0.081070	-0.227884
H	2.618806	1.486233	-1.578756
C	4.527289	-0.263723	-1.202780
C	5.524821	-1.181986	-0.904284
C	5.574804	-1.755579	0.366332
C	4.629267	-1.418224	1.341389
C	3.629756	-0.504340	1.051448
H	4.480639	0.191990	-2.186125
H	6.262399	-1.447976	-1.651250
H	6.357001	-2.467885	0.602431
H	4.684762	-1.868203	2.325255
H	2.890620	-0.229384	1.793350

S-1Mo

Mo	-1.585152	-0.093572	-0.001064
C	-3.406607	1.277933	0.631783

C	-3.477758	1.050697	-0.782280
C	-3.740620	-0.329828	-0.983567
C	-3.826799	-0.945103	0.301045
C	-3.643274	0.047713	1.293883
C	-1.193619	-2.269518	-0.092847
C	-0.354900	-0.263000	1.554191
H	-0.609391	1.463301	-0.010760
C	-0.400100	-0.146112	-1.589407
H	-3.412610	1.800824	-1.553526
H	-3.913915	-0.811309	-1.933586
H	-4.035665	-1.987559	0.488314
H	-3.678354	-0.104935	2.361790
H	-3.258966	2.229865	1.117648
H	-0.631526	-2.839498	1.829740
N	-0.821267	-3.134475	0.884233
C	-0.725453	-4.440349	0.431660
C	-1.053309	-4.407229	-0.882008
N	-1.331839	-3.081218	-1.172029
O	0.274108	-0.394640	2.513017
O	0.267864	-0.139460	-2.532253
H	-0.442175	-5.260148	1.068344
H	-1.112078	-5.191879	-1.615808
H	-1.596715	-2.731989	-2.079729
Si	0.274622	3.063378	0.055058
C	-1.169206	3.747820	-0.961870
C	0.130554	3.337653	1.897531
H	-1.172017	3.338862	-1.975605
H	-2.137958	3.545301	-0.507856
H	-0.818153	2.977054	2.297245
H	0.197339	4.413507	2.091910
H	0.941233	2.848507	2.439745
O	1.687380	1.447497	0.215361
C	1.726661	4.029099	-0.682126
H	-1.042571	4.832359	-1.047074
H	1.924011	3.774732	-1.728331
H	1.445905	5.087340	-0.675917
H	2.654883	3.924643	-0.118143
C	2.568807	1.064944	-0.565854
C	3.575203	0.081070	-0.227884
H	2.618806	1.486233	-1.578756
C	4.527289	-0.263723	-1.202780
C	5.524821	-1.181986	-0.904284
C	5.574804	-1.755579	0.366332
C	4.629267	-1.418224	1.341389
C	3.629756	-0.504340	1.051448
H	4.480639	0.191990	-2.186125
H	6.262399	-1.447976	-1.651250
H	6.357001	-2.467885	0.602431
H	4.684762	-1.868203	2.325255
H	2.890620	-0.229384	1.793350

S-TS2Mo

C	2.178963	-1.715554	-0.735388
C	1.278740	-2.806955	-0.487051
C	0.344820	-2.859522	-1.552669
C	0.653512	-1.794867	-2.446121
C	1.784869	-1.096371	-1.946048
Mo	0.021389	-0.837567	-0.322770
Si	-2.061937	-2.369101	0.649078
C	-1.337218	-4.024485	1.219065
C	0.515080	1.364714	0.007375
N	-0.323615	2.447536	0.087456
C	0.382986	3.634477	0.253144
C	1.687656	3.308698	0.293615
N	1.760645	1.925993	0.153880
C	-1.450993	-0.129621	-1.546586
O	-2.294529	0.165704	-2.253391
C	0.373174	-0.779794	1.678739
O	0.520975	-0.736617	2.810868
C	-2.984366	-1.674969	2.150228
C	-3.335682	-2.664141	-0.712855
H	1.350551	-3.510577	0.326456
H	-0.418092	-3.605147	-1.704019
H	0.143915	-1.584192	-3.374924
H	2.266532	-0.259373	-2.423032
H	3.039987	-1.459805	-0.140727
C	3.047497	1.279987	0.248584
H	2.569551	3.910820	0.423601
H	-0.117411	4.582386	0.342477
C	-1.766788	2.487853	0.068145
H	-4.077666	-3.378800	-0.340336
H	-3.871749	-1.750823	-0.980087
H	-2.909101	-3.082170	-1.627414
H	-2.160113	-4.615527	1.636618
H	-0.888909	-4.617985	0.420353
H	-0.597184	-3.898697	2.013286
H	-3.714593	-2.418616	2.486162
H	-2.320634	-1.467139	2.993545
H	-3.531360	-0.760134	1.911525
H	-1.402626	-0.523220	0.586997
C	3.456657	0.736318	1.464744
C	4.731835	0.185164	1.572733
C	5.595792	0.196411	0.478197
C	5.189551	0.771230	-0.724888
C	3.914631	1.321641	-0.841206
H	2.790092	0.754623	2.317532
H	5.054285	-0.237801	2.516611
H	6.589199	-0.226390	0.567836
H	5.866313	0.800121	-1.570336
H	3.596778	1.790018	-1.765540
C	-2.488289	2.078539	1.187189
C	-3.874350	2.216542	1.192074
C	-4.528167	2.771395	0.093050
C	-3.795516	3.195462	-1.013515
C	-2.409945	3.058969	-1.027725
H	-1.969403	1.676863	2.048428
H	-4.440219	1.907984	2.062924
H	-5.605592	2.883994	0.104528
H	-4.299703	3.634420	-1.865772
H	-1.831525	3.386296	-1.883593

S-2Mo

C	1.878555	1.256792	1.631690
C	0.960016	2.352583	1.670882
C	-0.203895	1.923024	2.367623
C	-0.003867	0.559635	2.759473
C	1.277926	0.165898	2.307578
Mo	-0.077689	0.691109	0.370345
Si	-1.451695	2.909324	-0.687360
C	-0.279479	4.321571	-1.150662
C	0.444007	-1.445352	-0.168846
N	-0.390660	-2.516481	-0.336643
C	0.313419	-3.675667	-0.638332
C	1.618252	-3.341778	-0.664859
N	1.690432	-1.981350	-0.384874
C	-2.042473	0.366050	0.585586
O	-3.172543	0.281162	0.747377
C	0.788140	1.282003	-1.347081
O	1.254565	1.625674	-2.335122
C	-2.399221	2.368220	-2.227198
C	-2.668840	3.621276	0.574304
H	1.147786	3.346432	1.298572
H	-1.056461	2.530793	2.622164

H	-0.687043	-0.041177	3.339739
H	1.719223	-0.805247	2.455402
H	2.867744	1.269485	1.201880
C	2.980364	-1.331175	-0.352693
H	2.499290	-3.925643	-0.865441
H	-0.185916	-4.613229	-0.808275
C	-1.830489	-2.556629	-0.243495
H	-3.256632	4.390617	0.060631
H	-3.371888	2.889715	0.974763
H	-2.163292	4.116706	1.406845
H	-0.892674	5.132965	-1.559145
H	0.254072	4.732656	-0.290059
H	0.452951	4.052851	-1.912835
H	-2.940026	3.229000	-2.634791
H	-1.735890	1.998271	-3.013070
H	-3.136733	1.592427	-2.007882
H	-0.875759	0.260786	-1.060437
C	3.424710	-0.607731	-1.456216
C	4.700788	-0.048243	-1.439108
C	5.534129	-0.233065	-0.337388
C	5.096133	-0.990667	0.747821
C	3.819256	-1.547077	0.740374
H	2.787549	-0.493855	-2.322587
H	5.047375	0.517158	-2.295676
H	6.528913	0.195953	-0.332104
H	5.749423	-1.157653	1.595735
H	3.481996	-2.157732	1.569829
C	-2.596748	-2.306308	-1.379439
C	-3.981880	-2.430092	-1.305417
C	-4.587448	-2.812660	-0.109876
C	-3.809480	-3.078074	1.015415
C	-2.424025	-2.955405	0.951454
H	-2.112533	-2.026484	-2.307447
H	-4.585655	-2.236338	-2.183742
H	-5.664963	-2.911503	-0.057471
H	-4.279496	-3.385307	1.941780
H	-1.806384	-3.171404	1.815210

