

Supporting Information

DFT Study on the Mechanism of Bimetallic Pd–Zn-Catalyzed Cycloaddition of Alkynyl Aryl Ethers with Internal Alkynes

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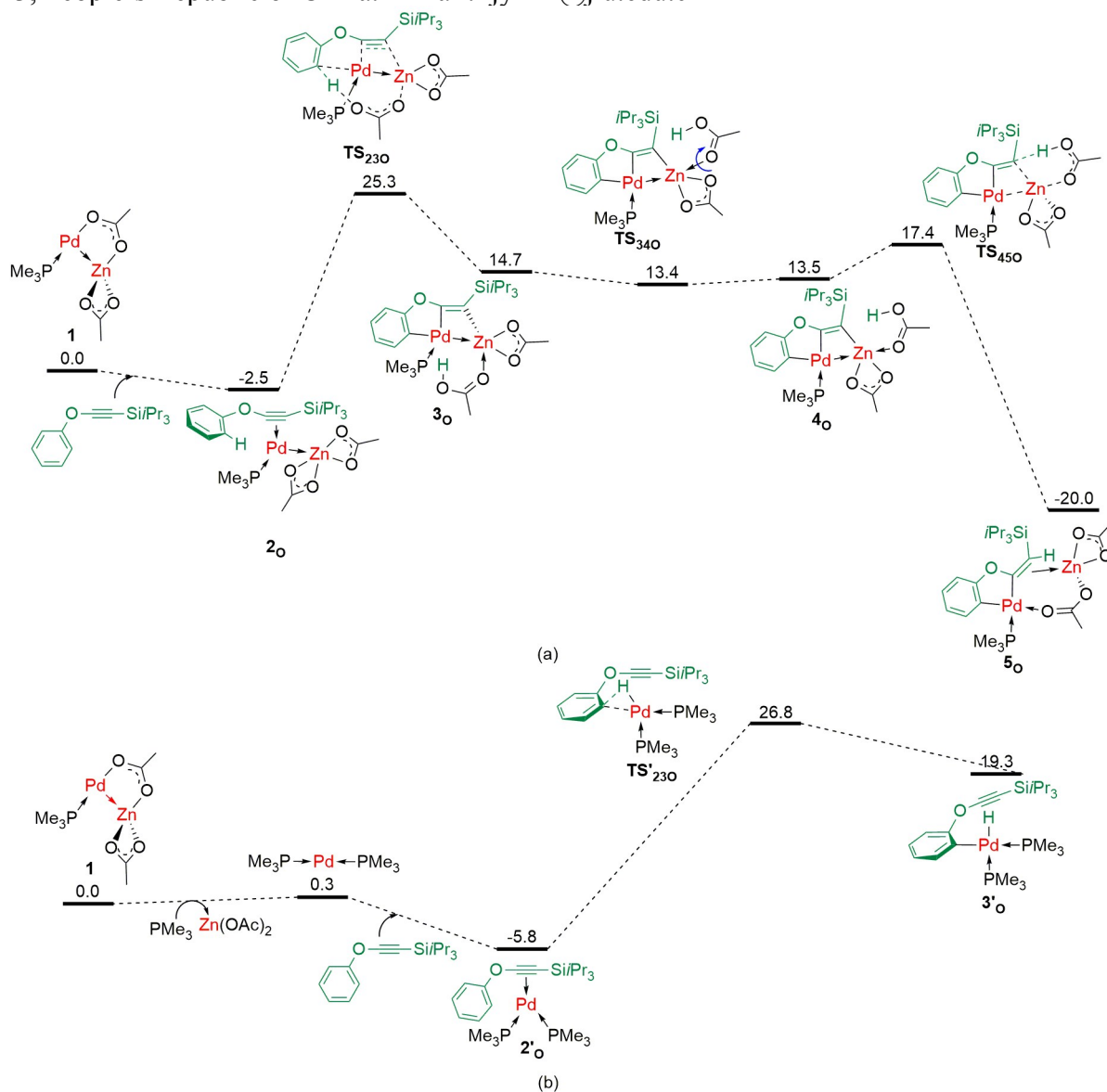


Figure S1. Free energy profiles at ω B97XD/6-311+G(d,p)-SDD-SMD//M06/6-31g(d,p)-LANL2DZ level for (a) bimetallic Pd–Zn complex 1 catalyzed coordination of substrate $C_6H_5OC\equiv CSiPr_3$, C–H activation, acetic acid rotation and H transformation steps and (b) monometallic $Pd(PMe_3)_2$ catalyzed C–H activation step. The free energies are in kcal/mol.

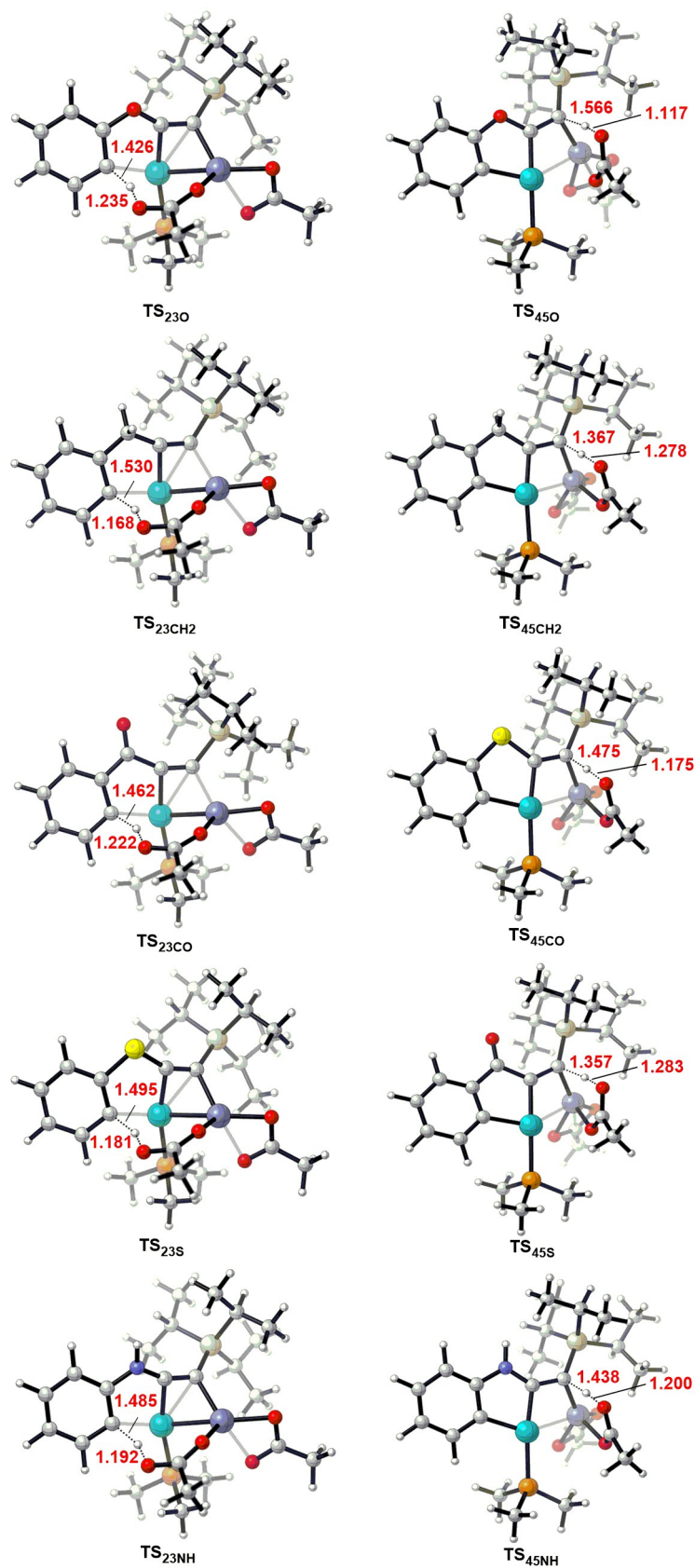


Figure S2. The optimized 3D structures of transition states TS_{23X} and TS_{45X} (X = O, CH₂, CO, S, and NH). The lengths are given in angstrom.

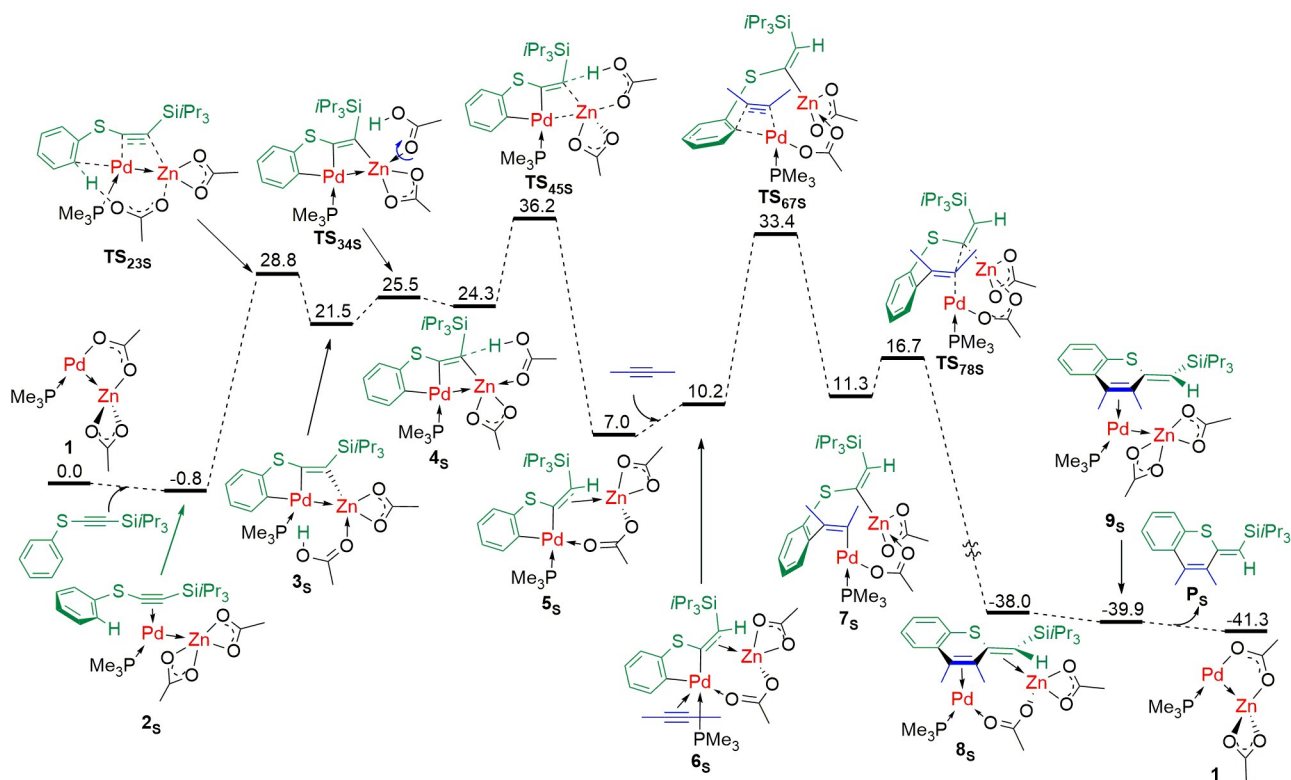


Figure S3. Free energy profile for the reaction of $\text{C}_6\text{H}_5\text{SC}\equiv\text{CSiPr}_3$ with $\text{MeC}\equiv\text{CMe}$ to generate the cycloaddition product P_5 . The free energies are given in kcal/mol.

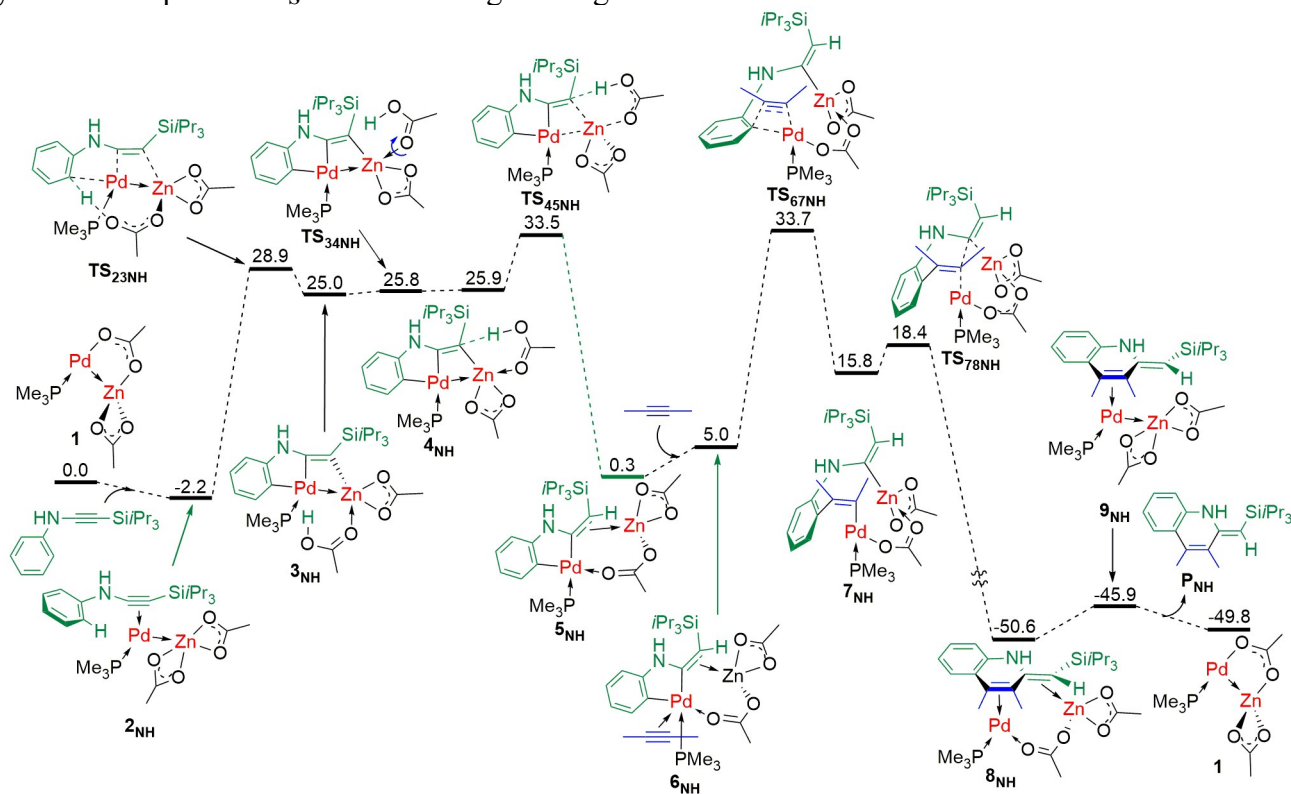


Figure S4. Free energy profile for the reaction of $\text{C}_6\text{H}_5\text{N(H)C}\equiv\text{CSiPr}_3$ with $\text{MeC}\equiv\text{CMe}$ to generate the cycloaddition product P_{NH} . The free energies are given in kcal/mol.

Table S1. Calculated thermodynamic corrections, solution-phase single-point energies in toluene and solution-phase Gibbs free energies in toluene of all the intermediates and transition states at M06/6-311+G(d,p)-SDD-SMD//M06/6-31g(d,p)-LANL2DZ level (in Hartree).