S-TS3Mo

C	4.297450	-3.064181	0.218183
C	3.536041	-2.418000	-0.752538
C	2.648538	-3.126145	-1.558363
C	2.510489	-4.499394	-1.374715
C	3.259782	-5.154977	-0.399767
C	4.152831	-4.438350	0.394229
N	3.734410	-1.008065	-0.985992
C	2.980116	0.033283	-0.515354
N	3.575491	1.136074	-1.077522
C	4.673994	0.778403	-1.854479
C	4.769853	-0.564319	-1.799552
Mo	1.215563	-0.036909	0.852709
C	0.488288	0.125262	-0.982981
O	0.162061	0.210901	-2.092434
C	3.193670	2.523442	-0.965640
C	2.099640	3.010136	-1.677573
C	1.793467	4.367855	-1.613177
C	2.583504	5.233808	-0.858765
C	3.691696	4.742766	-0.171324
C	4.002112	3.385941	-0.226884
C	1.258441	2.174138	1.844337
C	0.163134	1.450419	2.398305
C	0.685476	0.360662	3.153632
C	2.100686	0.411524	
3.070551			
C	2.448845	1.522096	2.258967
Si	-2.086507	-0.254455	0.353366
C	-2.456577	-0.839619	2.093694
C	0.540126	-1.875583	0.891940
O	0.181480	-2.968783	1.012747
C	-2.299120	1.555384	-0.115239
C	-2.188085	-1.568481	-0.981983
H	-0.872269	1.742912	2.340769
H	0.113206	-0.351587	3.727393
H	2.789640	-0.266300	3.550392
H	3.453905	1.830731	2.022357
H	1.201039	3.083519	1.267402
H	5.260847	1.513547	-2.376226
H	5.459465	-1.247888	-2.262360
H	-3.505744	-1.139769	2.136314
H	-1.843822	-1.701882	2.357594
H	-2.305070	-0.057041	2.837914
H	-3.012435	2.024818	0.566059
H	-1.367894	2.117729	-0.095305
H	-2.711803	1.618764	-1.124633
H	-3.058194	-2.199502	-0.785658
H	-2.292023	-1.115257	-1.969429
H	-1.314785	-2.217539	-0.999568
H	2.215277	-1.372002	1.068153
H	1.504666	2.338969	-2.282084
H	0.945452	4.750481	-2.168682
H	2.345450	6.290052	-0.818899
H	4.318702	5.413691	0.403466
H	4.870415	2.998352	0.293348
H	2.077554	-2.604949	-2.317386
H	1.819935	-5.056770	-1.996011
H	3.150388	-6.223848	-0.260982
H	4.740043	-4.947247	1.149157
H	4.991250	-2.496001	0.826363
O	-4.531699	-0.124603	0.173758
C	-5.345321	-0.346404	-0.718729
C	-6.782608	-0.135831	-0.601900
H	-4.998081	-0.737146	-1.692141
C	-7.602938	-0.433100	-1.700898
C	-8.976375	-0.242164	-1.614765
C	-9.531500	0.245334	-0.432045
C	-8.719501	0.543684	0.667376
C	-7.349327	0.355202	0.586782
H	-7.160704	-0.812830	-2.616212
H	-9.612917	-0.470882	-2.460662
H	-10.602937	0.394289	-0.363489
H	-9.163960	0.921111	1.580373
H	-6.702186	0.579072	1.425825

S-3Mo

C	3.757854	-2.637266	-1.696511
C	4.422671	-1.504718	-1.234974
C	5.676823	-1.612047	-0.635575
C	6.256910	-2.867212	-0.469571
C	5.586749	-4.008014	-0.907058
C	4.341362	-3.890084	-1.521302
N	3.878237	-0.187919	-1.463287
C	2.898805	0.464540	-0.748378
N	2.841263	1.688915	-1.366925
C	3.739452	1.782276	-2.425507
C	4.393944	0.606200	-2.481892
Mo	1.717946	-0.369206	0.987270
C	2.934795	0.346258	2.964301
C	1.857886	-0.509319	3.325706
C	2.130739	-1.811090	2.793521
C	3.373992	-1.753897	2.107832
C	3.850275	-0.419959	2.198694
C	2.045662	2.828467	-0.997742
C	1.012150	3.236108	-1.836802
C	0.300125	4.394502	-1.534483

C	0.620109	5.135440	-0.399398
C	1.658881	4.721322	0.432734
C	2.381018	3.570855	0.131876
C	0.418576	1.080535	0.858587
O	-0.458661	1.852507	0.932902
C	0.957530	-1.553889	-0.396537
O	0.453075	-2.279053	-1.149204
Si	-3.459890	0.712374	0.441800
C	-2.595066	0.003948	-1.048604
C	-3.043243	-0.044383	2.086305
C	-3.709860	2.552424	0.417713
O	-5.207666	0.138464	0.254835
C	-5.724981	-0.682106	-0.549131
C	-7.106701	-1.028112	-0.530026
C	-7.999191	-0.463629	0.409673
C	-9.330497	-0.831749	0.387669
C	-9.784245	-1.757524	-0.561918
C	-8.910710	-2.321198	-1.494888
C	-7.573633	-1.960278	-1.482631
H	1.019662	-0.242840	3.950330
H	1.530386	-2.694477	2.944790
H	3.871636	-2.575179	1.616943
H	4.773441	-0.052300	1.777854
H	3.043672	1.384567	3.237012
H	5.167056	0.253541	-3.141557
H	3.830547	2.675840	-3.017344
H	0.108943	-0.856596	1.255519
H	-3.096843	-1.135452	2.056427
H	-2.022004	0.232772	2.356382
H	-3.715420	0.317503	2.868359
H	-4.130454	2.892547	-0.532109
H	-4.369997	2.877447	1.225502
H	-2.738974	3.035258	0.554239
H	-3.057928	0.323092	-1.987372
H	-1.568226	0.377262	-1.051404
H	-2.526491	-1.086926	-1.035031
H	-5.083703	-1.153838	-1.300853
H	-6.883596	-2.390433	-2.200390
H	-9.277276	-3.035189	-2.221420
H	-10.830504	-2.040650	-0.571877
H	-10.024803	-0.407261	1.101977
H	-7.628072	0.249841	1.134379
H	0.773016	2.649328	-2.716006
H	-0.499939	4.719637	-2.189382
H	0.068113	6.038724	-0.167422
H	1.915300	5.301005	1.311544
H	3.198774	3.244896	0.761712
H	6.191759	-0.717922	-0.304443
H	7.230219	-2.951576	-0.000976
H	6.037980	-4.984750	-0.778020
H	3.822896	-4.773710	-1.874055
H	2.795983	-2.541497	-2.180749

S-6Mo

C	2.301600	-2.844548	0.969100
C	1.772042	-2.688870	-0.309768
C	2.584152	-2.778319	-1.437364
C	3.950137	-2.994554	-1.278505
C	4.493984	-3.125172	-0.002669
C	3.669749	-3.053755	1.119106
N	0.346059	-2.551565	-0.484762
C	-0.450923	-1.462538	-0.240307
N	-1.711998	-1.928193	-0.531932
C	-1.682608	-3.250430	-0.953375
C	-0.392542	-3.640315	-0.926532
Mo	0.132416	0.620174	0.440874
C	1.963639	0.269582	-0.293213
O	3.069527	0.248378	-0.603999
C	-2.993874	-1.268170	-0.397082
C	-3.577799	-0.657727	-1.503499
C	-4.857973	-0.119574	-1.391772
C	-5.555654	-0.211653	-0.189784
C	-4.977768	-0.854994	0.903713
C	-3.697316	-1.392530	0.800261
C	-1.504103	0.792974	2.207761
C	-0.705411	-0.348969	2.492058
C	0.632932	0.066642	2.728162
C	0.681179	1.468300	2.541060
C	-0.648762	1.918697	2.215667
C	-0.916944	1.137377	-1.187541
O	-1.489720	1.537350	-2.100204
Si	1.341677	3.643492	-0.681132
C	2.757315	4.107784	0.450425
C	1.873300	3.243888	-2.425816
C	-0.117963	4.808731	-0.587257
H	1.460757	-0.566241	3.005108
H	1.549294	2.092627	2.685733
H	-0.957858	2.943189	2.077295
H	-2.565348	0.800109	2.021509
H	-1.062138	-1.364086	2.566412
H	-2.580360	-3.778846	-1.222072
H	0.072087	-4.581180	-1.163452
H	2.151697	-2.667111	-2.424635
H	4.588108	-3.057720	-2.151538
H	5.557424	-3.293032	0.117860
H	4.089053	-3.176828	2.110548
H	1.646805	-2.822504	1.831144
H	-3.255764	-1.923063	1.634993
H	-5.527772	-0.952849	1.832072
H	-6.554187	0.200961	-0.109719
H	-5.311190	0.361773	-2.249826
H	-3.039038	-0.603569	-2.440191
H	0.814736	2.284595	-0.089174
H	0.166420	5.775573	-1.016082
H	-0.971649	4.434196	-1.156426
H	-0.437734	4.989447	0.441555
H	3.230093	5.022906	0.078181
H	2.421735	4.306481	1.471009
H	3.523816	3.329849	0.478575
H	2.269246	4.149839	-2.896826
H	2.660926	2.487891	-2.445767
H	1.036669	2.892755	-3.033622

S-TS7Mo

C	-1.959629	-0.201467	2.972728
C	-2.817951	-1.071215	2.253801
C	-2.066443	-2.180934	1.782710
C	-0.718596	-1.977521	2.175143
C	-0.652119	-0.749339	2.916001
Mo	-1.154918	-0.217227	0.690132
C	-0.518713	1.656970	0.728862
O	0.004173	2.667938	0.933153
C	-0.658303	-0.827287	-1.127429
O	-0.316254	-1.211567	-2.164466
C	-2.998388	0.411722	-0.477505
N	-3.430440	1.652826	-0.866396
C	-4.609831	1.588377	-1.598495
C	-4.946518	0.286759	-1.678042
N	-3.961534	-0.423834	-1.000885
C	-2.834297	2.935736	-0.592334
C	-3.168430	3.610106	0.578990
C	-2.656611	4.885491	0.799489
C	-1.830635	5.481707	-0.151228

C	-1.515378	4.804372	-1.327192
C	-2.019864	3.527066	-1.554333
C	-4.073291	-1.859672	-0.898550
C	-3.305662	-2.690768	-1.710200
C	-3.489737	-4.070218	-1.643603
C	-4.447312	-4.613366	-0.788857
C	-5.233039	-3.773148	-0.002278
C	-5.050478	-2.393637	-0.059047
O	4.636999	-0.088904	-0.016496
C	5.530580	-0.931435	-0.209496
C	6.925269	-0.598714	-0.346080
C	7.846226	-1.641433	-0.559078
C	9.196776	-1.354345	-0.694414
C	9.630109	-0.030043	-0.618502
C	8.720247	1.012974	-0.407312
C	7.371648	0.735790	-0.270751
H	0.094810	-2.669227	2.021372
H	0.220077	-0.344470	3.403745
H	-2.249090	0.707974	3.475856
H	-3.877544	-0.925085	2.117968
H	-2.453920	-3.027878	1.240101
H	-5.776023	-0.206327	-2.153286
H	-5.085772	2.472069	-1.985238
H	-2.578593	-2.266577	-2.388189
H	-2.891761	-4.718704	-2.272851
H	-4.590795	-5.686533	-0.746160
H	-5.990148	-4.188231	0.652189
H	-5.664853	-1.732362	0.540691
H	-1.784170	2.987694	-2.463877
H	-0.878466	5.270174	-2.069654
H	-1.436716	6.475975	0.022718
H	-2.907024	5.414611	1.711151
H	-3.818865	3.137141	1.304735
H	5.260791	-1.992973	-0.283395
H	7.496631	-2.666795	-0.616732
H	9.910479	-2.151980	-0.858148
H	10.685154	0.194576	-0.724526
H	9.074089	2.035007	-0.351150
H	6.651526	1.527517	-0.106850
H	0.613157	-0.181978	0.507261
Si	2.631252	-0.184071	0.218633
C	2.767560	0.508056	1.955200
C	2.556040	-2.042516	-0.051304
C	2.346898	0.965919	-1.229790
H	3.298393	1.284031	-1.660631
H	1.762641	0.470116	-2.006645
H	1.802124	1.854885	-0.909600
H	3.755771	0.943125	2.118934
H	2.021167	1.285773	2.117918
H	2.614201	-0.277893	2.698623
H	2.995586	-2.314379	-1.015583
H	3.092090	-2.577374	0.738764
H	1.527797	-2.397977	-0.055103

1W $[CpW(CO)_2(IMes)]^+$

1W

C	-4.194339	0.442634	1.218872
C	-1.429568	0.591102	0.611040
C	-2.132008	-1.933213	1.674807
C	-1.928582	-1.807859	-1.658064
C	-3.232700	-2.341159	-1.463943
C	-4.183893	-1.274828	-1.668643
C	-3.458988	-0.094426	-1.988912
C	-2.077398	-0.426219	-1.962523
O	-4.916590	1.201505	1.689321
N	-1.513422	1.944413	0.685341
C	-0.312260	2.527043	1.032215
C	0.576190	1.507473	1.169457
N	-0.124926	0.350216	0.901443
O	-1.599303	-2.621370	2.423529
H	-1.002844	-2.361025	-1.627814
H	-3.468129	-3.378048	-1.270538
H	-5.260618	-1.368093	-1.651437
H	-3.882268	0.864891	-2.243166
H	-1.268132	0.259352	-2.163950
H	-2.371807	2.450434	0.523456
H	-0.190522	3.589436	1.154523
H	1.619674	1.512340	1.433244
H	0.265520	-0.580078	0.935646
W	-3.002417	-0.836632	0.239806

TS2W

C	-2.445154	-2.207160	-1.699094
C	-3.848831	-2.174217	-1.511490
C	-4.286171	-0.836331	-1.684440
C	-3.143621	-0.030041	-2.003339
C	-2.001145	-0.886706	-2.009149
W	-2.839444	-0.774725	0.183131
Si	-4.457433	-2.455080	1.767911
C	-3.841384	-4.219802	1.520508
C	-1.433075	0.831929	0.677904
N	-0.757757	1.660766	-0.159269
C	0.043922	2.566526	0.525797
C	-0.129200	2.303242	1.839427
N	-1.029502	1.247884	1.904760
C	-4.057089	0.614879	0.997744
O	-4.756668	1.390372	1.464590
C	-1.372128	-1.798276	1.125077
O	-0.553800	-2.385485	1.667361
C	-4.473280	-2.098524	3.626066
C	-6.219516	-2.221250	1.135808
H	-4.476084	-3.025391	-1.302137
H	-5.309361	-0.495257	-1.644622
H	-3.172017	1.014196	-2.275623
H	-0.988713	-0.618758	-2.271011
H	-1.821658	-3.087628	-1.651665
H	-1.361207	0.827495	2.758871
H	0.296536	2.760489	2.715199
H	0.651524	3.299073	0.024185
H	-0.837311	1.624220	-1.161784
H	-6.883097	-2.858630	1.730848
H	-6.563209	-1.191671	1.261192
H	-6.354294	-2.501017	0.089493
H	-4.501636	-4.897544	2.072999
H	-3.838868	-4.542702	0.477600
H	-2.832838	-4.356019	1.918446
H	-5.164219	-2.794036	4.113788
H	-3.491509	-2.237781	4.087000
H	-4.817305	-1.085505	3.852224
H	-3.186265	-1.081085	1.864503