Complexes	Gas-Phase Gibbs Free Energies Corrections	Solution-Phase Single-Point Energies	Solution-Phase Gibbs Free Energies
PdPMe₃	0.079732	-588.9546168	-588.8748848
Pd(PMe₃)₂	0.181006	-1050.028762	-1049.847756
PdPCy₃	0.433120	-1174.718168	-1174.285048
Pd(PCy₃)₂	0.890356	-2221.558495	-2220.668139
Zn(OAc)₂	0.062284	-684.1090987	-684.0468147
1	0.167984	-1273.129937	-1272.961953
1'	0.523707	-1858.899023	-1858.375316
PMe₃	0.083283	-461.0191604	-460.9358774
PCy₃	0.433889	-1046.778242	-1046.344353
C₆H₅OC≡CSiPr₃	0.337631	-1027.768331	-1027.430700
2_O	0.532103	-2300.923950	-2300.391847
TS_{23O}	0.529317	-2300.874390	-2300.345073
3_O	0.532175	-2300.892762	-2300.360587
TS_{34O}	0.531108	-2300.893318	-2300.362210
4_O	0.533357	-2300.894807	-2300.361450
TS_{45O}	0.530214	-2300.884551	-2300.354337
5_O	0.534992	-2300.941322	-2300.406330
2'_O	0.549147	-2077.826032	-2077.276885
TS'_{23O}	0.542735	-2077.771499	-2077.228764
3'_O	0.543041	-2077.780660	-2077.237619
MeC≡CMe	0.057374	-155.8933942	-155.8360202
6_O	0.617411	-2456.838359	-2456.220948
TS_{67O}	0.605666	-2456.802460	-2456.196794
TS_{67Oa}	0.501448	-1995.736908	-1995.235460
TS_{67Ob}	0.576762	-2151.643539	-2151.066777
7_O	0.616280	-2456.839701	-2456.223421
TS_{78O}	0.616260	-2456.832518	-2456.216258
8_O	0.624160	-2456.938718	-2456.314558
9_O	0.623928	-2456.936145	-2456.312217
P_O	0.425511	-1183.782913	-1183.357402
6'_O	0.617411	-2456.838359	-2456.220948
TS'_{67O}	0.611908	-2456.795611	-2456.183703
7'_O	0.619144	-2456.830863	-2456.211719
10_O	0.439149	-1616.764616	-1616.325467
11_O	0.519117	-1772.687515	-1772.168398
TS_{1112O}	0.521797	-1772.652000	-1772.130203
12_O	0.525462	-1772.681966	-1772.156504
TS_{57OR}	0.900958	-3328.687774	-3327.786816

7 _{OR}	0.904178	-3328.724259	-3327.820081
6' _{OR}	0.904297	-3328.708935	-3327.804638
TS' _{67OR}	0.903473	-3328.668923	-3327.765450
7' _{OR}	0.891390	-3328.724008	-3327.832618
C ₆ H ₅ OC≡CSiMe ₃	0.168536	-792.0322286	-791.8636926
2 _{OMe}	0.368537	-2065.186272	-2064.817735
TS _{23OMe}	0.361209	-2065.138461	-2064.777252
3 _{OMe}	0.367540	-2065.158968	-2064.791428
TS _{34OMe}	0.368436	-2065.160337	-2064.791901
4 _{OMe}	0.367158	-2065.161566	-2064.794408
TS _{45OMe}	0.365432	-2065.148622	-2064.783190
5 _{OMe}	0.367571	-2065.204218	-2064.836647
6 _{OMe}	0.444055	-2221.106258	-2220.662203
TS _{67OMe}	0.446340	-2221.067889	-2220.621549
7 _{OMe}	0.448303	-2221.105334	-2220.657031
TS _{78OMe}	0.447351	-2221.096619	-2220.649268
8 _{OMe}	0.455780	-2221.200874	-2220.745094
9 _{OMe}	0.455002	-2221.197497	-2220.742495
P _{OMe}	0.259954	-948.0492885	-947.7893345
6 _{ORMe}	0.570725	-2857.238026	-2856.667301
TS _{67ORMe}	0.568474	-2857.222009	-2856.653535
7 _{ORMe}	0.574095	-2857.259686	-2856.685591
TS _{78ORMe}	0.574987	-2857.249385	-2856.674398
8 _{ORMe}	0.576781	-2857.356876	-2856.780095
9 _{ORMe}	0.573616	-2857.343289	-2856.769673
P _{ORMe}	0.377182	-1584.193316	-1583.816134
C ₆ H ₅ CH ₂ C≡CSiPr ₃	0.360163	-991.8669487	-991.5067857
2 _{CH2}	0.554119	-2265.028090	-2264.473971
TS _{23CH2}	0.551457	-2264.957224	-2264.405767
3 _{CH2}	0.554388	-2264.970912	-2264.416524
TS _{34CH2}	0.553622	-2264.970110	-2264.416488
4 _{CH2}	0.554133	-2264.970095	-2264.415962
TS _{45CH2}	0.552394	-2264.944448	-2264.392054
5 _{CH2}	0.559889	-2265.005797	-2264.445908
10 _{CH2}	0.462278	-1580.834660	-1580.372382
C ₆ H ₅ C(O)C≡CSiPr ₃	0.340319	-1065.877254	-1065.536935
2 _{CO}	0.536778	-2339.032802	-2338.496024
TS _{23CO}	0.532398	-2338.971678	-2338.439280
3 _{CO}	0.535745	-2338.990061	-2338.454316
TS _{34CO}	0.535237	-2338.987008	-2338.451771
4 _{CO}	0.535633	-2338.986940	-2338.451307
TS _{45CO}	0.534649	-2338.960958	-2338.426309
5 _{CO}	0.537990	-2339.024197	-2338.486207
10 _{CO}	0.445270	-1654.855120	-1654.409850
C ₆ H ₅ SC≡CSiPr ₃	0.330700	-1350.751899	-1350.421199
2 _S	0.526884	-2623.911342	-2623.384458
TS _{23S}	0.522351	-2623.859650	-2623.337299
3 _S	0.525145	-2623.874056	-2623.348911
TS _{34S}	0.528952	-2623.871483	-2623.342531

4_s	0.527684	-2623.872057	-2623.344373
TS_{45S}	0.525455	-2623.850895	-2623.325440
5_s	0.533469	-2623.905469	-2623.372000
6_s	0.609557	-2779.812530	-2779.202973
TS_{67S}	0.608377	-2779.774263	-2779.165886
7_s	0.616013	-2779.817204	-2779.201191
TS_{78S}	0.616299	-2779.808797	-2779.192498
8_s	0.617500	-2779.897309	-2779.279809
9_s	0.616841	-2779.899677	-2779.282836
10_s	0.436113	-1939.734991	-1939.298878
P_s	0.421656	-1506.744767	-1506.323111
C₆H₅N(H)C≡CSiPr₃	0.347238	-1007.912872	-1007.565634
2_{NH}	0.543507	-2281.074642	-2280.531135
TS_{23NH}	0.539402	-2281.020926	-2280.481524
3_{NH}	0.544734	-2281.032527	-2280.487793
TS_{34NH}	0.543164	-2281.029565	-2280.486401
4_{NH}	0.545689	-2281.031970	-2280.486281
TS_{45NH}	0.543727	-2281.017868	-2280.474141
5_{NH}	0.549893	-2281.076947	-2280.527054
6_{NH}	0.625609	-2436.981317	-2436.355708
TS_{67NH}	0.625979	-2436.935931	-2436.309952
7_{NH}	0.629185	-2436.967597	-2436.338412
TS_{78NH}	0.627965	-2436.962311	-2436.334346
8_{NH}	0.635478	-2437.079752	-2436.444274
9_{NH}	0.635318	-2437.072031	-2436.436713
10_{NH}	0.450914	-1596.895550	-1596.444636
P_{NH}	0.437986	-1163.919005	-1163.481019
TS_{23O-PCy3}	0.884748	-2886.647207	-2885.762459
2_{S-PCy3}	0.885123	-3209.686051	-3208.800928
TS_{45S-PCy3}	0.876500	-3209.615520	-3208.739020
2_{NH-PCy3}	0.900325	-2866.850240	-2865.949915
TS_{45NH-PCy3}	0.889404	-2866.785416	-2865.896012

Table S2. Calculated thermodynamic corrections, solution-phase single-point energies in toluene and solution-phase Gibbs free energies in toluene of several intermediates and transition states at ω B97XD/6-311+G(d,p)-SDD-SMD//M06/6-31g(d,p)-LANL2DZ level (in Hartree).

Complexes	Gas-Phase Gibbs Free Energies Corrections	Solution-Phase Single-Point Energies	Solution-Phase Gibbs Free Energies
1	0.167984	-1273.294735	-1273.126751
C₆H₅OC≡CSiPr₃	0.337631	-1028.113930	-1027.776299
2_O	0.532103	-2301.439115	-2300.907012
TS₂₃₀	0.529317	-2301.392110	-2300.862793
3_O	0.532175	-2301.411793	-2300.879618
TS₃₄₀	0.531108	-2301.412865	-2300.881757
4_O	0.533357	-2301.414883	-2300.881526
TS₄₅₀	0.530214	-2301.405551	-2300.875337
5_O	0.534992	-2301.469939	-2300.934947
PMe₃	0.083283	-461.1029837	-461.0197007
Zn(OAc)₂	0.062284	-684.1814199	-684.1191359
Pd(PMe₃)₂	0.181006	-1050.207767	-1050.026761
2'_O	0.549147	-2078.361972	-2077.812825
TS'₂₃₀	0.542735	-2078.303586	-2077.760851
3'_O	0.543041	-2078.315759	-2077.772718

Cartesian coordinates for all of the calculated structures

PdPMe₃

Pd	2.677842	-0.177965	-2.052277
P	0.839149	-0.384185	-3.294123
C	0.602044	0.815310	-4.670914
H	0.582787	1.832951	-4.268553
H	1.443940	0.744094	-5.366601
H	-0.333793	0.622685	-5.213442
C	0.589969	-1.970893	-4.194303
H	-0.345612	-1.962076	-4.770221
H	1.430563	-2.140839	-4.874386
H	0.564866	-2.797405	-3.477322
C	-0.785923	-0.230965	-2.442275
H	-1.619806	-0.346329	-3.148306
H	-0.863695	-0.996352	-1.663753
H	-0.854035	0.749096	-1.959789

Pd (PMe₃)₂

Pd	2.386631	4.420709	-1.393741
P	3.567093	6.221042	-0.531979
C	2.611612	7.469741	0.429293
H	3.257647	8.278877	0.795720
H	1.826114	7.893723	-0.204387
H	2.128513	6.980240	1.281013
C	4.445893	7.324973	-1.716134
H	3.727750	7.737627	-2.431877
H	4.953900	8.148718	-1.197180
H	5.183626	6.742855	-2.277496
C	4.930439	5.873351	0.657811
H	5.402827	6.799678	1.011448
H	4.533644	5.320871	1.515461
H	5.685321	5.245817	0.173332
P	1.194191	2.633439	-2.266809
C	-0.178779	1.938065	-1.253345
H	-0.674363	1.101954	-1.764806
H	0.216682	1.589791	-0.293749
H	-0.914631	2.722407	-1.049251
C	2.120679	1.089073	-2.655196
H	2.600770	0.715005	-1.745305
H	1.457205	0.313021	-3.059666
H	2.906362	1.308319	-3.385128
C	0.314370	2.897806	-3.863866
H	-0.205803	1.988643	-4.194083
H	-0.413622	3.706960	-3.746694
H	1.033589	3.201124	-4.631289

PdPCy₃

Pd	2.350035	4.414789	-1.411167
P	1.212283	2.663900	-2.262936
C	2.362001	1.380452	-2.997098
C	0.193634	1.802413	-0.945291
C	0.030179	3.200212	-3.615829
C	3.182877	0.737505	-1.872982
C	1.804024	0.325936	-3.957175
H	3.061889	2.009119	-3.576248
C	-0.890331	2.763919	-0.444711
C	-0.378089	0.403633	-1.204540
H	0.927913	1.706164	-0.125417
C	0.835331	3.729807	-4.808294
C	-1.090175	2.257991	-4.068351
H	-0.453519	4.077611	-3.150029
C	4.281967	-0.162342	-2.427130
H	2.521985	0.133277	-1.229571
H	3.604168	1.528417	-1.234974
C	2.921365	-0.567894	-4.492084
H	1.051045	-0.296521	-3.451399
H	1.292243	0.809945	-4.799106
C	-1.605352	2.211310	0.783100
H	-1.636664	2.931402	-1.239212
H	-0.435488	3.742226	-0.229523
C	-1.103567	-0.125985	0.032245
H	-1.079112	0.422588	-2.052582
H	0.424552	-0.292574	-1.481536
C	-0.068478	4.382047	-5.848792
H	1.380534	2.899909	-5.287766
H	1.595105	4.437616	-4.445060

C	-1.973520	2.926239	-5.120754
H	-0.673673	1.327911	-4.483711
H	-1.708908	1.964738	-3.210639
C	3.704718	-1.219755	-3.360354
H	4.835938	-0.631364	-1.603590
H	5.007552	0.453536	-2.982300
H	2.504115	-1.327786	-5.165694
H	3.607937	0.044430	-5.099292
C	-2.190199	0.833482	0.498641
H	-2.389464	2.907030	1.108945
H	-0.887215	2.135453	1.615509
H	-1.524367	-1.118111	-0.177823
H	-0.371749	-0.263536	0.844971
C	-1.156279	3.418801	-6.307750
H	0.528613	4.729339	-6.701951
H	-0.538411	5.276855	-5.409846
H	-2.756016	2.229631	-5.449174
H	-2.491294	3.783653	-4.660733
H	4.501086	-1.860429	-3.760383
H	3.030356	-1.877748	-2.787281
H	-2.699007	0.436300	1.386434
H	-2.957181	0.922059	-0.288892
H	-1.807041	3.894779	-7.052558
H	-0.686973	2.555097	-6.807930

Pd(PCy₃)₂

Pd	2.482508	4.420334	-1.475115
P	3.624945	6.244605	-0.550769
C	4.007346	5.924801	1.253773
C	5.246209	6.585281	-1.421974
C	2.586440	7.797372	-0.652321
C	5.008161	4.764952	1.339535
C	4.398714	7.073311	2.187651
H	3.041237	5.527664	1.615445
C	4.949264	7.004001	-2.867272
C	6.302177	7.495757	-0.788584
H	5.680806	5.570330	-1.475684
C	1.313025	7.592481	0.178922
C	3.207971	9.170526	-0.386545
H	2.269516	7.780681	-1.711285
C	5.191255	4.288403	2.775517
H	5.987754	5.090049	0.950822
C	4.666881	3.943836	0.690349
H	4.594774	6.572287	3.617652
H	5.326462	7.552144	1.841832
H	3.626852	7.853334	2.179857
C	6.221643	7.050719	-3.705383
H	4.486166	8.005214	-2.874698
H	4.213666	6.311086	-3.303662
C	7.566157	7.539696	-1.645471
H	5.909903	8.517511	-0.673949
H	6.558247	7.146403	0.220237
C	0.310217	8.717056	-0.049054
H	1.570113	7.563267	1.250928
C	0.873362	6.613651	-0.066763
H	2.185300	10.285090	-0.601034
H	3.594450	9.223971	0.642241
H	4.066330	9.337582	-1.049286
C	5.612132	5.440167	3.680075
H	5.927826	3.475257	2.813585
H	4.240500	3.868384	3.141700
H	4.896671	7.403836	4.267995
H	3.629034	6.207843	4.004538
C	7.258109	7.972177	-3.073672
H	5.989074	7.372080	-4.729093
H	6.639693	6.034216	-3.783376
H	8.307193	8.208732	-1.188516
H	8.020831	6.535738	-1.664255
C	0.937336	10.073744	0.247091
H	-0.582911	8.558278	0.569265
H	-0.026289	8.694299	-1.098151
H	2.642157	11.260045	-0.385586
H	1.897188	10.304378	-1.664929
H	5.742432	5.095350	4.714094
H	6.593824	5.817826	3.348598
H	8.175559	7.995414	-3.676074
H	6.864786	9.002372	-3.061609
H	0.214072	10.882161	0.078566