2W

C	-1.957221	-2.040978	-1.559951
C	-3.336950	-2.362934	-1.368368
C	-4.094518	-1.179813	-1.598555
C	-3.178168	-0.124133	-1.930323
C	-1.865247	-0.670415	-1.905379
W	-2.812827	-0.782997	0.300475
Si	-4.618019	-2.376259	1.708356
C	-4.113572	-4.199903	1.735134
C	-1.333325	0.801141	0.674592
N	-1.507694	2.144482	0.625788
C	-0.343076	2.841343	0.906396

C	0.606875	1.904961	1.138779
N	-0.020080	0.678101	0.989345
C	-4.288338	0.440550	0.878669
O	-5.143570	1.126315	1.216480
C	-1.708530	-2.024968	1.436041
O	-1.082645	-2.722296	2.095586
C	-4.751680	-1.770399	3.490133
C	-6.317523	-2.273153	0.882119
H	-3.731969	-3.343707	-1.161506
H	-5.170133	-1.106140	-1.595469
H	-3.445420	0.879062	-2.223528
H	-0.953319	-0.135877	-2.121347
H	-1.132088	-2.733830	-1.487758
H	0.431632	-0.213820	1.120216
H	1.648030	2.001453	1.392716
H	-0.293932	3.916149	0.917829
H	-2.399813	2.573945	0.435450
H	-7.023074	-2.855249	1.485277
H	-6.705778	-1.253786	0.825994
H	-6.330512	-2.705683	-0.121763
H	-4.890594	-4.754828	2.272486
H	-4.038257	-4.643159	0.738869
H	-3.171214	-4.378288	2.256374
H	-5.471577	-2.396261	4.028193
H	-3.798699	-1.842011	4.021120
H	-5.102186	-0.737790	3.559151
H	-2.807793	-0.398381	1.971176

3W

W	2.546151	-0.513258	0.001870
C	3.518986	-2.629247	0.453708
C	4.437220	-1.686500	0.986545
C	4.921002	-0.898686	-0.085827
C	4.327189	-1.364346	-1.299870
C	3.448835	-2.439629	-0.961019
H	1.132385	-1.396608	0.436562
C	1.165490	-0.120269	-1.336536
C	1.693476	0.170441	1.633254
O	1.187332	0.545371	2.617006
O	0.346476	0.048786	-2.147523
Si	-2.497820	-0.062040	0.796348
O	-4.303914	0.144866	0.524969
C	-5.096911	-0.492388	-0.221861
C	-6.482930	-0.189003	-0.327339
C	-7.270283	-0.972100	-1.200781
C	-8.623163	-0.707550	-1.331760
C	-9.194735	0.333572	-0.596259
C	-7.071702	0.862810	0.412098
C	-8.422284	1.116435	0.273106
C	3.033754	1.598489	-0.286927
N	3.646243	2.151683	-1.370467
C	3.842568	3.518799	-1.236630
C	3.336614	3.851142	-0.026516
N	2.856902	2.674522	0.528395
H	2.446968	2.590573	1.445578
H	3.280627	4.799955	0.477507
H	4.313670	4.119708	-1.994473
H	3.876294	1.607605	-2.186058
C	-2.049661	-1.600708	-0.149737
C	-2.410675	-0.218654	2.644704
C	-1.836159	1.533137	0.114457
H	2.890589	-3.047208	-1.655435
H	2.991666	-3.382996	1.016886
H	4.710014	-1.582175	2.025451
H	5.641340	-0.099242	0.001100
H	4.570658	-1.039257	-2.299494
H	-2.303101	2.396151	0.595454
H	-0.760346	1.573751	0.307834
H	-1.973969	1.605658	-0.966366
H	-2.857019	-1.149312	3.003191
H	-1.359399	-0.205009	2.950535
H	-2.907722	0.619224	3.140104
H	-2.607389	-2.480346	0.184552
H	-2.160056	-1.484083	-1.230691
H	-0.988095	-1.801982	0.029980
H	-4.700160	-1.319801	-0.818678
H	-6.812052	-1.776404	-1.765930
H	-9.234309	-1.302095	-1.998787
H	-10.253834	0.540185	-0.699162
H	-8.886663	1.918072	0.833591
H	-6.456755	1.455223	1.077481

4W

C	2.058879	1.283604	-2.376446
C	2.501448	2.352024	-1.539587
C	3.727265	1.969585	-0.933750
C	4.038369	0.660960	-1.374989
C	3.018101	0.228929	-2.279226
C	2.804139	-1.334723	0.706419
C	0.361104	-0.621377	-0.321555
H	0.632506	1.516952	0.181337
C	1.877643	1.019276	1.719356
N	3.316707	-2.403348	0.034181
C	3.793863	-3.392024	0.884605
C	3.575750	-2.940285	2.140378
N	2.979478	-1.695401	2.006447
O	-0.630610	-1.241633	-0.463446
O	1.852486	1.374260	2.822220
Si	-4.345089	-2.485218	-0.422956
C	-3.550885	-2.608071	-2.102930
C	-3.315801	-3.190412	0.959931
C	-6.147196	-2.935341	-0.365505
O	-4.424950	-0.704239	-0.083731
C	-3.472618	0.129367	0.037394
C	-3.695648	1.506309	0.304715
C	-4.998693	2.040419	0.445090
C	-5.154770	3.386650	0.706801
C	-4.025212	4.209209	0.832872
C	-2.735449	3.692097	0.696976
C	-2.562800	2.343036	0.431659
H	1.197497	1.300317	-3.025097
H	2.007202	3.302346	-1.413492
H	4.312500	2.565458	-0.250426
H	4.916782	0.100512	-1.093026
H	3.021587	-0.674768	-2.869342
H	3.295990	-2.463377	-0.970399
H	4.237011	-4.305441	0.528919
H	3.790206	-3.383415	3.096916
H	2.721555	-1.095196	2.774318
H	-2.522707	-2.237365	-2.083149
H	-3.516625	-3.656822	-2.415096
H	-4.113876	-2.058852	-2.861917
H	-2.288614	-2.819520	0.919719
H	-3.275723	-4.280255	0.863831
H	-3.739619	-2.964139	1.941743
H	-6.273054	-4.005760	-0.555082
H	-6.582863	-2.720752	0.613595
H	-6.721251	-2.396268	-1.123270
H	-5.856042	1.387015	0.344979
H	-6.145281	3.810338	0.816106
H	-4.157950	5.264988	1.040168
H	-1.874605	4.340464	0.799877
H	-1.565551	1.927955	0.321960
H	-2.444826	-0.230338	-0.072487

W	1.955991	0.473483	-0.182531

TS5W

C	-3.524115	-1.064715	-1.233058
C	-3.021286	-0.921923	0.071360
C	-3.198608	-1.951726	1.011404
C	-3.880495	-3.106525	0.653463
C	-4.374597	-3.244565	-0.644955
C	-4.194137	-2.226173	-1.585762
C	-2.376856	0.306413	0.496917
O	-2.500304	1.370561	-0.210919
Si	-2.353011	3.103443	0.178405
C	-3.902473	3.789254	-0.596133
C	-2.322718	3.244202	2.039762
C	-0.790036	3.680277	-0.652194
C	0.450076	0.349609	-1.528394
O	0.080276	0.822383	-2.521707
W	1.058672	-0.571652	0.107668
C	0.917160	0.790001	1.523417
O	0.811828	1.535284	2.407887
C	0.635216	-2.519111	1.286341
C	0.268195	-2.762800	-0.079946
C	1.453159	-2.755596	-0.864260
C	2.541399	-2.485157	0.001579
C	2.051962	-2.352311	1.332178
C	2.914211	0.520386	-0.320694
N	3.962968	0.713634	0.522599
C	4.989996	1.438665	-0.059965
C	4.581585	1.716063	-1.321289
N	3.327718	1.144243	-1.454723
H	-0.679295	-0.175743	0.221426
H	-0.726094	-2.971858	-0.442059
H	1.514485	-2.924140	-1.928317
H	3.575159	-2.409054	-0.300124
H	2.646716	-2.221470	2.222917
H	-0.022898	-2.550402	2.140145
H	3.952520	0.386962	1.476089
H	5.898703	1.688122	0.459194
H	5.064398	2.256850	-2.116321
H	2.763885	1.181200	-2.290068
H	-3.213140	2.811598	2.504897
H	-1.432719	2.791249	2.482879
H	0.096557	3.241076	-0.190674
H	-0.713573	4.768818	-0.565021
H	-0.788295	3.425712	-1.714323
H	-2.307916	4.305557	2.308860
H	-4.803280	3.366163	-0.144487
H	-3.941561	4.874390	-0.459409
H	-3.932131	3.590033	-1.670319
H	-2.105779	0.406815	1.547560
H	-2.815410	-1.834801	2.019460
H	-4.032095	-3.895485	1.379793
H	-4.905761	-4.146864	-0.924618
H	-4.584069	-2.342223	-2.589616
H	-3.383063	-0.265017	-1.948777

5W

W	-1.228904	0.179931	0.091520
C	0.448611	-0.156752	1.663335
C	-0.176109	1.103084	1.968562
C	-1.503713	0.864408	2.394676
C	-1.729026	-0.532981	2.312656
C	-0.521696	-1.171113	1.881409
C	-2.535750	1.472958	-0.664280
C	-2.960257	-1.137638	-0.165874
C	-0.619064	-0.963733	-1.411832
O	-0.235497	-1.702111	-2.211470
O	-3.374062	2.201343	-0.984313
N	-4.279722	-0.832971	-0.257326
C	-5.071262	-1.954153	-0.427494
C	-4.227175	-3.014620	-0.432873
N	-2.956611	-2.491739	-0.269890
Si	4.708863	-1.319819	0.036564
O	3.364014	-0.274236	0.016529
C	2.771719	0.273984	-1.147281
C	1.948702	1.493029	-0.787736
C	4.252232	-2.933059	-0.813935
C	6.151573	-0.495452	-0.838774
C	5.052082	-1.572468	1.858014
C	2.453716	2.439557	0.097351
C	1.755353	3.624312	0.354366
C	0.529528	3.875317	-0.254914
C	0.003746	2.935182	-1.140067
C	0.696323	1.734261	-1.400574
H	1.479943	-0.302450	1.373597
H	0.296623	2.070642	1.905763
H	-2.218123	1.608746	2.711374
H	-2.645576	-1.035442	2.581055
H	-0.358188	-2.235033	1.805023
H	-4.628957	0.113589	-0.231012
H	-6.141201	-1.902161	-0.529545
H	-4.416520	-4.068505	-0.538728
H	-2.107623	-3.036189	-0.262127
H	3.996518	-2.787618	-1.867805
H	3.401254	-3.416430	-0.324999
H	5.091344	-3.634876	-0.780156
H	5.955594	-0.317167	-1.900147
H	7.038805	-1.134023	-0.782655
H	6.409026	0.462040	-0.377081
H	5.903995	-2.243586	2.002316
H	5.289005	-0.627068	2.353322
H	4.193845	-2.015526	2.370791
H	3.540175	0.585639	-1.869304
H	2.143457	-0.468058	-1.651394
H	3.410049	2.258460	0.571855
H	2.186111	4.362180	1.022186
H	0.003001	4.803753	-0.071172
H	-0.897097	3.161950	-1.694426
H	0.390875	1.127963	-2.244991

6W

C	-3.396864	-0.069517	-2.258604
C	-2.024806	-0.322206	-2.003103
C	-1.847000	-1.714298	-1.752348
C	-3.128431	-2.328871	-1.824284
C	-4.088786	-1.301722	-2.133228
C	-1.683328	0.460416	0.792395
C	-2.494945	-2.028100	1.463017
H	-4.760196	-1.814690	0.449525
C	-4.393719	0.458087	0.858257
N	-1.746556	1.799450	1.004844
C	-0.566559	2.311716	1.513772
C	0.284248	1.261998	1.619502
N	-0.416437	0.155713	1.172679
O	-2.019155	-2.725204	2.250811
O	-5.079321	1.287754	1.272670
Si	-5.758682	-2.786571	1.213741
C	-5.126339	-4.525445	0.961045
C	-5.769630	-2.223469	2.991949
C	-7.343486	-2.413190	0.293388
H	-5.143819	-1.447951	-2.306739
H	-3.833789	0.884224	-2.511480
H	-1.237987	0.416146	-2.030036
H	-0.906480	-2.219420	-1.596278

H	-3.325542	-3.386775	-1.750166
H	-2.576984	2.344713	0.828830
H	-0.436705	3.353154	1.751248
H	1.301510	1.208829	1.966123
H	-0.052938	-0.784973	1.155513
H	-7.611944	-1.356401	0.361711
H	-7.283079	-2.689916	-0.761765
H	-8.161358	-2.990938	0.737298
H	-5.070802	-4.794338	-0.096257
H	-4.144014	-4.674666	1.413773
H	-5.819400	-5.226221	1.439303
H	-6.032377	-1.167239	3.082313
H	-4.806338	-2.386046	3.479247
H	-6.521675	-2.799695	3.541786
W	-3.220181	-0.904015	-0.001655

TS7W

W	1.957367	0.346938	-0.087157
C	1.542560	2.408207	-1.117033
C	2.798472	2.001274	-1.639613
C	3.712880	1.936343	-0.559336
C	3.046517	2.332568	0.635848
C	1.692393	2.620414	0.296231
H	0.163327	0.230160	-0.063361
C	1.503010	-0.451275	1.666045
C	1.503813	-1.031718	-1.424230
O	1.264576	-1.788330	-2.270252
O	1.237127	-0.841527	2.721836
Si	-1.667318	0.001415	-0.005069
O	-3.791255	-0.250561	-0.049916
C	-4.751892	0.323492	0.478131
C	-6.134809	-0.025839	0.238154
C	-7.137919	0.704272	0.899282
C	-8.474157	0.393126	0.688805
C	-8.810828	-0.645321	-0.179839
C	-6.483048	-1.072378	-0.636775
C	-7.817787	-1.376860	-0.841522
C	3.690816	-0.980630	0.193582
N	4.565444	-0.979916	1.234254
C	5.551587	-1.943997	1.103347
C	5.297815	-2.580027	-0.065238
N	4.173177	-1.973804	-0.597392
H	3.733941	-2.239360	-1.465816
H	5.808763	-3.391993	-0.552325
H	6.327801	-2.090487	1.833749
H	4.464014	-0.361634	2.023740
C	-1.805580	1.166290	1.466694
C	-1.796176	0.645357	-1.765611
C	-1.477407	-1.833418	0.310403
H	0.943311	3.015163	0.964147
H	0.651579	2.589814	-1.696581
H	3.018563	1.781518	-2.672906
H	4.751689	1.653434	-0.637358
H	3.497291	2.456986	1.608301
H	-2.453056	-2.314775	0.392461
H	-0.928824	-2.308556	-0.504848
H	-0.925040	-2.009399	1.235359
H	-1.794480	1.738768	-1.778335
H	-0.958245	0.296718	-2.369560
H	-2.721368	0.304682	-2.233381
H	-2.201955	2.140968	1.167519
H	-2.466169	0.746627	2.230190
H	-0.835756	1.328855	1.934066
H	-4.569544	1.153168	1.177135
H	-6.864146	1.509558	1.572819
H	-9.250916	0.952321	1.195308
H	-9.854055	-0.889094	-0.344367
H	-8.095697	-2.180417	-1.512475
H	-5.699233	-1.626161	-1.138205