H	1.214700	10.117142	1.313549	H	3.919034	1.218243	-8.144085
P	1.250959	2.620843	-2.319349	H	2.487933	2.073362	-7.547123
C	2.334685	1.246624	-2.983681	H	4.052144	2.902034	-7.521635
C	0.164090	1.880242	-0.986263	O	4.492116	-0.142438	-0.934004
C	0.128864	3.166752	-3.717462	C	5.586970	0.072504	-1.507658
C	3.129533	0.630255	-1.826296	O	5.737740	0.350091	-2.743039
C	1.733040	0.167617	-3.886687	C	6.847524	0.010428	-0.689995
H	3.061806	1.814695	-3.592465	H	7.528338	-0.724698	-1.129724
C	-0.852191	2.937223	-0.535658	H	7.353430	0.979694	-0.736506
C	-0.502481	0.517253	-1.194929	H	6.632375	-0.249564	0.347162
H	0.882385	1.767967	-0.153575	P	0.805028	-0.367964	-3.307276
C	0.995660	3.587776	-4.910753	C	0.586300	0.825698	-4.685626
C	-1.044337	2.285487	-4.157635	H	0.758710	1.850261	-4.341908
H	-0.302266	4.096720	-3.303921	H	1.325306	0.585569	-5.458702
C	4.189630	-0.341848	-2.332993	H	-0.420209	0.742660	-5.114908
H	2.445960	0.085722	-1.153333	C	0.628534	-1.956616	-4.205625
H	3.583761	1.435553	-1.229012	H	-0.299068	-1.980188	-4.791923
C	2.809217	-0.799612	-4.375312	H	1.484911	-2.074470	-4.878546
H	0.957591	-0.397402	-3.347393	H	0.631982	-2.789480	-3.495928
H	1.236569	0.628535	-4.750403	C	-0.802707	-0.229967	-2.428941
C	-1.617463	2.486973	0.703238	H	-1.640735	-0.372590	-3.123040
H	-1.574925	3.127886	-1.346718	H	-0.857859	-0.984290	-1.637841
C	-0.327325	3.887432	-0.351987	H	-0.883282	0.758158	-1.965375
H	-1.277965	0.091274	0.050323				
H	-1.185858	0.548445	-2.057367	1'			
H	0.252337	-0.245434	-1.425846	Pd	2.508587	-0.106940	-2.018460
C	0.164067	4.249569	-6.004184	Zn	4.189155	0.646883	-3.658735
H	1.494058	2.701895	-5.337940	O	4.050503	2.076066	-5.178213
H	1.793402	4.260130	-4.559163	C	4.183316	1.135610	-6.018505
C	-1.854593	2.966264	-5.259344	O	4.373548	-0.056906	-5.628046
H	-0.684473	1.311379	-4.523563	C	4.051147	1.432123	-7.481175
H	-1.700061	2.071374	-3.303703	H	4.327534	0.566278	-8.086108
C	3.567933	-1.421891	-3.210318	H	3.006482	1.699277	-7.684067
H	4.725832	-0.790781	-1.486645	H	4.660726	2.299520	-7.747867
H	4.938708	0.214372	-2.919252	O	4.263888	0.016573	-0.777596
H	2.357906	-1.577319	-5.005406	O	5.404702	0.342787	-1.182634
H	3.519253	-0.251446	-5.015993	O	5.704205	0.670503	-2.378607
C	-2.297083	1.144004	0.466947	C	6.538162	0.362201	-0.193851
H	-2.352969	3.249559	0.990896	H	7.341475	-0.288635	-0.551843
H	-0.914928	2.394332	1.547284	H	6.949610	1.374843	-0.138950
H	-1.767424	-0.875833	-0.125372	H	6.205680	0.040894	0.794083
H	-0.565905	-0.066122	0.877100	P	0.721694	-0.214785	-3.443491
C	-0.977545	3.342087	-6.446218	C	-0.455666	-1.436677	-2.657355
H	0.803047	4.514241	-6.856826	C	-0.133452	1.441377	-3.566272
H	-0.252682	5.194495	-5.619624	C	1.102640	-0.797797	-5.171487
H	-2.680237	2.315169	-5.575588	C	-0.908946	-0.889969	-1.296939
H	-2.316284	3.880434	-4.851508	C	-1.637713	-1.982751	-3.464618
H	4.336617	-2.115119	-3.575906	H	0.214413	-2.290410	-2.447661
H	2.868316	-2.021299	-2.603816	C	0.712938	2.396289	-4.418051
H	-2.841141	0.820319	1.363833	C	-1.609493	1.490146	-3.974942
H	-3.049055	1.255975	-0.332103	H	-0.072150	1.807941	-2.525565
H	-1.575159	3.824535	-7.230531	C	1.688732	-2.213997	-5.123864
H	-0.558487	2.424121	-6.891336	C	0.037149	-0.670829	-6.263849
				H	1.937104	-0.137956	-5.463700
Zn(OAc) ₂				C	-1.697650	-1.930290	-0.510291
Zn	1.463138	-1.241913	-2.501610	H	-1.544430	-0.002032	-1.446551
O	0.662623	-2.513302	-1.130333	H	-0.034466	-0.551560	-0.720208
C	-0.463884	-2.316946	-1.687083	C	-2.421023	-3.011858	-2.651250
O	-0.541705	-1.538378	-2.688356	H	-2.311948	-1.165992	-3.762601
C	-1.687619	-2.978992	-1.145135	H	-1.282268	-2.446988	-4.393075
H	-2.006155	-2.440592	-0.246201	C	0.162754	3.816750	-4.370238
H	-2.497086	-2.956503	-1.875817	H	0.717341	2.054286	-5.467187
H	-1.456674	-4.004240	-0.847250	H	1.761206	2.380143	-4.089128
O	2.670904	0.390705	-2.423099	C	-2.136623	2.923156	-3.930783
C	3.386977	-0.161647	-3.317893	H	-1.742367	1.088504	-4.990730
O	3.057339	-1.302388	-3.769056	H	-2.213538	0.859172	-3.310145
C	4.608891	0.534036	-3.820579	C	2.251401	-2.614590	-6.483475
H	4.342366	1.541889	-4.150914	H	0.904278	-2.932119	-4.830181
H	5.319524	0.646186	-2.995913	H	2.469177	-2.265366	-4.350146
H	5.071617	-0.024157	-4.634864	C	0.613059	-1.088399	-7.615974
				H	-0.835192	-1.299424	-6.030537
1				H	-0.330217	0.361786	-6.327405
Pd	2.611385	-0.249656	-1.960627	C	-2.884864	-2.439391	-1.318208
Zn	4.063543	0.557877	-3.783452	H	-2.029796	-1.505677	0.445564
O	3.951256	2.208647	-5.050286	H	-1.035694	-2.776120	-0.264753
C	3.782977	1.404643	-6.013602	H	-3.274932	-3.375806	-3.236952
O	3.747399	0.149450	-5.808331	H	-1.776404	-3.885810	-2.463322
C	3.565410	1.932753	-7.398179	C	-1.298898	3.853719	-4.797979

H	0.773607	4.472789	-5.002699	H	0.030455	-2.216113	2.788107
H	0.250286	4.202924	-3.342121	H	-1.650152	-1.920627	2.342448
H	-3.189292	2.941919	-4.241305	H	-7.843541	1.568954	-0.115872
H	-2.111912	3.281690	-2.888874	H	-6.718840	1.341803	-1.454943
C	1.187911	-2.498511	-7.568468	H	-0.448136	1.629300	-5.545325
H	2.647848	-3.636948	-6.438434	H	-0.225199	0.515465	-4.195582
H	3.100144	-1.952798	-6.717231				
H	-0.158590	-1.005642	-8.392415	C ₆ H ₅ OC≡CSiPr ₃			
H	1.414324	-0.382828	-7.894583	C	0.317098	-1.746678	-0.514020
H	-3.445990	-3.192207	-0.750329	C	0.332041	-0.477766	-1.082560
H	-3.580223	-1.604362	-1.505421	C	1.225998	0.491708	-0.635838
H	-1.690841	4.877773	-4.753060	C	2.098875	0.158014	0.388700
H	-1.376632	3.534094	-5.850537	C	2.106149	-1.101199	0.972463
H	1.600948	-2.776703	-8.546490	C	1.206511	-2.053973	0.513188
H	0.372449	-3.211113	-7.359089	H	-0.385315	-2.495634	-0.870296
				H	-0.358773	-0.231773	-1.885368
PMe ₃				H	1.248912	1.488804	-1.070873
P	-0.797599	-0.141558	-0.015555	H	1.201515	-3.044016	0.962506
C	0.107406	0.707138	-1.396675	O	3.029630	1.059461	0.904628
H	-0.048755	0.161801	-2.333560	C	3.062360	2.263826	0.422911
H	-0.285237	1.720660	-1.531108	C	3.097016	3.399970	-0.017136
H	1.186453	0.770081	-1.202050	Si	3.064394	5.089460	-0.734300
C	0.277262	-1.648500	0.116524	C	3.047562	4.949030	-2.635956
H	0.007820	-2.219185	1.011699	H	1.979810	4.884372	-2.909865
H	0.117630	-2.296339	-0.752026	C	1.464884	5.907598	-0.120878
H	1.343220	-1.389753	0.171213	H	1.573934	5.974044	0.974367
C	-0.079137	0.820075	1.399605	C	4.590447	6.019168	-0.096999
H	-0.474132	1.841616	1.392752	H	4.591006	7.005386	-0.591006
H	-0.369669	0.357195	2.348811	C	4.508248	6.232854	1.413333
H	1.017107	0.866226	1.350638	H	4.435614	5.271681	1.941834
				H	5.405032	6.743926	1.790415
PCy ₃				H	3.638959	6.835981	1.704060
P	-2.097051	2.387825	-0.034763	C	5.882884	5.291720	-0.464414
C	-1.144351	0.936867	0.688992	H	6.763493	5.834280	-0.093218
C	-3.921841	2.020369	0.244042	H	5.905714	4.287492	-0.019338
C	-1.830390	2.318600	-1.894185	H	6.003342	5.171614	-1.548807
C	-1.493470	0.841251	2.180864	C	0.244827	5.039661	-0.420225
C	-1.149283	-0.447958	0.033679	H	0.341058	4.037905	0.016596
H	-0.101949	1.304529	0.641237	H	-0.674785	5.492860	-0.024545
C	-4.737561	3.055288	-0.542841	H	0.098347	4.917740	-1.503579
C	-4.503173	0.614090	0.064468	C	1.279739	7.317029	-0.679218
H	-4.045244	2.276921	1.313018	H	2.134351	7.972303	-0.463342
C	-0.321701	2.393736	-2.163885	H	1.148756	7.293381	-1.770676
C	-2.491304	1.240121	-2.757310	H	0.383692	7.797194	-0.262137
H	-2.251511	3.287454	-2.222648	C	3.738782	3.690480	-3.157001
C	-0.584641	-0.139154	2.914142	H	4.804240	3.678603	-2.887616
H	-2.537453	0.505149	2.296055	H	3.295829	2.776687	-2.744267
H	-1.437500	1.838361	2.640904	H	3.680223	3.633612	-4.253043
C	-0.244911	-1.421367	0.788950	C	3.628597	6.195284	-3.306601
H	-2.170289	-0.855824	0.004047	H	3.523032	6.139934	-4.398870
H	-0.814657	-0.379934	-1.009705	H	3.144722	7.123679	-2.977099
C	-6.217813	3.004811	-0.181553	H	4.701938	6.294976	-3.093813
H	-4.632320	2.860305	-1.622997	H	2.812450	-1.309526	1.771432
H	-4.330178	4.061822	-0.369238				
C	-5.988128	0.583486	0.423345	2o			
H	-4.376123	0.274224	-0.974375	C	-3.963284	3.730487	-0.420588
H	-3.963543	-0.105493	0.693788	C	-2.710394	4.272318	-0.699597
C	-0.018384	2.586506	-3.645620	C	-1.574982	3.760201	-0.080480
H	0.158420	1.460357	-1.826886	C	-1.725828	2.709753	0.810911
H	0.123994	3.203483	-1.568308	C	-2.955412	2.144186	1.103351
C	-2.168037	1.442066	-4.236687	C	-4.082339	2.671029	0.475472
H	-2.153966	0.240463	-2.445570	H	-4.849431	4.136236	-0.902626
H	-3.580017	1.256452	-2.617161	H	-2.615164	5.100641	-1.397308
C	-0.628209	-1.514309	2.260267	H	-0.582731	4.160837	-0.276688
H	-0.870445	-0.202205	3.972385	H	-5.059344	2.241819	0.686879
H	0.449842	0.240045	2.890793	O	-0.588014	2.206176	1.466040
H	-0.280698	-2.411166	0.314859	C	0.249423	1.529280	0.721897
H	0.799187	-1.076094	0.710969	C	1.305330	1.017750	0.277266
C	-6.779940	1.603134	-0.385311	Si	3.099137	0.714322	-0.109445
H	-6.778774	3.738399	-0.775410	C	3.343625	-0.324337	-1.691225
H	-6.342753	3.294361	0.874301	H	3.384211	0.417551	-2.507913
H	-6.390911	-0.427165	0.274637	C	3.822280	2.453731	-0.381394
H	-6.102413	0.809851	1.496260	H	3.651814	2.980137	0.572897
C	-0.664635	1.486478	-4.478710	C	3.843656	-0.107076	1.426702
H	1.066883	2.612224	-3.809948	H	4.903464	-0.300946	1.187707
H	-0.408049	3.564334	-3.971915	Pd	-0.355880	0.148593	-0.840118
H	-2.634854	0.649151	-4.835850	C	3.782249	0.818527	2.640297
H	-2.613766	2.391993	-4.575118				