TS7W-II

C	-3.228547	1.192825	0.661366
C	-3.268238	1.035013	-0.766224
C	-3.515501	-0.340529	-1.040837
C	-3.621299	-1.016519	0.209262
C	-3.463752	-0.074676	1.255325
C	-0.188420	-0.235003	1.559969
C	-0.198006	-0.124266	-1.574416
C	-0.947124	-2.254529	-0.084932
H	-0.478393	1.482503	0.006704
Si	0.410543	3.099795	0.068163
C	0.395067	3.375281	1.914198
H	1.899235	3.724700	-1.873251
C	1.792618	4.028705	-0.827136
C	-1.119544	3.807706	-0.793858
O	1.834397	1.487279	0.215197
C	2.712018	1.104533	-0.569987
C	3.724201	0.126131	-0.231923
C	3.782120	-0.458133	1.047625
C	4.787474	-1.365649	1.338069
C	5.735171	-1.697622	0.363340
C	5.681086	-1.125677	-0.907847
C	4.677548	-0.214130	-1.206948
N	-1.063536	-3.080561	-1.157561
C	-0.731958	-4.391657	-0.859953
C	-0.393991	-4.402314	0.451989
N	-0.537837	-3.099477	0.896603
O	0.431899	-0.348132	2.532068
O	0.475467	-0.103484	-2.518449
H	3.040126	-0.188116	1.788631
H	4.845709	-1.814787	2.322188
H	6.521986	-2.404698	0.599871
H	6.419960	-1.387892	-1.654900
H	4.627018	0.239763	-2.190937
H	2.754202	1.519910	-1.585278
H	1.255652	2.919151	2.404241
H	2.765662	3.948110	-0.340502
H	1.511003	5.086244	-0.846838
H	0.432111	4.454923	2.096528
H	-0.512728	2.986668	2.378437
H	-1.006721	4.897261	-0.823178
H	-2.049276	3.573785	-0.277860
H	-1.196873	3.461071	-1.827411
H	-3.110848	2.120301	1.198934
H	-3.208859	1.823260	-1.498253
H	-3.667160	-0.775393	-2.016510
H	-3.811394	-2.070943	0.340961
H	-3.516122	-0.282511	2.313034
H	-1.339114	-2.745821	-2.067651
H	-0.765219	-5.183628	-1.587454
H	-0.074422	-5.206061	1.091972
H	-0.349355	-2.788408	1.837456
W	-1.393565	-0.103088	-0.004994

S-1W

C	-3.624302	3.108179	1.491768
C	-2.848386	2.641345	0.435242
C	-3.063634	3.087102	-0.867347
C	-4.101402	3.981006	-1.117936
C	-4.901821	4.434520	-0.070224
C	-4.659190	4.003372	1.231783
N	-1.710267	1.789375	0.714177
C	-1.613519	0.419678	0.626936
N	-0.299959	0.172480	0.953312

C	0.371355	1.339573	1.254890
C	-0.513511	2.354054	1.104861
C	0.407450	-1.091402	0.987257
C	0.597710	-1.732365	2.207584
C	1.359786	-2.897354	2.252257
C	1.934652	-3.403316	1.088850
C	1.759756	-2.738529	-0.124210
C	1.000705	-1.572449	-0.178251
W	-3.192161	-1.020507	0.199717
C	-2.507049	-2.310345	1.566251
O	-2.195699	-3.170751	2.261044
C	-2.261508	-0.536799	-2.011501
C	-2.122493	-1.925186	-1.748500
C	-3.431204	-2.450534	-1.553919
C	-4.372303	-1.371070	-1.713820
C	-3.637709	-0.187162	-2.005878
C	-4.552310	0.034241	1.218449
O	-5.449587	0.559203	1.707629
H	-1.203431	-2.486966	-1.722122
H	-3.673644	-3.489997	-1.383725
H	-5.449676	-1.452836	-1.685494
H	-4.056145	0.785226	-2.206714
H	-1.446258	0.147214	-2.192067
H	-0.403638	3.416100	1.239238
H	1.407296	1.339912	1.546260
H	0.151944	-1.328882	3.108607
H	1.504345	-3.405579	3.197588
H	2.529866	-4.307513	1.128655
H	2.226890	-3.117555	-1.025238
H	0.889229	-1.028978	-1.108638
H	-2.413518	2.757351	-1.668612
H	-4.273562	4.334794	-2.127353
H	-5.705245	5.133814	-0.267543
H	-5.272122	4.363679	2.048689
H	-3.425103	2.772286	2.502138

S-TS2W

C	1.827851	-1.186114	-1.765199
C	2.133824	-1.730347	-0.487048
C	1.186359	-2.774158	-0.220419
C	0.315089	-2.871487	-1.340926
C	0.712116	-1.890437	-2.287740
W	0.009483	-0.768200	-0.262619
C	-1.351423	0.003135	-1.543337
O	-2.124134	0.322866	-2.324263
C	0.590107	1.406046	-0.060500
N	-0.220738	2.516365	-0.033585
C	0.520225	3.689811	0.062457
C	1.815054	3.331685	0.115984
N	1.851661	1.941567	0.054690
C	-1.662636	2.602238	0.012706
C	-2.343392	3.151627	-1.071229
C	-3.719772	3.346107	-0.987925
C	-4.405191	3.003299	0.175387
C	-3.712684	2.470068	1.261588
C	-2.336034	2.273260	1.187125
C	3.118236	1.274256	0.232915
C	3.467390	0.794893	1.494564
C	4.727895	0.233517	1.686904
C	5.636582	0.170352	0.630739
C	5.289102	0.678738	-0.619404
C	4.028898	1.238984	-0.820530
C	0.176428	-0.472677	1.718513
O	0.257396	-0.301721	2.851133
Si	-2.268171	-2.209214	0.658580
C	-3.307817	-1.402000	2.014906
C	-3.382824	-2.553104	-0.820107
C	-1.589833	-3.810057	1.396651
H	1.189678	-3.426856	0.637445
H	-0.471494	-3.594553	-1.482868
H	0.254329	-1.721464	-3.251367
H	2.365267	-0.400461	-2.269104
H	2.974482	-1.466426	0.131803
H	2.713370	3.915539	0.211474
H	0.046145	4.654302	0.104425
H	-4.188474	-3.221174	-0.496704
H	-3.849664	-1.640782	-1.198128
H	-2.870223	-3.036683	-1.654346
H	-2.446291	-4.384670	1.767201
H	-1.057376	-4.445778	0.687767
H	-0.936540	-3.616419	2.250667
H	-4.083035	-2.109658	2.326671
H	-2.715913	-1.153644	2.899786
H	-3.805819	-0.493751	1.669227
H	-1.540008	-0.560028	0.521691
H	2.765397	0.869978	2.315605
H	5.004376	-0.138965	2.665997
H	6.618900	-0.259093	0.786424
H	6.000149	0.649281	-1.436164
H	3.757306	1.657328	-1.782961
H	-1.785900	1.887720	2.036234
H	-4.239707	2.224633	2.175812
H	-5.474853	3.162402	0.240635
H	-4.253106	3.768018	-1.830993
H	-1.802236	3.416499	-1.971678

S-2W

C	1.334994	-0.265292	-2.235352
C	1.951403	-1.228830	-1.394551
C	1.085435	-2.368929	-1.331274
C	-0.056856	-2.099033	-2.139332
C	0.105348	-0.790490	-2.698752
W	-0.068578	-0.632560	-0.309454
C	-1.975722	-0.172221	-0.751757
O	-3.074746	-0.011146	-1.030040
C	0.514944	1.492957	0.156978
N	-0.293789	2.589034	0.310982
C	0.439156	3.735099	0.590039
C	1.735425	3.371766	0.616523
N	1.774813	2.005698	0.360513
C	-1.733255	2.670103	0.235252
C	-2.324167	3.153319	-0.929430
C	-3.705841	3.319286	-0.973863
C	-4.482993	3.011729	0.140937
C	-3.879694	2.544920	1.307621
C	-2.498180	2.379151	1.362707
C	3.049298	1.327552	0.359999
C	3.449672	0.593209	1.473453
C	4.712087	0.003578	1.485036
C	5.574934	0.168990	0.402553
C	5.180152	0.936145	-0.692387
C	3.916507	1.522223	-0.714530
C	0.707560	-1.212927	1.444763
O	1.116235	-1.575660	2.453530
Si	-1.685472	-2.675299	0.717291
C	-2.493679	-2.082392	2.317750
C	-3.060997	-3.226830	-0.462275
C	-0.650515	-4.221839	1.073687
H	1.301123	-3.295452	-0.825102
H	-0.859889	-2.782426	-2.360542
H	-0.575626	-0.303006	-3.379638

H	1.732281	0.704772	-2.484497
H	2.920400	-1.145054	-0.931845
H	2.630693	3.937194	0.806092
H	-0.037760	4.685992	0.749547
H	-3.638208	-4.004165	0.050927
H	-3.755515	-2.429804	-0.729780
H	-2.682431	-3.674539	-1.384831
H	-1.300689	-4.955093	1.563767
H	-0.279069	-4.694610	0.160693
H	0.194022	-4.041129	1.741156
H	-3.108345	-2.888386	2.732066
H	-1.762333	-1.803847	3.080216
H	-3.150575	-1.225722	2.145445
H	-0.927548	-0.104717	1.070991
H	2.788760	0.492314	2.323790
H	5.025614	-0.570234	2.348741
H	6.559058	-0.283592	0.419971
H	5.856027	1.085819	-1.525663
H	3.609131	2.135058	-1.554088
H	-2.015820	2.037094	2.270346
H	-4.482049	2.320370	2.179605
H	-5.557614	3.143582	0.103801
H	-4.173393	3.690835	-1.877573
H	-1.708053	3.396214	-1.787191

S-TS3W

C	7.606968	0.251803	0.511724
C	6.941814	-0.319139	-0.587956
C	7.679331	-0.847747	-1.659714
C	9.067208	-0.806588	-1.634570
C	9.719661	-0.238476	-0.540589
C	8.991266	0.289765	0.530932
C	5.491185	-0.373161	-0.644413
O	4.740670	0.059864	0.230372
C	2.346153	0.781459	-1.337348
Si	2.423317	0.016760	0.374632
C	2.700789	-1.825660	0.629435
W	-1.069443	-0.055735	0.586967
C	-0.323110	1.755975	0.535447
O	0.122404	2.827223	0.560000
C	-2.877730	0.202861	-0.652694
N	-3.436868	1.368422	-1.109348
C	-4.604844	1.133470	-1.824760
C	-4.800572	-0.200018	-1.823502
N	-3.744414	-0.760000	-1.112772
C	-2.955270	2.715412	-0.922015
C	-3.346864	3.436031	0.203070
C	-2.944593	4.761884	0.338127
C	-2.166905	5.361191	-0.650734
C	-1.792001	4.635855	-1.779061
C	-2.188676	3.308571	-1.921073
C	-3.660731	-2.189080	-0.939286
C	-2.758959	-2.934651	-1.693683
C	-2.735195	-4.320347	-1.556206
C	-3.620097	-4.956592	-0.687605
C	-4.538389	-4.205551	0.044049
C	-4.562899	-2.818503	-0.082108
C	-0.156891	-1.298116	-0.643477
O	0.345552	-2.058856	-1.365222
C	-1.872788	-1.778801	2.066691
C	-0.581433	-1.334465	2.496059
C	-0.696604	0.028131	2.898140
C	-2.060608	0.430207	2.717724
C	-2.765633	-0.686692	2.201074
C	2.639278	1.109966	1.877278
H	0.298789	-1.949692	2.585984
H	0.082516	0.631871	3.333656
H	-2.478195	1.392535	2.966510
H	-3.814854	-0.700581	1.953566
H	-2.126084	-2.770291	1.727012
H	-5.571517	-0.806560	-2.265039
H	-5.173501	1.935834	-2.260608
H	3.686099	1.414076	1.939855
H	2.023106	2.005856	1.826838
H	2.399882	0.560494	2.790276
H	3.479790	-1.953577	1.384734
H	1.809454	-2.355722	0.956394
H	3.035912	-2.297591	-0.296458
H	3.336016	1.092763	-1.675773
H	1.936697	0.075439	-2.061509
H	1.712563	1.668262	-1.323458
H	-0.660892	0.585085	-0.947970
H	-2.083227	-2.438595	-2.376620
H	-2.030071	-4.901471	-2.138122
H	-3.602834	-6.035564	-0.590020
H	-5.238604	-4.696567	0.709248
H	-5.281667	-2.228513	0.474561
H	-1.908458	2.734814	-2.796456
H	-1.192686	5.102402	-2.551637
H	-1.857388	6.393863	-0.543531
H	-3.244567	5.327973	1.211885
H	-3.964353	2.963101	0.957151
H	5.063429	-0.837417	-1.549871
H	7.161126	-1.286879	-2.505878
H	9.640024	-1.212712	-2.459066
H	10.802868	-0.205506	-0.520016
H	9.511672	0.728143	1.373755
H	7.024090	0.655711	1.330079

S-3W

C	-3.995635	-0.313852	-1.727795
C	-3.325023	0.575281	-2.606532
C	-2.282033	-0.154439	-3.241498
C	-2.331045	-1.506164	-2.761007
C	-3.408212	-1.603120	-1.834359
W	-1.685086	-0.155561	-0.984736
C	-0.550414	1.448245	-0.942849
O	0.182100	2.344475	-1.086542
C	-0.559024	-1.352075	0.087419
O	0.147977	-2.088280	0.652516
C	-2.568712	0.391814	1.000684
N	-3.309689	-0.427790	1.826261
C	-3.699218	0.224820	2.989958
C	-3.205028	1.475898	2.917801
N	-2.531205	1.571187	1.705858
C	-3.740641	-1.785169	1.593341
C	-2.876540	-2.853628	1.815975
C	-3.345057	-4.155499	1.654209
C	-4.670757	-4.388273	1.292731
C	-5.536419	-3.314041	1.096758
C	-5.073500	-2.009487	1.250110
C	-1.966918	2.831023	1.298911
C	-0.826189	3.304259	1.940977
C	-0.327844	4.562350	1.612556
C	-0.968000	5.337944	0.649511
C	-2.115209	4.859685	0.018913
C	-2.624181	3.607388	0.347827
C	2.760557	0.296108	0.935227
Si	3.509484	0.138108	-0.763123
C	2.983873	-1.358951	-1.727969
O	5.280959	-0.211544	-0.483309
C	5.931615	-0.380729	0.589588
C	7.328927	-0.639634	0.617610
C	7.953139	-0.806707	1.874810