H	2.740131	1.067900	2.886919	H	-5.369005	0.948013	1.655297
H	4.210276	0.328960	3.525852	C	-2.855059	-1.459559	1.526651
H	4.327164	1.758868	2.487325	H	-3.229919	-2.041761	2.380726
C	3.155893	-1.434966	1.743729	H	-3.164363	-1.985403	0.611891
H	3.673814	-1.959202	2.558536	H	-1.758117	-1.484750	1.572079
H	2.124685	-1.264953	2.081878	C	-3.918819	-0.361936	-2.005553
H	3.106038	-2.118380	0.886693	H	-4.202132	-1.150777	-1.297089
C	3.076872	3.211332	-1.477452	H	-4.618977	-0.405605	-2.851186
H	1.998340	3.259744	-1.280114	H	-2.927706	-0.633898	-2.393319
H	3.449829	4.240385	-1.576652	C	-3.485922	2.078576	-2.404719
H	3.210498	2.729476	-2.456820	H	-3.559842	3.102299	-2.016413
C	5.322884	2.432656	-0.664434	H	-2.446993	1.923054	-2.730882
H	5.893906	1.911414	0.115341	H	-4.115998	2.020417	-3.303048
H	5.535433	1.932358	-1.620017	C	-1.642711	3.043076	1.931230
H	5.727953	3.451273	-0.742614	H	-1.988972	2.495479	2.819550
C	2.240388	-1.325802	-2.030313	H	-0.638955	2.669063	1.688767
H	2.061158	-2.041901	-1.217437	H	-1.541455	4.097160	2.225462
H	1.278050	-0.825290	-2.238208	C	-3.975956	3.503300	1.137245
C	2.506333	-1.900358	-2.930383	H	-3.872554	4.566128	1.396814
C	4.696561	-1.042543	-1.648497	H	-4.709768	3.434433	0.323424
H	4.906381	-1.532897	-2.608980	H	-4.407848	3.004733	2.017099
H	5.536254	-0.368200	-1.436245	Zn	-0.364293	-1.387551	-0.791652
H	4.701561	-1.826193	-0.879157	O	-0.198573	-3.286707	0.158498
Zn	-0.707429	-1.635136	0.982516	C	-1.204566	-3.646601	-0.523518
O	0.654439	-3.138954	0.373416	O	-1.756140	-2.840310	-1.332736
C	-0.314388	-3.758848	-0.152319	C	-1.790823	-5.012802	-0.336819
O	-1.503631	-3.333166	-0.024392	H	-1.052085	-5.704440	0.072320
C	-0.042536	-4.972681	-0.990179	H	-2.622268	-4.933320	0.373813
H	-0.949647	-5.560781	-1.142343	H	-2.195125	-5.387322	-1.279866
H	0.328068	-4.633449	-1.965996	O	1.101913	-1.524920	-2.188705
O	0.743874	-5.581543	-0.537930	C	2.338588	-1.361040	-2.328969
O	-0.244133	-1.142680	2.951559	C	3.059918	-0.484041	-1.756506
C	-1.432332	-0.738443	3.123888	C	3.067042	-2.310843	-3.240115
O	-2.288533	-0.834845	2.193211	H	3.994181	-1.869887	-3.610905
C	-1.815052	-0.080909	4.415539	H	3.317974	-3.209569	-2.664089
H	-2.866205	-0.267163	4.647207	H	2.419488	-2.616901	-4.064771
H	-1.170717	-0.415254	5.230763	H	2.589535	0.427233	-1.068140
H	-1.680970	1.001197	4.294163	P	2.085417	-1.311967	2.037510
H	-3.009689	1.286522	1.773800	C	1.136616	-2.488147	3.077263
P	-2.317105	-0.604156	-1.859261	H	0.492320	-1.936152	3.769396
C	-2.178189	-2.040244	-2.991352	H	0.508423	-3.095245	2.415929
H	-1.377238	-1.870135	-3.718641	H	1.810478	-3.139275	3.648864
H	-1.932231	-2.916735	-2.380441	C	3.150927	-2.458717	1.076409
H	-3.120947	-2.219867	-3.523262	H	3.740568	-3.106786	1.737199
C	-3.753936	-1.071277	-0.823944	H	2.506145	-3.079502	0.443464
H	-4.639062	-1.237041	-1.451441	H	3.817986	-1.876230	0.430187
H	-3.516524	-1.986538	-0.271887	C	3.281719	-0.612308	3.244999
H	-3.953634	-0.274619	-0.099158	H	3.821464	-1.404468	3.779391
C	-3.031621	0.707812	-2.928147	H	3.997709	0.022289	2.711949
H	-3.954729	0.367386	-3.414973	H	2.749796	0.012983	3.969126
H	-3.249010	1.586429	-2.308319				
H	-2.304205	0.999093	-3.692781				
				3o			
				C	-4.123108	3.701848	0.187767
				C	-3.249530	4.609025	0.779380
				C	-1.925432	4.250868	1.020251
				C	-1.529858	2.974509	0.657629
				C	-2.363967	2.020836	0.062087
				C	-3.678821	2.427522	-0.173089
				H	-5.158101	3.985658	0.006732
				H	-3.596141	5.602133	1.055711
				H	-1.216608	4.940374	1.471804
				H	-4.382800	1.737577	-0.639087
				O	-0.210312	2.597335	0.920321
				C	0.054712	1.388097	0.444122
				C	1.066596	0.565767	0.272627
				Si	2.819734	1.048464	-0.195858
				C	2.766803	2.858053	-0.786123
				H	2.390114	3.440336	0.070728
				C	3.902624	0.909666	1.361400
				H	4.944604	1.086940	1.046209
				C	3.465449	-0.040969	-1.628250
				H	3.234668	0.544139	-2.534976
				Pd	-1.290229	0.318064	-0.557217
				C	4.983521	-0.217430	-1.561006
				H	5.271219	-0.826289	-0.692876
				H	5.360078	-0.733684	-2.455193
				H	5.519503	0.737148	-1.482433
				C	2.785800	-1.398766	-1.776591
TS₂₃₀							
C	4.269569	3.399522	-0.079702				
C	3.428036	4.390046	-0.582640				
C	2.136887	4.072729	-0.995148				
C	1.739109	2.752402	-0.886678				
C	2.541210	1.701299	-0.428646				
C	3.826962	2.081602	-0.009914				
H	5.277274	3.656794	0.239260				
H	3.774571	5.418581	-0.650547				
H	1.451773	4.827275	-1.372540				
H	4.511933	1.304156	0.334040				
O	0.411374	2.457272	-1.265299				
C	-0.053988	1.397261	-0.661777				
C	-1.059254	0.607922	-0.415239				
Si	-2.783646	1.095541	0.156551				
C	-2.624362	2.891462	0.770416				
H	-2.214077	3.442802	-0.093598				
C	-3.902439	1.028820	-1.375408				
H	-4.921705	1.268615	-1.028002				
C	-3.396641	-0.033872	1.561910				
H	-3.022968	0.444230	2.484055				
Pd	1.078477	0.296963	0.610276				
C	-4.926040	-0.055344	1.624928				
H	-5.346592	-0.572195	0.751461				
H	-5.273939	-0.595549	2.516082				

H	3.172293	-1.938057	-2.653346	H	2.333780	-0.854677	2.140686
H	2.971225	-2.038110	-0.901288	C	2.640666	3.497619	1.293108
H	1.698088	-1.305291	-1.909537	H	3.124923	2.936083	2.102838
C	3.817440	-0.478355	1.991266	H	2.917147	4.554375	1.416970
H	4.059047	-1.287963	1.290097	H	1.555817	3.426654	1.438127
H	4.499263	-0.568344	2.848488	C	2.435736	3.850559	-1.192027
H	2.803563	-0.674204	2.369619	H	2.822910	3.588965	-2.184644
C	3.518165	1.979675	2.382218	H	1.343552	3.753871	-1.220830
H	3.678853	2.997711	2.005725	H	2.662443	4.912873	-1.022730
H	2.456723	1.896104	2.658395	C	2.512203	-0.729765	-2.522969
H	4.102406	1.872775	3.307053	H	3.024408	-1.510668	-1.941772
C	1.813140	3.076704	-1.959420	H	1.429180	-0.845234	-2.369478
H	2.139971	2.519928	-2.849471	H	2.707203	-0.933796	-3.585446
H	0.785952	2.762143	-1.736316	C	4.457099	0.852209	-2.538548
H	1.779240	4.137686	-2.244107	H	4.602323	0.680282	-3.614329
C	4.163842	3.370287	-1.139009	H	4.831716	1.859933	-2.314918
H	4.137393	4.432853	-1.418681	H	5.099262	0.132761	-2.010399
H	4.876909	3.267754	-0.310294	Zn	0.627119	-1.361266	0.186249
H	4.578355	2.826977	-2.000825	O	-0.829123	0.032963	2.956490
Zn	0.493097	-1.423381	0.513543	C	-0.593834	-1.257146	3.033002
O	0.050933	-3.329053	-0.332670	O	-0.150548	-1.940026	2.111346
C	1.044321	-3.785041	0.311191	C	-0.945052	-1.837192	4.360857
O	1.746644	-3.016859	1.033686	H	-2.033620	-1.950607	4.413910
C	1.404788	-5.237288	0.224892	H	-0.476812	-2.814539	4.478565
H	0.759790	-5.766747	-0.477991	H	-0.648569	-1.159630	5.165096
H	2.451811	-5.331601	-0.078496	O	0.326519	-3.230969	-0.773392
H	1.319432	-5.688129	1.218548	C	1.529392	-3.516806	-0.488450
O	-0.819006	-1.685532	2.192730	O	2.244055	-2.697642	0.163656
C	-1.905179	-1.387556	2.682314	C	2.134005	-4.805377	-0.953972
O	-2.767091	-0.553683	2.151389	H	2.690167	-5.273117	-0.137380
C	-2.380393	-1.960825	3.977159	H	1.373597	-5.485523	-1.340692
H	-3.349495	-2.446825	3.829908	H	2.854629	-4.580871	-1.748509
H	-1.652080	-2.673200	4.364436	H	-0.674657	0.367908	2.041804
H	-2.534584	-1.150597	4.696417	P	-2.911002	-1.807014	-0.872240
H	-2.416860	-0.134440	1.315033	C	-2.893713	-3.178453	0.349265
P	-2.454855	-1.343347	-1.816048	H	-1.870138	-3.559978	0.429461
C	-1.526607	-2.340594	-3.045891	H	-3.208441	-2.803269	1.329309
H	-1.049165	-1.676917	-3.774134	H	-3.563338	-3.990525	0.039207
H	-0.750891	-2.901048	-2.512310	C	-4.712592	-1.517671	-1.083454
H	-2.188880	-3.039980	-3.572330	H	-5.235086	-2.445862	-1.347617
C	-3.249427	-2.656035	-0.807185	H	-5.129877	-1.119886	-0.151754
H	-3.826743	-3.344725	-1.436995	H	-4.870493	-0.775092	-1.872944
H	-2.463299	-3.215082	-0.288197	C	-2.480495	-2.689311	-2.421401
H	-3.914397	-2.198138	-0.066448	H	-3.154161	-3.538205	-2.594847
C	-3.872621	-0.731984	-2.812116	H	-2.544350	-1.997132	-3.266964
H	-4.332309	-1.546239	-3.386705	H	-1.449624	-3.049348	-2.332683
H	-4.623251	-0.296986	-2.143880				
H	-3.533630	0.050827	-3.497922				
				4o			
				C	-4.163903	3.843660	-0.332974
				C	-3.188981	4.824159	-0.182292
				C	-1.847120	4.468676	-0.060213
				C	-1.530919	3.121160	-0.091438
				C	-2.476423	2.101669	-0.242316
				C	-3.807033	2.492255	-0.366348
				H	-5.210316	4.128159	-0.424709
				H	-3.469915	5.874539	-0.158223
				H	-1.063653	5.213764	0.055633
				H	-4.585444	1.739134	-0.487393
				O	-0.206473	2.737824	0.042198
				C	-0.079898	1.400668	-0.028605
				C	0.958360	0.580206	0.075871
				Si	2.776123	0.923661	-0.303019
				C	2.966110	0.680091	-2.183890
				H	2.399161	1.517623	-2.625042
				C	3.251370	2.709590	0.171547
				H	4.355018	2.709335	0.180969
				C	3.890149	-0.318996	0.633083
				H	3.923754	-1.220735	-0.002008
				Pd	-1.637626	0.217330	-0.342485
				C	5.319830	0.205192	0.791972
				H	5.351907	1.058842	1.483388
				H	5.974489	-0.571016	1.211762
				H	5.767958	0.534515	-0.153513
				C	3.363614	-0.752249	2.000309
				H	4.065918	-1.446315	2.482796
				H	3.235691	0.102322	2.680066
				H	2.403775	-1.279658	1.941630
				C	2.773145	3.071763	1.578440
TS ₃₄₀							
C	-4.542047	3.436012	-0.193687				
C	-3.683522	4.516332	-0.016510				
C	-2.310039	4.312278	0.094111				
C	-1.841921	3.010401	0.024902				
C	-2.666422	1.893026	-0.152791				
C	-4.033958	2.136200	-0.264646				
H	-5.614339	3.602810	-0.276310				
H	-4.081419	5.527228	0.036083				
H	-1.616705	5.138971	0.227298				
H	-4.722370	1.303179	-0.408271				
O	-0.479091	2.783557	0.144319				
C	-0.196521	1.473879	0.024085				
C	0.885498	0.722324	0.032880				
Si	2.695161	1.127675	-0.314127				
C	2.993562	0.667872	-2.140480				
H	2.383434	1.393859	-2.704096				
C	3.044143	2.986588	-0.089248				
H	4.142717	3.066845	-0.168906				
C	3.821133	0.110402	0.848233				
H	3.976557	-0.860836	0.349780				
Pd	-1.603108	0.124398	-0.354892				
C	5.185680	0.776861	1.038055				
H	5.093727	1.720664	1.593280				
H	5.859480	0.129574	1.616247				
H	5.685917	1.005174	0.088647				
C	3.191705	-0.174963	2.212248				
H	3.916432	-0.660027	2.881299				
H	2.846112	0.741902	2.711161				