C	9.313063	-1.056835	1.941615
C	10.057198	-1.142756	0.761957
C	9.448215	-0.979671	-0.489893
C	8.092176	-0.729017	-0.570306
C	3.581073	1.728792	-1.719066
H	-1.613773	0.226711	-3.997349
H	-1.714046	-2.322030	-3.102405
H	-3.731610	-2.494349	-1.321943
H	-4.833008	-0.054452	-1.098602
H	-3.566167	1.613905	-2.770922
H	-4.281239	-0.267516	3.748864
H	-3.276064	2.309026	3.594421
H	-0.127809	-0.367607	-1.675319
H	3.049244	-2.270591	-1.129489
H	1.938644	-1.239441	-2.029043
H	3.586882	-1.484143	-2.630721
H	4.109728	2.509345	-1.165486
H	4.068461	1.599797	-2.688261
H	2.558995	2.082533	-1.888794
H	3.221595	1.091446	1.528027
H	1.707599	0.562367	0.802030
H	2.777005	-0.639253	1.500083
H	5.393122	-0.323746	1.540223
H	7.363779	-0.737814	2.782644
H	9.798154	-1.185508	2.900914
H	11.121834	-1.338841	0.815355
H	10.042817	-1.050463	-1.392125
H	7.603080	-0.599444	-1.527293
H	-0.336000	2.687843	2.685310
H	0.560090	4.935332	2.109283
H	-0.578017	6.315976	0.393700
H	-2.619827	5.465890	-0.723954
H	-3.522022	3.229381	-0.124462
H	-5.740678	-1.167689	1.106221
H	-6.571182	-3.488695	0.826954
H	-5.030793	-5.403344	1.173541
H	-2.672014	-4.988313	1.819862
H	-1.850671	-2.670646	2.103471

S-6W

C	-1.529377	0.706890	2.142749
C	-0.717810	-0.420469	2.444314
C	0.615698	0.011144	2.674881
C	0.648720	1.415823	2.475734
C	-0.685969	1.847691	2.142328
W	0.109153	0.554058	0.394363
C	-0.942150	1.079654	-1.209452
O	-1.538393	1.483817	-2.111476
C	-0.442274	-1.515397	-0.281782
N	-1.698711	-1.997762	-0.575115
C	-1.652141	-3.316835	-0.999803
C	-0.356968	-3.691155	-0.972669
N	0.367839	-2.597062	-0.526156
C	-2.990293	-1.356433	-0.437932
C	-3.577243	-0.737927	-1.538011
C	-4.865767	-0.220552	-1.424629
C	-5.568273	-0.341549	-0.228081
C	-4.986732	-0.993170	0.858597
C	-3.698040	-1.510202	0.753684
C	1.794757	-2.723662	-0.346192
C	2.612451	-2.796681	-1.470605
C	3.978831	-3.006882	-1.307331
C	4.517329	-3.147331	-0.030444
C	3.687409	-3.092109	1.088067
C	2.318823	-2.889724	0.933537
C	1.933831	0.234878	-0.330829
O	3.044306	0.212427	-0.641769
H	1.450036	-0.609611	2.959586
H	1.508328	2.050350	2.625095
H	-1.011309	2.866889	2.004281
H	-2.590764	0.699592	1.957697
H	-1.061123	-1.440076	2.519496
H	-2.542762	-3.855520	-1.271756
H	0.119090	-4.625341	-1.213257
H	2.184237	-2.676710	-2.458650
H	4.621274	-3.056991	-2.177902
H	5.581175	-3.309978	0.093576
H	4.102666	-3.222904	2.080223
H	1.659870	-2.881131	1.792749
H	-3.253121	-2.047261	1.582592
H	-5.540096	-1.113522	1.782298
H	-6.573205	0.055046	-0.147056
H	-5.321237	0.267810	-2.277482
H	-3.034080	-0.659663	-2.470215
H	0.782660	2.213142	-0.113637
Si	1.292839	3.564145	-0.758982
C	1.799783	3.120710	-2.498070
C	-0.174618	4.716942	-0.664149
C	2.718496	4.044588	0.351108
H	0.093130	5.674126	-1.124542
H	-1.035474	4.319656	-1.206208
H	-0.474011	4.922411	0.366067
H	3.189152	4.952193	-0.041988
H	2.392754	4.261909	1.371025
H	3.483262	3.265261	0.384492
H	2.186764	4.016495	-2.995640
H	2.588821	2.366298	-2.509065
H	0.954881	2.753581	-3.084165

S-TS7W

C	-7.616136	-0.456300	-1.837380
C	-6.906065	-0.306502	-0.632191
C	-7.598044	-0.237490	0.592868
C	-8.979486	-0.318202	0.601874
C	-9.678873	-0.467239	-0.601689
C	-9.001221	-0.536441	-1.819448
C	-5.466965	-0.226378	-0.686864
O	-4.739693	-0.092095	0.309112
Si	-2.664280	-0.056364	0.421650
C	-2.774352	0.674917	2.141560
C	-2.467474	1.106574	-1.039256
C	-2.686288	-1.919073	0.160909
W	1.046375	-0.170528	0.663734
C	0.431478	-0.786260	-1.109723
O	0.026901	-1.180835	-2.123958
C	2.826100	0.359839	-0.607797
N	3.725473	-0.520668	-1.175128
C	4.685329	0.141707	-1.930683
C	4.397947	1.455637	-1.859239
N	3.274996	1.577878	-1.052062
C	3.800268	-1.957605	-1.051073
C	2.950940	-2.780809	-1.785847
C	3.099363	-4.163669	-1.701624
C	4.101079	-4.719209	-0.907503
C	4.967791	-3.887934	-0.200660
C	4.821974	-2.504892	-0.275119
C	2.746702	2.889228	-0.770837
C	1.890219	3.489383	-1.689777
C	1.454670	4.791910	-1.463445
C	1.879217	5.484542	-0.331668
C	2.746272	4.878422	0.575122
C	3.190274	3.577918	0.354685

C	2.020281	-0.140183	2.862942
C	0.683028	-0.619328	2.915002
C	0.632168	-1.864935	2.196537
C	1.939578	-2.148230	1.715060
C	2.777589	-1.071207	2.107047
C	0.502674	1.723577	0.725075
O	0.051464	2.767780	0.950286
H	-0.127425	-0.161382	3.458834
H	-0.221855	-2.519327	2.122850
H	2.244259	-3.027023	1.170506
H	3.829113	-0.981966	1.888329
H	2.393514	0.762145	3.321317
H	5.464249	-0.389475	-2.448454
H	4.875450	2.313857	-2.297883
H	-0.742081	-0.085553	0.617463
H	-3.111877	-2.161775	-0.816882
H	-1.690297	-2.354290	0.203983
H	-3.310717	-2.391705	0.923874
H	-3.767185	1.095220	2.312555
H	-2.598111	-0.090371	2.901313
H	-2.035668	1.466805	2.270809
H	-3.418231	1.557543	-1.332090
H	-1.586526	4.579274	0.337370
H	0.299085	-3.496100	0.694473
H	-0.704860	-0.148473	3.799911
H	-4.456475	-2.073442	1.450357
H	-4.990737	-0.389688	1.492621
H	-5.790788	-1.546074	0.421380
H	-2.875921	-3.169058	-1.022387
H	-4.165412	-2.656270	-2.113163
H	-2.511514	-2.088970	-2.380223
H	-4.441792	1.491786	-0.992972
H	-3.566236	0.841319	-2.392493
H	-5.216004	0.307636	-2.048664
H	-0.359516	-2.116974	-1.198271
H	1.663643	-3.385005	-1.159632
H	4.085067	-3.620024	-1.589881
H	5.415809	-1.646638	-2.290321
H	4.310476	0.557489	-2.559634
H	1.882187	0.788784	-2.117755
H	-1.791019	1.919368	-0.773816
H	-2.045129	0.588591	-1.902475
H	-5.007526	-0.287427	-1.684475
H	-7.077555	-0.508843	-2.777685
H	-9.553253	-0.651835	-2.743805
H	-10.760886	-0.529371	-0.586954
H	-9.521385	-0.265754	1.538139
H	-7.037860	-0.121791	1.512198
H	1.569000	2.937813	-2.565150
H	0.785753	5.265342	-2.172156
H	1.538078	6.498167	-0.158199
H	3.081504	5.419180	1.451996
H	3.871394	3.096830	1.046184
H	5.500538	-1.851586	0.260931
H	5.759608	-4.312510	0.404786
H	4.215397	-5.795208	-0.851151
H	2.437518	-4.805831	-2.270484
H	2.187970	-2.349524	-2.418205