H	3.111838	2.352132	2.336488	H	2.461153	1.820872	2.613260
H	3.146950	4.060610	1.879504	C	3.732462	3.154246	0.540263
H	1.676520	3.112887	1.621541	H	4.114808	3.305885	-0.477372
C	2.798743	3.760231	-0.841797	H	2.664254	3.407396	0.531000
H	3.223181	3.590197	-1.839096	H	4.239106	3.879397	1.193312
H	1.706339	3.777647	-0.940621	C	2.190108	0.072620	-2.733323
H	3.112026	4.764341	-0.521581	H	2.416768	-1.004666	-2.683015
C	2.345966	-0.619677	-2.694088	H	1.143461	0.213165	-2.429628
H	2.812414	-1.502429	-2.231837	H	2.258624	0.356805	-3.793145
H	1.265156	-0.662001	-2.498374	C	4.562416	0.847543	-2.456711
H	2.480396	-0.718360	-3.780636	H	4.588439	1.242136	-3.482469
C	4.421147	0.784825	-2.637880	H	5.280428	1.429120	-1.862347
H	4.499168	0.753581	-3.733707	H	4.934647	-0.185825	-2.503647
H	4.906452	1.710125	-2.299767	Zn	0.385796	-1.546876	-0.231361
H	5.010445	-0.058759	-2.251597	O	0.531994	-0.815194	2.817495
Zn	0.542232	-1.458590	0.123524	C	-0.575926	-1.415936	2.589320
O	0.062150	0.201443	2.961783	O	-0.950668	-1.795815	1.446894
C	-0.325050	-1.050018	3.016001	C	-1.484759	-1.635353	3.753980
O	-0.154290	-1.871903	2.113505	H	-2.342735	-0.960968	3.632028
C	-1.021618	-1.397813	4.287160	H	-1.866133	-2.660000	3.741793
H	-1.990816	-0.887141	4.303456	H	-0.986462	-1.414742	4.698892
H	-1.171590	-2.475787	4.351521	O	-0.913526	-2.310786	-1.722259
H	-0.450733	-1.031843	5.144702	C	-0.168197	-3.336734	-1.751346
O	-0.109757	-3.217898	-0.831033	O	0.853254	-3.408371	-0.999678
C	1.064362	-3.685115	-0.687819	C	-0.498064	-4.463497	-2.681566
O	1.957345	-2.997004	-0.112961	H	0.179203	-5.306350	-2.537875
C	1.388655	-5.042462	-1.231857	H	-1.533407	-4.777852	-2.519102
H	2.321455	-5.419612	-0.809701	H	-0.429463	-4.106625	-3.714022
H	0.566560	-5.734272	-1.032168	H	0.955061	-0.455043	1.848219
H	1.497005	-4.967481	-2.319372	P	-3.799446	-0.580503	-0.022876
H	0.427083	0.421898	2.063121	C	-3.873685	-2.388778	0.275632
P	-3.201075	-1.593037	-0.596613	H	-3.018026	-2.845724	-0.232875
C	-3.125024	-2.883875	0.708414	H	-3.783726	-2.597101	1.346581
H	-2.153581	-3.384795	0.639758	H	-4.808741	-2.816327	-0.107383
H	-3.214010	-2.422172	1.697978	C	-5.388418	-0.008079	0.702882
H	-3.926477	-3.622146	0.578172	H	-6.235543	-0.559912	0.276774
C	-4.973348	-1.109494	-0.541132	H	-5.371900	-0.160184	1.787236
H	-5.626112	-1.990907	-0.575388	H	-5.528798	1.061240	0.513712
H	-5.170474	-0.544572	0.376475	C	-4.116266	-0.500628	-1.825553
H	-5.199101	-0.463066	-1.396120	H	-5.060922	-0.990768	-2.092238
C	-3.140759	-2.622510	-2.113500	H	-4.133826	0.542972	-2.156444
H	-3.933592	-3.381307	-2.102840	H	-3.282841	-1.005891	-2.326588
H	-3.257808	-1.989860	-2.998837				
H	-2.162878	-3.113935	-2.154186				
				5o			
				C	2.918432	4.143649	0.064097
				C	1.673328	4.750569	0.182742
				C	0.513644	4.007809	-0.018425
				C	0.638302	2.664897	-0.337882
				C	1.870714	2.009837	-0.444809
				C	3.011499	2.783714	-0.241015
				H	3.825547	4.726443	0.208383
				H	1.600285	5.806780	0.430157
				H	-0.477256	4.448626	0.066514
				H	4.000715	2.335317	-0.327212
				O	-0.505700	1.939345	-0.559790
				C	-0.277962	0.643284	-0.874778
				C	-1.353459	-0.212716	-0.814158
				Si	-3.175343	0.201977	-0.491749
				C	-3.370372	1.750457	0.598589
				H	-2.943851	2.581084	0.014423
				C	-3.956687	0.515959	-2.201395
				H	-5.045349	0.603386	-2.049484
				C	-3.966253	-1.312302	0.369148
				H	-3.866400	-1.105560	1.448947
				Pd	1.697543	0.064382	-0.922273
				C	-5.454228	-1.447334	0.041217
				H	-5.606862	-1.706132	-1.016032
				H	-5.916405	-2.248110	0.635165
				H	-6.019778	-0.527570	0.234070
				C	-3.253561	-2.636788	0.096060
				H	-3.766372	-3.465739	0.603166
				H	-3.235037	-2.878579	-0.977123
				H	-2.217468	-2.642382	0.456479
				C	-3.699499	-0.649378	-3.156349
				H	-4.063380	-1.607669	-2.762702
				H	-4.189729	-0.484927	-4.126069
				H	-2.624402	-0.760971	-3.355546
				C	-3.444770	1.819881	-2.810551
TS ₄₅₀							
C	-2.992707	4.347493	-0.897472				
C	-1.779297	5.019020	-1.000473				
C	-0.582514	4.361803	-0.724019				
C	-0.636010	3.029685	-0.344051				
C	-1.839958	2.328668	-0.226963				
C	-3.020714	3.003930	-0.513541				
H	-3.923849	4.866692	-1.113949				
H	-1.759133	6.064083	-1.300494				
H	0.379539	4.862643	-0.803309				
H	-3.979562	2.491996	-0.432331				
O	0.525476	2.351627	-0.084059				
C	0.308435	1.056262	0.279584				
C	1.302120	0.150064	0.446512				
Si	3.097840	0.400813	-0.032914				
C	3.150170	0.896403	-1.876126				
H	2.803529	1.942409	-1.897304				
C	3.957880	1.727309	1.037104				
H	5.038606	1.516104	0.973531				
C	3.979189	-1.290601	0.183758				
H	3.787871	-1.838576	-0.756734				
Pd	-1.630727	0.435062	0.398629				
C	5.492905	-1.141425	0.343240				
H	5.739546	-0.666227	1.303371				
H	5.991145	-2.121061	0.334720				
H	5.949089	-0.533318	-0.447322				
C	3.437300	-2.149485	1.325765				
H	3.999753	-3.090077	1.408624				
H	3.514960	-1.637193	2.295231				
H	2.383787	-2.428534	1.190873				
C	3.531968	1.599281	2.499521				
H	3.698778	0.590741	2.902931				
H	4.081110	2.304340	3.139704				

H	-3.709632	2.696443	-2.206561	C	3.735685	8.040272	-2.432845
H	-2.349124	1.808969	-2.907071	H	4.444103	8.602789	-3.054649
H	-3.856865	1.975234	-3.817591	H	2.749613	8.514137	-2.499929
C	-2.609598	1.671783	1.920516	H	4.061559	8.093545	-1.388027
H	-2.917051	0.800128	2.515556	C	3.308721	6.585937	-4.771508
H	-1.524192	1.609754	1.767327	H	2.320382	7.034345	-4.918279
H	-2.797992	2.567669	2.529868	H	4.073206	7.260913	-5.177713
C	-4.846932	2.047432	0.865865	H	3.334991	5.642446	-5.326431
H	-4.964763	2.987507	1.422646	C	5.374518	5.797811	-3.028070
H	-5.440278	2.136059	-0.053831	H	5.978291	6.528146	-3.582380
H	-5.303191	1.257045	1.478860	H	5.763447	5.706376	-2.008174
Zn	-0.137169	-0.998160	0.927619	H	5.463682	4.817624	-3.509368
O	1.346044	-2.013498	-1.602893	C	-0.733877	-0.061452	-4.675839
C	0.972086	-2.935019	-0.838497	H	0.125157	-0.527277	-5.180601
O	0.559337	-2.780169	0.356646	H	-1.400831	-0.879366	-4.367760
C	1.009727	-4.349936	-1.348852	H	-1.271512	0.535374	-5.424706
H	1.600284	-4.966410	-0.663054	C	0.451759	-0.117076	-2.464457
H	-0.005773	-4.759607	-1.347507	H	0.731961	0.440415	-1.563505
H	1.428155	-4.396642	-2.355544	H	-0.174813	-0.965761	-2.154269
O	0.687735	-0.203286	2.662972	H	1.371600	-0.542211	-2.892013
C	-0.333870	-0.622607	3.292522	C	-1.594242	3.801292	-4.349223
O	-1.246145	-1.256750	2.682416	H	-2.215638	2.920766	-4.143404
C	-0.488952	-0.321918	4.750664	H	-1.393395	4.294486	-3.386656
H	0.470355	-0.066586	5.203882	H	-2.195848	4.495546	-4.953343
H	-1.162934	0.537301	4.849988	C	0.475273	4.709611	-5.425145
H	-0.952620	-1.165751	5.266917	H	0.755637	5.265414	-4.518520
H	-1.148353	-1.180622	-1.286060	H	1.402286	4.493042	-5.974029
P	3.902624	-0.586537	-0.246807	H	-0.132896	5.377757	-6.052772
C	4.132375	-2.402642	-0.142381	C	2.108700	1.505135	-6.396619
H	3.369469	-2.814940	0.527918	H	1.254329	0.854628	-6.623592
H	4.008385	-2.853802	-1.131821	H	1.922624	2.468957	-6.891162
H	5.126834	-2.643630	0.251983	H	2.993271	1.065081	-6.878873
C	5.422047	-0.065688	-1.136154	C	3.557520	2.566207	-4.642754
H	6.317532	-0.412413	-0.605921	H	3.754000	2.696844	-3.571236
H	5.413884	-0.491838	-2.144244	H	4.455654	2.143878	-5.117187
H	5.461644	1.024197	-1.229140	H	3.410536	3.571952	-5.063999
C	4.214218	-0.077384	1.484084				
H	5.160416	-0.489050	1.856396	TS' 230			
H	4.231433	1.014201	1.556737	C	-1.014635	-0.726535	1.955818
H	3.382099	-0.432125	2.103326	C	-1.235218	0.607381	2.290069
				C	-0.568933	1.601909	1.588239
2'o				C	0.295117	1.243982	0.559062
C	-1.646815	4.907423	2.735383	C	0.530810	-0.068712	0.168913
C	-1.180510	3.624149	3.016956	C	-0.137975	-1.047459	0.925179
C	-0.481830	2.903911	2.057579	H	-1.519138	-1.519375	2.504316
C	-0.250773	3.474403	0.808293	H	-1.912028	0.874118	3.098008
C	-0.725723	4.746970	0.501272	H	-0.707056	2.656678	1.814925
C	-1.421010	5.457263	1.477410	H	0.038303	-2.096342	0.685998
H	-2.190486	5.470017	3.490060	O	0.862647	2.358545	-0.083011
H	-1.356512	3.181275	3.994660	C	1.744498	2.297296	-1.023673
H	-0.098071	1.905866	2.253743	C	2.560635	2.470024	-1.918739
H	-0.541986	5.167228	-0.485257	Si	3.789581	3.067123	-3.132893
H	-1.795593	6.451845	1.242971	C	5.524365	2.570357	-2.542257
O	0.440930	2.700680	-0.085987	H	6.245016	2.963395	-3.279537
C	1.001407	3.273251	-1.163875	C	3.418342	2.402449	-4.881224
C	1.203667	3.157200	-2.420200	H	2.637048	3.077241	-5.273984
Si	0.767820	2.281128	-3.976149	C	3.598992	4.961055	-3.113392
C	2.333857	1.689123	-4.894982	H	3.823493	5.245982	-2.071640
H	2.545603	0.695776	-4.462084	H	2.109925	-0.714437	-0.244755
C	-0.274962	0.765077	-3.476498	Pd	1.337337	-0.661540	-1.658690
H	-1.164024	1.186600	-2.976710	P	2.573290	-2.269595	-2.907401
C	-0.287704	3.442282	-5.053364	C	2.050779	-3.915452	-2.267059
H	-0.527595	2.893532	-5.979913	H	0.969802	-4.027184	-2.407300
Pd	2.271661	4.848493	-1.537419	H	2.569525	-4.737631	-2.777354
P	2.914828	5.778719	0.563848	H	2.257817	-3.962331	-1.192766
C	2.207914	7.399779	1.082113	C	2.337397	-2.546966	-4.713676
H	2.629102	7.734906	2.038915	H	2.844502	-3.460878	-5.049181
H	2.397775	8.159044	0.315873	H	1.264369	-2.634853	-4.918709
H	1.123256	7.286737	1.190357	H	2.722158	-1.693341	-5.281335
C	4.721353	6.095597	0.781854	C	4.400639	-2.417064	-2.768486
H	5.089601	6.795362	0.023470	H	4.764789	-3.344874	-3.228616
H	4.939308	6.506281	1.776239	H	4.883560	-1.561823	-3.253410
H	5.264118	5.151285	0.660570	H	4.677798	-2.400842	-1.708899
C	2.607142	4.805828	2.097072	C	4.578593	5.684487	-4.034793
H	3.113944	5.260430	2.958407	H	4.510541	6.774300	-3.910078
H	1.531182	4.764801	2.297116	H	5.623848	5.398667	-3.855950
H	2.966170	3.779353	1.963995	H	4.353477	5.474478	-5.090423
P	3.595805	6.278423	-2.974580	C	2.164374	5.388170	-3.416027

H	1.442974	4.905551	-2.745419	H	5.657325	0.601942	-3.406119
H	2.043368	6.476052	-3.316730	H	6.675233	0.805197	-1.972280
H	1.881959	5.131146	-4.447801	H	4.919600	0.635767	-1.789945
C	5.675921	1.051456	-2.477623	C	5.829375	3.244101	-1.155095
H	5.598747	0.589101	-3.471565	H	5.799396	4.340170	-1.200430
H	6.650876	0.763963	-2.058304	H	5.088738	2.923113	-0.409711
H	4.898811	0.602136	-1.840050	H	6.820447	2.957096	-0.776628
C	5.829410	3.193740	-1.181755	C	2.935874	0.946971	-4.869846
H	5.805816	4.290433	-1.208964	H	2.635558	0.633185	-5.882523
H	5.097620	2.865589	-0.430734	H	3.705320	0.238614	-4.526668
H	6.824072	2.894389	-0.822607	H	2.079276	0.820024	-4.193283
C	2.861646	0.983047	-4.898279	C	4.699324	2.462070	-5.791324
H	2.564172	0.684630	-5.916202	H	5.501449	1.797463	-5.440682
H	3.620008	0.261828	-4.558152	H	4.452181	2.151605	-6.816444
H	1.999467	0.855126	-4.229486	H	5.118837	3.473882	-5.845995
C	4.634324	2.497960	-5.804527	P	-0.578482	-0.051010	-2.897399
H	5.430816	1.815594	-5.476112	C	-0.863877	-0.637646	-4.620160
H	4.374230	2.213440	-6.833855	H	-0.888897	-1.733561	-4.633716
H	5.066067	3.505582	-5.840834	H	-1.812076	-0.257338	-5.020728
P	-0.571325	-0.011199	-3.017269	H	-0.044120	-0.302253	-5.265474
C	-0.917622	-0.685559	-4.698086	C	-0.837991	1.757007	-3.097479
H	-1.012578	-1.776437	-4.640405	H	-0.885453	2.226299	-2.108683
H	-1.840796	-0.271276	-5.123436	H	0.002821	2.204057	-3.639783
H	-0.077566	-0.448532	-5.362086	H	-1.772739	1.953782	-3.637309
C	-0.756817	1.793389	-3.333038	C	-2.151445	-0.542908	-2.088328
H	-0.709950	2.335953	-2.381998	H	-2.188463	-1.632942	-1.984507
H	0.065989	2.152391	-3.962056	H	-2.180742	-0.110544	-1.081559
H	-1.713115	2.008018	-3.827185	H	-3.020470	-0.201502	-2.664377
C	-2.155828	-0.367172	-2.155244				
H	-2.246101	-1.445054	-1.981694	MeC≡CMe			
H	-2.142772	0.126528	-1.176194	C	0.604344	0.000053	0.000219
H	-3.021637	-0.016828	-2.731230	C	-0.604335	-0.000038	-0.000205
				C	2.057955	-0.000002	0.000003
3'o				H	2.458780	0.929711	0.420575
C	-1.072335	-0.628157	1.949334	H	2.458653	-0.829383	0.594509
C	-1.249759	0.713284	2.279854	H	2.458336	-0.100487	-1.015604
C	-0.590825	1.683905	1.540500	C	-2.057959	-0.000010	-0.000012
C	0.222082	1.290253	0.481483	H	-2.458797	-0.928502	-0.423259
C	0.414104	-0.025070	0.088061	H	-2.458338	0.097564	1.015878
C	-0.251453	-0.977363	0.881011	H	-2.458664	0.831079	-0.592126
H	-1.572400	-1.404427	2.525550				
H	-1.887104	1.002833	3.111934	6'o			
H	-0.688541	2.743771	1.764991	C	2.532329	2.815444	3.055804
H	-0.130512	-2.033895	0.639927	C	1.291735	2.978370	3.663160
O	0.788526	2.395527	-0.191179	C	0.167140	2.353706	3.134051
C	1.717333	2.320522	-1.080628	C	0.310852	1.566426	1.998503
C	2.570545	2.478795	-1.943417	C	1.546017	1.376065	1.362394
Si	3.820970	3.070006	-3.134478	C	2.652102	2.018093	1.915938
C	5.549110	2.596490	-2.509826	H	3.411285	3.309198	3.464360
H	6.278766	2.981377	-3.242670	H	1.194463	3.599677	4.550369
C	3.477864	2.372063	-4.875423	H	-0.820523	2.473211	3.574335
H	2.690709	3.029740	-5.285120	H	3.631343	1.925317	1.447745
C	3.621402	4.963191	-3.154609	O	-0.803364	0.993646	1.464852
H	3.833011	5.268872	-2.116134	C	-0.583880	0.378180	0.256027
H	2.474018	-1.128812	-0.541102	C	-1.666884	-0.117540	-0.389168
Pd	1.354991	-0.744703	-1.618254	Si	-3.482545	0.155793	0.055560
P	2.510354	-2.288752	-2.978245	C	-3.805227	-0.080246	1.913003
C	2.050484	-3.959195	-2.366359	H	-3.260858	0.729805	2.423699
H	0.972145	-4.106809	-2.491109	C	-3.903835	1.940679	-0.470440
H	2.589705	-4.749489	-2.904214	H	-4.996489	2.050788	-0.362280
H	2.278745	-4.018747	-1.297419	C	-4.498313	-1.119487	-0.945601
C	2.268065	-2.520231	-4.788770	H	-4.622546	-1.980454	-0.266298
H	2.828905	-3.393019	-5.146987	Pd	1.405408	0.369207	-0.369078
H	1.203758	-2.671923	-4.999465	C	-5.894218	-0.604351	-1.301494
H	2.603092	-1.631462	-5.333119	H	-5.841552	0.227120	-2.017859
C	4.338930	-2.353556	-2.853125	H	-6.497438	-1.393702	-1.771671
H	4.740399	-3.240733	-3.359016	H	-6.450232	-0.244443	-0.426508
H	4.777156	-1.454236	-3.298542	C	-3.786738	-1.629764	-2.199795
H	4.617627	-2.372313	-1.794412	H	-4.430512	-2.320534	-2.762445
C	4.609527	5.672490	-4.077961	H	-3.525304	-0.806880	-2.883066
H	4.538759	6.764158	-3.972317	H	-2.860207	-2.167553	-1.960662
H	5.653290	5.391356	-3.883601	C	-3.534306	2.195142	-1.931572
H	4.395246	5.444779	-5.132199	H	-3.989055	1.469347	-2.619461
C	2.189479	5.380624	-3.481646	H	-3.850260	3.197211	-2.253906
H	1.462445	4.912483	-2.807022	H	-2.444029	2.143640	-2.064684
H	2.065747	6.470311	-3.408639	C	-3.223890	2.976590	0.424306
H	1.918410	5.100005	-4.510361	H	-3.506793	2.870190	1.479448
C	5.708102	1.079701	-2.417454				

H	-2.128922	2.884196	0.370804	H	4.010530	-1.123473	2.966287
H	-3.483623	3.997773	0.111473	H	3.336517	-2.540593	2.152402
C	-3.262731	-1.409886	2.430041	C	3.577308	1.813263	1.896142
H	-3.685778	-2.264075	1.880634	H	3.928043	1.108370	2.662262
H	-2.171506	-1.478401	2.353019	H	3.858184	2.825611	2.224944
H	-3.523316	-1.556108	3.487926	H	2.479597	1.760607	1.881260
C	-5.293054	0.059253	2.236158	C	3.691809	2.566810	-0.488609
H	-5.469251	-0.005695	3.318970	H	4.129612	2.418291	-1.484108
H	-5.714345	1.014026	1.892857	H	2.601593	2.562250	-0.613549
H	-5.879189	-0.746999	1.771829	H	3.983153	3.571400	-0.146315
Zn	0.182716	-1.830618	0.314574	C	3.634364	-1.860386	-2.395594
O	1.092059	-0.721953	-2.284422	H	4.190053	-2.680282	-1.917089
C	0.608247	-1.870182	-2.443387	H	2.568204	-2.034546	-2.205442
O	0.169466	-2.623501	-1.517829	H	3.805456	-1.951646	-3.477939
C	0.540933	-2.422278	-3.841831	C	5.557941	-0.255910	-2.246572
H	1.221691	-3.277071	-3.920176	H	5.706829	-0.295845	-3.335312
H	-0.467229	-2.797780	-4.041429	H	5.929719	0.718259	-1.900374
H	0.817640	-1.666072	-4.579401	H	6.207195	-1.029394	-1.811429
O	1.909272	-2.699470	1.306018	Zn	-0.757544	-1.620296	-0.244314
C	1.078269	-3.127220	2.151910	O	-2.545282	-0.604666	2.382003
O	-0.168619	-2.889810	2.013029	C	-2.307152	-1.841983	2.301231
C	1.523332	-3.916812	3.344908	O	-1.633047	-2.413396	1.400843
H	2.594406	-4.120272	3.306546	C	-2.910879	-2.731206	3.357338
H	1.286065	-3.354313	4.253410	H	-3.727600	-3.304019	2.903281
H	0.961152	-4.853817	3.392649	H	-2.168157	-3.455006	3.703283
H	-1.447579	-0.548732	-1.366876	H	-3.302543	-2.150033	4.193967
P	3.737697	-0.060548	-0.659404	O	-2.016666	-2.193665	-1.843678
C	4.030674	-1.399267	-1.874404	C	-1.295559	-3.238235	-1.996399
H	3.482000	-2.287516	-1.538888	O	-0.308211	-3.455358	-1.250778
H	3.648422	-1.105748	-2.856259	C	-1.661641	-4.203233	-3.086219
H	5.099277	-1.636314	-1.942405	H	-2.665504	-4.596829	-2.897471
C	4.862713	1.270048	-1.231867	H	-1.698860	-3.677059	-4.044992
H	5.889511	0.902691	-1.349904	H	-0.946714	-5.025733	-3.137854
H	4.499136	1.654554	-2.190813	H	1.828753	-1.776514	0.847882
H	4.858688	2.097042	-0.513378	P	-3.681761	0.406149	-0.468610
C	4.567380	-0.742140	0.823586	C	-4.587450	-1.165275	-0.230830
H	5.605703	-1.015708	0.598469	H	-3.955522	-1.988460	-0.579757
H	4.549766	-0.017815	1.643253	H	-4.811656	-1.293214	0.833389
H	4.002705	-1.626972	1.142882	H	-5.523685	-1.154037	-0.801960
C	0.527934	2.494819	-2.654565	C	-4.966614	1.652543	-0.061660
C	0.973345	3.184274	-1.762869	H	-5.879507	1.471854	-0.642699
C	1.471568	4.056638	-0.710088	H	-5.199166	1.595628	1.006894
C	0.918307	3.904245	0.226238	H	-4.596948	2.657932	-0.287337
H	1.376901	5.111529	-0.993052	C	-3.513423	0.545689	-2.282116
H	2.528578	3.862422	-0.487877	H	-4.499861	0.512418	-2.760835
C	-0.050370	1.705451	-3.730184	H	-3.016382	1.489009	-2.533736
H	-0.693584	0.909499	-3.330563	H	-2.906524	-0.296879	-2.631504
H	0.724432	1.218226	-4.332453	C	-0.152566	1.348674	2.145550
H	-0.658689	2.332125	-4.393346	C	-0.076295	2.402000	1.453052
TS₆₇₀				C	0.385183	3.794354	1.316729
C	-1.485428	3.933889	-1.974295	H	0.942766	3.947737	0.384487
C	-0.459490	3.524973	-2.831659	H	1.044347	4.017166	2.165410
C	0.328531	2.438873	-2.497620	H	-0.450793	4.501783	1.331923
C	0.116963	1.727350	-1.305709	C	0.293645	0.478294	3.240329
C	-0.923336	2.116942	-0.438902	H	0.849870	-0.368297	2.812596
C	-1.701414	3.232775	-0.799184	H	-0.558588	0.085984	3.803378
H	-2.102337	4.795014	-2.219913	H	0.964336	1.019623	3.919410
H	-0.269828	4.063355	-3.757086	TS_{670a}			
H	1.148069	2.109845	-3.133903	C	3.534781	3.939102	-0.138130
H	-2.476835	3.566674	-0.108356	C	2.322812	4.552735	0.172111
O	1.033287	0.771336	-1.065091	C	1.167880	3.791220	0.309781
C	0.846776	-0.338696	-0.243097	C	1.239077	2.411252	0.182757
C	1.973386	-0.839988	0.297686	C	2.476303	1.746983	-0.004929
Si	3.747084	-0.297605	-0.013447	C	3.605395	2.555448	-0.228968
C	4.096204	-0.499880	-1.877643	H	4.430756	4.536501	-0.284785
H	3.477614	0.272808	-2.364801	H	2.267216	5.634113	0.270579
C	4.136142	1.501342	0.509781	H	0.191216	4.249462	0.449208
H	5.237273	1.541325	0.568510	H	4.562112	2.068040	-0.399656
C	4.874063	-1.485053	0.988111	O	0.058305	1.733577	0.126700
H	5.001253	-2.369355	0.339089	C	0.054359	0.636517	-0.720505
Pd	-1.739334	0.754972	0.888799	C	-1.171163	0.023901	-0.856616
C	6.262598	-0.904779	1.260928	Si	-2.888869	0.633227	-0.334558
H	6.207121	-0.061552	1.964109	C	-2.851709	1.648143	1.277405
H	6.921381	-1.656288	1.718932	H	-2.243426	2.537552	1.049835
H	6.760817	-0.539480	0.354329	C	-3.497347	1.761411	-1.747755
C	4.256933	-1.965413	2.302396	H	-4.545898	2.017521	-1.520295
H	4.957416	-2.610430	2.852420	C	-4.011938	-0.899201	-0.128231

C	0.659271	2.539265	0.391367	H	-0.908317	-1.059265	4.572936
C	1.732464	2.580846	-0.500655	H	-1.129723	-2.816576	4.491134
C	2.738613	3.520867	-0.230633	H	0.520771	-2.100206	4.485378
H	3.464040	5.067604	1.065299				
H	1.531241	4.918379	2.626419	9%			
H	-0.295099	3.256229	2.161342	C	0.638736	5.106706	0.375974
H	3.587885	3.605040	-0.904118	C	-0.656842	4.993375	0.877314
O	-0.366099	1.655881	0.210163	C	-1.438175	3.894200	0.546828
C	-0.474570	0.860798	-0.873014	C	-0.916619	2.908684	-0.283584
C	-1.607298	0.018719	-0.840600	C	0.386217	2.994114	-0.803276
H	-1.736731	-0.521779	-1.785270	C	1.149468	4.117892	-0.453664
Pd	2.029712	-0.324581	-0.891512	H	1.249980	5.969156	0.628187
P	3.747484	-0.466118	0.741982	H	-1.063069	5.766039	1.525333
C	5.498946	0.028398	0.468867	H	-2.457296	3.779024	0.909297
H	5.531123	1.079607	0.160557	H	2.158237	4.217558	-0.845137
H	6.092700	-0.089822	1.384609	O	-1.732506	1.870189	-0.578896
H	5.942581	-0.577608	-0.327211	C	-1.276093	0.737841	-1.229511
C	3.310991	0.551955	2.204394	C	-2.096570	-0.328960	-1.212631
H	4.035484	0.419623	3.018611	H	-1.751112	-1.192669	-1.774112
H	3.271990	1.610126	1.917861	Pd	1.258652	0.668791	0.203585
H	2.314566	0.242203	2.539266	P	2.013782	0.158646	2.326445
C	3.914597	-2.133352	1.484866	C	1.788210	1.725579	3.262031
H	4.611553	-2.135432	2.332719	H	0.729079	2.007824	3.227284
H	2.918184	-2.440813	1.820007	H	2.104267	1.615452	4.307596
H	4.248260	-2.843478	0.722451	H	2.367552	2.523940	2.786065
C	1.738106	1.649573	-1.633412	C	1.143135	-1.051601	3.388521
C	0.528821	0.905414	-1.904565	H	1.513480	-0.977884	4.419064
Si	-3.274867	0.530897	-0.103937	H	0.067206	-0.850678	3.375799
C	-4.305666	-1.041549	0.220855	H	1.328048	-2.058498	2.999175
C	-3.120257	1.563306	1.495057	C	3.769659	-0.253896	2.629243
C	-4.107671	1.632757	-1.427395	H	3.992855	-0.205384	3.702369
H	-4.040180	-1.343333	1.248395	H	3.980826	-1.260421	2.253542
C	-3.968353	-2.218198	-0.695557	H	4.411405	0.440102	2.078826
C	-5.811706	-0.774485	0.167659	C	0.874600	1.903521	-1.664516
H	-2.577946	2.476693	1.201375	C	0.049224	0.802569	-1.869200
C	-2.326703	0.893613	2.614508	Si	-3.630080	-0.539303	-0.165573
C	-4.493554	1.984524	2.022283	C	-3.832827	-2.416150	0.164709
H	-5.108171	1.889641	-1.040830	C	-3.419368	0.347647	1.513158
C	-3.326230	2.927106	-1.643610	C	-5.147267	0.164761	-1.077699
C	-4.285817	0.910280	-2.761326	H	-3.291453	-2.590441	1.112821
H	-4.135479	-1.974206	-1.754332	C	-3.187448	-3.308732	-0.895802
H	-2.931368	-2.562321	-0.600935	C	-5.289736	-2.827573	0.384787
H	-4.603692	-3.083427	-0.461320	H	-3.408584	1.424821	1.289059
H	-6.376369	-1.664729	0.477397	C	-2.093280	-0.001152	2.139366
H	-6.127010	0.053908	0.812388	C	-4.586704	0.066593	2.457835
H	-6.137040	-0.531855	-0.853718	H	-6.038304	-0.113513	-0.490643
H	-1.288643	0.693853	2.321425	C	-5.092864	1.688653	-1.173743
H	-2.302173	1.536078	3.508284	C	-5.275841	-0.449253	-2.470967
H	-2.778633	-0.061919	2.916333	H	-3.612894	-3.125880	-1.893683
H	-5.108440	2.491459	1.266869	H	-2.102550	-3.155708	-0.964982
H	-5.058904	1.114613	2.384266	H	-3.358796	-4.371173	-0.666717
H	-4.390377	2.671325	2.874127	H	-5.360333	-3.885614	0.674313
H	-2.304118	2.715686	-1.995554	H	-5.788391	-2.239976	1.166018
H	-3.800362	3.555680	-2.410681	H	-5.877708	-2.709830	-0.535572
H	-3.239919	3.531080	-0.731619	H	-1.224218	0.259213	1.559668
H	-4.770458	1.559448	-3.504223	H	-1.985389	0.519388	3.149264
H	-3.313410	0.615030	-3.182362	H	-2.027432	-1.080721	2.394356
H	-4.893294	0.001067	-2.674564	H	-5.557236	0.334453	2.018441
C	0.135764	0.377093	-3.261578	H	-4.631527	-0.996982	2.731730
H	0.936367	0.509252	-3.992508	H	-4.486139	0.631504	3.395666
H	-0.096439	-0.694672	-3.233850	H	-4.194978	2.018701	-1.714563
H	-0.753909	0.897559	-3.647124	H	-5.964899	2.083041	-1.714752
C	2.733525	1.927831	-2.728377	H	-5.072571	2.168949	-0.186594
H	2.779443	1.116558	-3.458409	H	-6.167491	-0.075394	-2.994097
H	2.493907	2.860282	-3.261836	H	-4.404199	-0.193597	-3.089606
H	3.742633	2.031657	-2.315353	H	-5.344989	-1.544710	-2.442996
Zn	-0.670080	-1.572357	0.240334	C	0.324502	-0.271432	-2.879943
O	1.853174	-2.622745	-1.076526	H	1.340926	-0.243179	-3.272379
C	0.883333	-3.384119	-1.255772	H	0.176339	-1.266921	-2.449543
O	-0.324570	-3.139581	-0.913272	H	-0.382110	-0.168774	-3.715045
C	1.105045	-4.718755	-1.922466	C	2.167257	2.108232	-2.401284
H	2.152229	-4.852241	-2.198677	H	2.550538	1.176296	-2.822638
H	0.789929	-5.519611	-1.246339	H	2.041334	2.838798	-3.212973
H	0.471818	-4.788907	-2.812650	H	2.944067	2.495230	-1.731671
O	-1.588823	-2.270405	2.024050	Zn	2.326285	-1.568125	-0.391871
C	-0.568776	-1.867740	2.651040	O	1.937330	-3.075546	1.017477
O	0.397511	-1.315104	2.032422	C	0.825824	-3.303334	0.443386
C	-0.510579	-1.987103	4.143890	O	0.524178	-2.717868	-0.635189

C	-0.159932	-4.232842	1.086864	H	0.022826	4.536186	0.000288
H	-0.925941	-3.623659	1.585395	H	-4.174679	1.886790	0.182364
H	-0.668395	-4.837083	0.331080	O	0.323826	2.036385	0.620717
H	0.324497	-4.867788	1.831185	C	0.217942	0.701706	0.830570
O	3.271857	-1.263448	-2.237283	C	1.321766	-0.089501	0.656219
C	4.372946	-1.094081	-1.622413	Si	3.143927	0.412831	0.446323
O	4.437539	-1.213845	-0.367618	C	3.351020	1.857470	-0.781669
C	5.588930	-0.714411	-2.414854	H	2.449155	2.475829	-0.647990
H	5.690674	-1.372866	-3.281749	C	3.735479	0.952968	2.181850
H	5.453917	0.303677	-2.797912	H	4.788448	1.262120	2.063658
H	6.488593	-0.751483	-1.798691	C	4.066206	-1.136040	-0.179286
				H	3.803589	-1.193614	-1.248772
Po				Pd	-1.663219	-0.083978	0.973057
C	4.882659	-1.743909	0.161973	C	5.580275	-0.957182	-0.063935
C	3.811576	-2.635208	0.193636	H	5.900504	-0.869692	0.984044
C	2.509362	-2.163006	0.112193	H	6.115426	-1.816899	-0.491654
C	2.288605	-0.795259	-0.003012	H	5.935080	-0.060875	-0.588915
C	3.341242	0.126397	-0.029538	C	3.633917	-2.460282	0.451206
C	4.645079	-0.381137	0.053017	H	4.196659	-3.297211	0.011397
H	5.903219	-2.112417	0.224892	H	3.818983	-2.488135	1.533255
H	3.990893	-3.703746	0.284304	H	2.567656	-2.674525	0.296377
H	1.650111	-2.828934	0.140473	C	3.679395	-0.174721	3.210320
H	5.487143	0.306145	0.033274	H	4.348126	-1.006874	2.961299
O	1.000292	-0.392077	-0.086843	H	3.964153	0.187245	4.208855
C	0.642337	0.939124	-0.119805	H	2.661727	-0.585609	3.295383
C	-0.684317	1.191679	-0.122527	C	2.936141	2.151412	2.692946
C	-0.961727	2.242946	-0.141465	H	2.961701	3.009187	2.009359
C	3.020043	1.546400	-0.133094	H	1.877557	1.886608	2.827487
C	1.715883	1.932240	-0.165848	H	3.314482	2.489900	3.668022
C	4.180298	2.490203	-0.184525	C	3.393262	1.398203	-2.239893
H	3.885483	3.533691	-0.295397	H	4.289993	0.794462	-2.440453
H	4.785857	2.412740	0.727974	H	2.522098	0.802452	-2.535342
H	4.842090	2.243628	-1.024628	H	3.430230	2.266232	-2.912274
C	1.258234	3.355146	-0.244403	C	4.573275	2.726125	-0.477209
H	0.634274	3.512914	-1.133095	H	4.639753	3.560886	-1.188877
H	0.638585	3.609495	0.624883	H	4.552298	3.155370	0.531606
H	2.081348	4.069092	-0.283633	H	5.509890	2.158112	-0.569866
Si	-2.059857	-0.077570	-0.049262	Zn	0.308351	-0.506835	-1.395464
C	-3.694842	0.790040	-0.551359	O	-1.558874	-0.184444	-2.370489
C	-1.739716	-1.506771	-1.268626	C	-1.132263	0.965652	-2.704144
C	-2.222865	-0.763130	1.724403	O	0.043483	1.324523	-2.409649
H	-3.785298	0.611769	-1.637123	C	-2.055634	1.926436	-3.387850
C	-3.699799	2.302246	-0.333831	H	-2.592885	2.478351	-2.604003
C	-4.918769	0.165690	0.120758	H	-1.496361	2.646270	-3.988854
H	-0.851787	-2.034124	-0.886475	H	-2.790011	1.395585	-3.998678
C	-1.409642	-0.988180	-2.666165	O	1.727639	-1.590759	-2.497220
C	-2.901050	-2.498049	-1.327408	C	1.254390	-2.674563	-2.044237
H	-3.160929	-1.343667	1.740999	O	0.274073	-2.664852	-1.240329
C	-1.078742	-1.697728	2.110813	C	1.862218	-3.975813	-2.477599
C	-2.343704	0.370433	2.741728	H	1.484930	-4.229261	-3.474087
H	-3.516574	2.560812	0.719347	H	2.948176	-3.871872	-2.554311
H	-2.936581	2.810780	-0.934649	H	1.600025	-4.780698	-1.787583
H	-4.672726	2.736434	-0.605383	H	1.160045	-1.119873	0.993854
H	-5.849573	0.588488	-0.283205	P	-3.693640	-1.201147	0.251385
H	-4.968972	-0.922022	-0.010108	C	-3.193206	-2.484512	-0.957731
H	-4.923845	0.361953	1.202103	H	-2.839087	-1.961732	-1.852593
H	-0.531762	-0.331595	-2.663022	H	-2.359330	-3.084510	-0.584522
H	-1.209203	-1.815371	-3.362035	H	-4.042647	-3.133914	-1.204816
H	-2.248317	-0.414609	-3.087760	C	-4.687015	-2.135968	1.484394
H	-3.152632	-2.916680	-0.343630	H	-5.432970	-2.773676	0.994092
H	-3.809985	-2.024937	-1.726336	H	-4.024858	-2.756896	2.096715
H	-2.667803	-3.342179	-1.992018	H	-5.199446	-1.433395	2.149973
H	-0.116460	-1.168297	2.100194	C	-5.005501	-0.360355	-0.718134
H	-1.220464	-2.099138	3.124557	H	-5.678837	-1.107638	-1.155854
H	-0.988473	-2.551730	1.426917	H	-5.594286	0.315817	-0.089897
H	-2.497709	-0.016618	3.759124	H	-4.532628	0.213129	-1.523673
H	-1.426310	0.975156	2.757503	C	-0.984393	-2.288193	2.230553
H	-3.177445	1.049294	2.517541	C	-0.977808	-1.298123	2.949047
				C	-0.886359	-0.270725	3.983069
6'o				H	-1.779511	0.363420	4.000634
C	-3.308365	3.822368	-0.141344	H	-0.022845	0.381683	3.805267
C	-2.140658	4.576411	-0.200278	H	-0.773354	-0.735240	4.969685
C	-0.909081	3.978526	0.046828	C	-0.885661	-3.575741	1.554665
C	-0.881603	2.626409	0.352772	H	-0.362736	-3.488344	0.592136
C	-2.031140	1.827083	0.392382	H	-1.875109	-4.012668	1.371094
C	-3.249267	2.454824	0.143528	H	-0.331023	-4.277343	2.188936
H	-4.272922	4.293919	-0.316996				
H	-2.186015	5.636500	-0.438228	TS' 6to			

C	-2.109171	4.182192	-0.197053	H	1.542982	-0.364303	3.816392
C	-0.890246	4.676440	0.256927	H	0.125517	-0.721918	4.842344
C	0.040014	3.810619	0.821267	C	-1.662040	-2.971551	2.784697
C	-0.290003	2.466211	0.925496	H	-1.349052	-3.704086	2.028952
C	-1.501636	1.920369	0.488523	H	-2.757786	-2.995203	2.810963
C	-2.399774	2.821195	-0.085704	H	-1.286990	-3.308202	3.760853
H	-2.838932	4.857549	-0.640365				
H	-0.654516	5.733647	0.160770	7'			
H	1.017365	4.154380	1.154861	C	-2.201310	1.094287	3.573525
H	-3.352857	2.461780	-0.471672	C	-1.219291	0.551318	4.393395
O	0.688972	1.630737	1.449375	C	-0.175738	-0.168955	3.828673
C	0.461952	0.300916	1.299889	C	-0.105600	-0.326537	2.447543
C	1.411246	-0.479124	0.717700	C	-1.050640	0.252312	1.564415
Si	3.125460	0.089324	0.088299	C	-2.110912	0.932779	2.193822
C	2.978539	1.572217	-1.107955	H	-3.034653	1.646439	4.002106
H	2.031907	2.075342	-0.849672	H	-1.266020	0.677051	5.472689
C	4.183962	0.556556	1.614055	H	0.598103	-0.629110	4.439535
H	5.133793	0.908998	1.174884	H	-2.867989	1.409645	1.571507
C	3.890618	-1.405925	-0.814102	O	0.974853	-1.089751	2.029291
H	3.383914	-1.415038	-1.791973	C	0.894296	-1.716028	0.792754
Pd	-1.605121	-0.085921	1.059431	C	1.584457	-1.193506	-0.261548
C	5.387443	-1.195716	-1.049291	Si	2.965987	0.122854	-0.201415
H	5.953757	-1.211715	-0.107159	C	2.499356	1.660998	0.831163
H	5.802917	-1.990916	-1.684067	H	1.398728	1.682456	0.847718
H	5.604929	-0.239353	-1.543652	C	4.427272	-0.895425	0.534463
C	3.634863	-2.770539	-0.176956	H	5.264532	-0.175551	0.583272
H	4.095153	-3.568557	-0.778092	C	3.409682	0.608439	-1.994667
H	4.055935	-2.851005	0.833781	H	2.766963	1.476607	-2.192798
H	2.564609	-3.003784	-0.104200	Pd	-1.070123	-1.191806	-0.100535
C	4.499259	-0.639642	2.512048	C	4.865597	1.054542	-2.135542
H	5.103994	-1.400463	2.005014	H	5.571414	0.224604	-1.997229
H	5.054602	-0.323518	3.406777	H	5.051207	1.465284	-3.137882
H	3.580595	-1.134993	2.862243	H	5.135585	1.834612	-1.412206
C	3.612359	1.692183	2.462200	C	3.054003	-0.441401	-3.045642
H	3.318852	2.569155	1.873818	H	3.316528	-0.087056	-4.053322
H	2.713478	1.369238	3.001305	C	3.585184	-1.391537	-2.893743
H	4.345024	2.018051	3.214067	H	1.978443	-0.661269	-3.048606
C	2.889178	1.131209	-2.570686	C	4.838803	-2.043441	-0.392224
C	3.844444	0.706430	-2.911307	H	5.089457	-1.720046	-1.407970
H	2.108191	0.386987	-2.752420	H	5.715581	-2.570055	0.010226
H	2.667061	1.994223	-3.212213	H	4.032790	-2.788562	-0.472673
C	4.114132	2.587678	-0.961878	C	4.214658	-1.473542	1.932637
H	3.979049	3.413201	-1.674313	H	4.028206	-0.713094	2.694302
H	4.178679	3.027528	0.039890	C	3.362249	-2.166985	1.950438
H	5.091648	2.135499	-1.184764	H	5.099934	-2.047001	2.243385
Zn	-0.325598	-0.540950	-1.278211	C	2.952526	2.968277	0.181666
O	-1.977081	-0.054835	-2.534605	H	4.049716	3.041023	0.147744
C	-1.367629	1.026641	-2.808334	H	2.561120	3.086281	-0.834851
O	-0.224903	1.266045	-2.323263	H	2.584114	3.818777	0.769006
C	-2.023472	2.059965	-3.673587	C	2.953417	1.627216	2.288344
H	-2.339071	2.886399	-3.024549	H	2.624388	2.539613	2.803935
H	-1.302638	2.466626	-4.387492	H	2.539749	0.770941	2.833103
H	-2.892334	1.652369	-4.194658	H	4.049709	1.584599	2.364479
O	1.021839	-1.778432	-2.308978	Zn	-0.805450	1.543705	-0.281098
C	0.444849	-2.802209	-1.831407	O	-2.353789	2.989581	-0.160536
O	-0.516664	-2.680512	-1.017338	C	-1.537827	3.779159	0.410847
C	0.897191	-4.168507	-2.257363	O	-0.346540	3.428644	0.636052
H	0.286450	-4.490538	-3.107948	C	-2.017951	5.128644	0.861694
H	1.941961	-4.144772	-2.576395	H	-2.443518	5.026922	1.866721
H	0.754954	-4.890279	-1.449207	H	-1.187751	5.835927	0.914851
H	1.215994	-1.550413	0.798944	H	-2.803564	5.500579	0.200061
P	-3.709832	-0.784648	0.287331	O	0.482165	1.648387	-1.896946
C	-3.677076	-2.380240	-0.602109	C	-0.383264	1.276883	-2.753097
H	-3.098187	-2.254311	-1.522153	O	-1.545403	0.947309	-2.409424
H	-3.172075	-3.135678	0.007311	C	-0.002254	1.244438	-4.208387
H	-4.696755	-2.707508	-0.840534	H	-0.643579	1.936140	-4.763621
C	-4.889855	-1.086286	1.661819	H	1.045378	1.516827	-4.353917
H	-5.842703	-1.472085	1.278454	H	-0.184293	0.242173	-4.611200
H	-4.470460	-1.806162	2.371585	H	1.566345	-1.834329	-1.144683
H	-5.069749	-0.147156	2.194972	P	-3.221757	-1.216762	-0.938064
C	-4.718188	0.261572	-0.823654	C	-3.331467	-1.626255	-2.712239
H	-5.620531	-0.285669	-1.123434	H	-2.840673	-0.813543	-3.256739
H	-5.016017	1.179828	-0.307632	H	-2.805305	-2.565516	-2.911661
H	-4.122431	0.504620	-1.709798	H	-4.379428	-1.716762	-3.023666
C	-1.146252	-1.641491	2.416460	C	-4.324462	-2.434821	-0.127761
C	-0.289729	-0.745869	2.768713	H	-5.347459	-2.335251	-0.511131
C	0.461730	-0.213853	3.931210	H	-3.973428	-3.453728	-0.312691
H	0.289004	0.861723	4.050776	H	-4.325211	-2.254871	0.952636

C	-4.198846	0.315230	-0.778837	C	-1.287527	4.613936	0.073912
H	-5.173771	0.171865	-1.261813	C	-0.188165	3.776392	-0.084769
H	-4.357137	0.537195	0.281991	C	-0.389551	2.401667	-0.072975
H	-3.675026	1.157041	-1.239187	C	-1.657167	1.821645	0.084563
C	-0.677519	-3.198711	-0.212132	C	-2.732624	2.688565	0.262706
C	0.289868	-3.099986	0.711681	H	-3.414754	4.729357	0.391643
C	0.839489	-4.153902	1.623723	H	-1.146874	5.692652	0.066879
H	0.684418	-3.873748	2.673253	H	0.821587	4.164359	-0.203889
H	1.922518	-4.272535	1.478524	H	-3.732072	2.292978	0.423063
C	0.355179	-5.120939	1.453887	O	0.682044	1.583335	-0.194596
H	-1.390084	-4.408201	-0.695657	C	0.379108	0.248095	-0.011572
H	-1.806785	-4.271797	-1.700691	C	1.408375	-0.612775	0.066840
H	-2.222387	-4.677405	-0.030016	H	1.140574	-1.657069	0.223021
H	-0.715718	-5.274759	-0.737927	Pd	-1.616018	-0.202809	0.052676
10 _o				P	-4.000840	-0.759731	-0.100245
C	-3.175296	3.481339	0.143414	C	-5.375509	0.460765	-0.135299
C	-1.987227	4.204726	0.142831	H	-5.447952	0.979035	0.826591
C	-0.759397	3.551557	0.092280	H	-6.328152	-0.044721	-0.336305
C	-0.744693	2.163846	0.041165	H	-5.193256	1.206172	-0.916025
C	-1.928604	1.413351	0.038307	C	-4.664115	-1.971107	1.117499
C	-3.142934	2.084739	0.090854	H	-5.683646	-2.277635	0.852886
H	-4.131576	3.997949	0.185252	H	-4.674487	-1.528739	2.119418
H	-2.013014	5.291263	0.183789	H	-4.019425	-2.856782	1.133009
H	0.180684	4.097587	0.093982	C	-4.327018	-1.664342	-1.169538
H	-4.081207	1.530335	0.094337	H	-5.378755	-1.967630	-1.742849
O	0.431122	1.492797	-0.000890	H	-3.695573	-2.558812	-1.706815
C	0.235292	0.131088	-0.035423	C	-4.076458	-1.025070	-2.522714
C	1.262346	-0.726560	-0.075022	H	-1.108590	-2.525152	-0.597331
Si	3.095259	-0.294109	-0.049860	C	-1.251427	-2.554352	0.616946
C	3.411431	1.284759	-1.062934	C	-1.269289	-2.696782	2.067394
H	2.819021	2.067917	-0.565036	H	-0.404019	-2.175317	2.495923
C	3.622363	-0.014023	1.760819	H	-1.220748	-3.751824	2.360748
H	4.719632	0.099923	1.765247	H	-2.169133	-2.255012	2.510101
C	4.082466	-1.749920	-0.810182	C	-0.780864	-2.593785	-2.015478
H	4.159011	-1.511288	-1.885138	H	-1.552320	-2.127366	-2.638365
Pd	-1.650418	-0.574448	-0.043042	H	-0.653701	-3.633237	-2.339421
C	5.503912	-1.840653	-0.251813	H	0.157244	-2.049631	-2.189990
H	5.496745	-2.136734	0.806454	Si	3.224551	-0.162971	-0.027878
H	6.092368	-2.597118	-0.790462	C	3.549842	1.103633	-1.413248
H	6.049799	-0.891129	-0.317543	C	4.211122	-1.758505	-0.446771
C	3.385287	-3.103957	-0.689724	C	3.787944	0.546102	1.652865
H	4.005904	-3.907448	-1.111837	H	3.029173	2.023992	-1.106989
H	3.190154	-3.367485	0.360239	C	5.038723	1.407311	-1.572543
H	2.424177	-3.119955	-1.216911	C	2.948546	0.651021	-2.741601
C	3.258840	-1.212872	2.635143	H	4.339601	-1.722773	-1.542816
H	3.729402	-2.143352	2.290475	C	5.607478	-1.775357	0.175388
H	3.566219	-1.055817	3.678989	C	3.473619	-3.056288	-0.119839
H	2.171542	-1.374185	2.636156	H	4.887539	0.629290	1.617725
C	3.004803	1.261308	2.329719	C	3.411445	-0.392752	2.798186
H	3.302069	2.155664	1.767438	C	3.209359	1.936929	1.911820
H	1.907510	1.212478	2.306302	H	5.594869	0.515896	-1.898334
H	3.303744	1.413799	3.376802	H	5.500642	1.758104	-0.639772
C	2.907393	1.156849	-2.498133	H	5.210006	2.181835	-2.333913
H	3.460024	0.380954	-3.048034	H	3.134697	1.388706	-3.535504
H	1.843365	0.896657	-2.540102	H	1.863949	0.504228	-2.669482
H	3.045246	2.096314	-3.052173	H	3.390869	-0.297693	-3.081412
C	4.881864	1.697913	-1.047671	H	6.186686	-0.875073	-0.065194
H	5.032291	2.651584	-1.573443	H	6.186381	-2.643185	-0.172578
H	5.277223	1.818554	-0.030172	H	5.556218	-1.844777	1.270800
H	5.507930	0.952755	-1.559732	H	2.529627	-3.145376	-0.673015
H	0.982194	-1.785793	-0.075449	H	3.231865	-3.128646	0.950902
P	-3.895183	-1.491971	-0.081537	H	4.087020	-3.934296	-0.369986
C	-4.129288	-3.313859	-0.197069	H	2.320700	-0.526091	2.841191
H	-3.663749	-3.690829	-1.113281	H	3.729876	0.011946	3.769831
H	-3.653516	-3.806249	0.656899	H	3.861223	-1.389412	2.696089
H	-5.195637	-3.571761	-0.207903	H	3.563103	2.338276	2.872562
C	-4.934716	-1.097605	1.379976	H	2.111939	1.905135	1.951640
H	-5.960009	-1.466094	1.250796	H	3.482308	2.657704	1.130194
H	-4.494466	-1.560355	2.268933	TS ₁₁₁₂₀			
H	-4.954222	-0.015334	1.543221	C	1.747605	4.055432	-0.290985
C	-4.940982	-0.919622	-1.478302	C	0.596760	4.265451	-1.041995
H	-5.967250	-1.296479	-1.387292	C	-0.177533	3.178482	-1.437152
H	-4.955985	0.174342	-1.513268	C	0.234874	1.903820	-1.071749
H	-4.508420	-1.275775	-2.418808	C	1.399101	1.632808	-0.338798
11 _o				C	2.131106	2.756434	0.051271
C	-2.556554	4.074563	0.254313	H	2.354600	4.902067	0.024500
				H	0.291729	5.273663	-1.313325

H	-1.100357	3.304609	-2.001280	P	-3.354991	0.235926	-1.037951
H	3.042760	2.638768	0.641848	C	-3.164155	1.250554	-2.551332
O	-0.600568	0.855671	-1.421778	H	-2.521551	2.111312	-2.339441
C	-0.318048	-0.307372	-0.761492	H	-4.138538	1.602178	-2.913268
C	-1.244411	-0.927119	-0.013213	H	-2.681742	0.651655	-3.330456
H	-0.954161	-1.913592	0.348365	C	-4.368939	1.297776	0.052110
Pd	1.690978	-0.445140	-0.242455	H	-5.273392	1.646889	-0.461093
P	3.677970	-0.387754	0.977797	H	-3.766419	2.153397	0.375019
C	3.474658	0.428456	2.607085	H	-4.652594	0.728442	0.943273
H	3.009788	1.410008	2.470959	C	-4.553742	-1.037728	-1.586323
H	4.436094	0.539418	3.124039	H	-5.430499	-0.577832	-2.059481
H	2.801014	-0.177767	3.221501	H	-4.879005	-1.629953	-0.724978
C	5.064658	0.534611	0.211357	H	-4.066151	-1.713133	-2.296806
H	5.909491	0.630109	0.904902	C	-1.669989	-2.342700	0.670841
H	4.722125	1.527911	-0.094220	C	-0.775166	-2.131319	1.661536
H	5.392510	0.001133	-0.686776	C	-0.660154	-2.732805	3.028101
C	4.513833	-1.949883	1.464251	H	0.306689	-3.236879	3.165482
H	5.385043	-1.749425	2.100647	H	-1.455244	-3.459703	3.222039
H	4.843539	-2.487288	0.568776	H	-0.721527	-1.948192	3.792843
H	3.809883	-2.589438	2.006853	C	-2.747024	-3.367464	0.649084
C	1.569399	-2.415063	-1.036737	H	-2.785422	-3.886946	-0.316947
C	0.707013	-1.810080	-1.760152	H	-3.733020	-2.900538	0.786498
C	-0.009894	-1.737167	-3.050293	H	-2.635560	-4.133113	1.432272
H	-1.077697	-1.958799	-2.927560	Si	2.420344	-0.181552	-0.561979
H	0.424787	-2.458084	-3.753153	C	2.147658	1.613623	-1.127222
H	0.068005	-0.735654	-3.487157	C	3.003253	-1.180021	-2.097983
C	2.339967	-3.666677	-0.902853	C	3.765357	-0.282282	0.786604
H	2.207416	-4.114483	0.089444	H	1.738029	2.155294	-0.261539
H	3.413579	-3.473931	-1.020668	C	3.454924	2.288347	-1.544882
H	2.046074	-4.414512	-1.651434	C	1.130880	1.705326	-2.265114
Si	-2.923573	-0.202580	0.451423	H	2.570340	-0.642044	-2.958229
C	-2.776516	1.659605	0.806763	C	4.526020	-1.143234	-2.259495
C	-3.535729	-1.102916	2.026420	C	2.516222	-2.625912	-2.178704
C	-4.132000	-0.490958	-0.994853	H	4.699377	-0.006119	0.268340
H	-2.466455	2.115986	-0.146352	C	3.924790	-1.707271	1.316054
C	-4.118045	2.266884	1.215895	C	3.562093	0.687126	1.948413
C	-1.705579	1.983129	1.846912	H	3.896293	1.793020	-2.421711
H	-3.170995	-0.482873	2.863871	H	4.211719	2.292223	-0.749960
C	-5.061859	-1.153566	2.114208	H	3.276512	3.334667	-1.829994
C	-2.961187	-2.507193	2.209084	H	0.879985	2.754318	-2.480073
H	-5.139539	-0.247119	-0.618717	H	0.195961	1.182237	-2.019692
C	-4.129532	-1.954388	-1.434073	H	1.532219	1.273157	-3.193123
C	-3.828527	0.426704	-2.178200	H	4.938638	-0.126813	-2.231592
H	-4.462183	1.858386	2.177181	H	4.826256	-1.592235	-3.216696
H	-4.909951	2.085153	0.476534	H	5.025829	-1.718398	-1.467846
H	-4.034738	3.355046	1.346439	H	1.425407	-2.695577	-2.264821
H	-1.597907	3.070443	1.971176	H	2.817118	-3.209960	-1.296849
H	-0.718839	1.589725	1.570384	H	2.942744	-3.131589	-3.056761
H	-1.968022	1.569730	2.832242	H	3.015873	-2.032711	1.842402
H	-5.530095	-0.166991	2.009623	H	4.753764	-1.774379	2.034752
H	-5.386186	-1.570332	3.078283	H	4.119754	-2.437190	0.519164
H	-5.482992	-1.798812	1.330790	H	4.436731	0.686928	2.614451
H	-1.871030	-2.499549	2.322655	H	2.692419	0.390814	2.547766
H	-3.198519	-3.156980	1.353643	H	3.392558	1.720776	1.620608
H	-3.380910	-2.990155	3.103233				
H	-3.133211	-2.254676	-1.791631	TS _{570R}			
H	-4.836273	-2.128417	-2.257884	C	1.660293	0.144291	-4.168600
H	-4.399588	-2.637619	-0.617773	C	0.435248	-0.394797	-4.566529
H	-4.512098	0.230379	-3.016669	C	-0.581775	-0.579452	-3.643895
H	-2.802710	0.283008	-2.543448	C	-0.415048	-0.213432	-2.300160
H	-3.924664	1.487869	-1.913785	C	0.804039	0.371063	-1.885933
				C	1.828115	0.515203	-2.841965
12o				H	2.478087	0.250369	-4.877401
C	-0.541117	3.890408	0.985909	H	0.279483	-0.694748	-5.600375
C	0.195104	3.644330	2.138803	H	-1.534419	-1.023746	-3.926536
C	0.481403	2.334047	2.511011	H	2.788387	0.915717	-2.513796
C	0.022375	1.286751	1.719656	O	-1.430517	-0.573996	-1.497282
C	-0.730402	1.488099	0.546016	C	-1.662318	-0.061243	-0.214344
C	-0.990162	2.817407	0.212171	C	-2.278095	-0.907820	0.630156
H	-0.767903	4.912364	0.687539	Si	-3.058253	-2.592494	0.327495
H	0.554417	4.468284	2.751279	C	-4.502955	-2.305334	-0.883919
H	1.060705	2.111260	3.404866	H	-4.009502	-1.997348	-1.822468
H	-1.551931	3.041409	-0.698441	C	-1.909582	-3.943285	-0.380549
O	0.328395	0.005361	2.187494	H	-2.478389	-4.882112	-0.264325
C	0.175019	-1.027934	1.287420	C	-3.726154	-3.172134	2.027476
C	0.884830	-1.085032	0.100988	H	-4.663159	-2.603004	2.164604
H	0.732602	-2.045580	-0.390429	Pd	0.953282	1.546569	-0.204130
Pd	-1.363109	-0.412877	-0.111159	C	-4.073466	-4.661204	2.063364

H	-3.166125	-5.278637	2.000244	H	4.636027	0.649683	1.060983
H	-4.572877	-4.928324	3.005595	H	3.480208	1.987663	1.245192
C	-4.733300	-4.968962	1.242982	H	5.022819	2.014584	2.122985
H	-2.809216	-2.839971	3.206943	C	1.060117	-1.549139	4.785470
H	-3.250784	-3.180045	4.154957	H	0.119267	-1.732987	5.323893
H	-1.835090	-3.341631	3.111309	H	1.621124	-2.491253	4.779088
H	-2.609162	-1.766163	3.306215	H	1.636793	-0.826164	5.380547
C	-0.623476	-4.056699	0.434242	C	-0.170795	0.168537	3.411219
H	-0.800369	-4.422521	1.454524	H	-0.464378	0.471373	2.399318
H	0.097267	-4.742537	-0.040148	H	-1.090736	-0.082708	3.960291
H	-0.127187	-3.079687	0.517896	H	0.277458	1.038599	3.910214
C	-1.583816	-3.781460	-1.863058	C	2.609570	-3.515965	1.793846
H	-2.480147	-3.667376	-2.487141	H	2.032931	-3.391722	0.872053
H	-0.958278	-2.896086	-2.028820	H	3.270837	-4.382363	1.653366
H	-1.032016	-4.658608	-2.236105	H	1.898616	-3.784026	2.588615
C	-5.402315	-1.156793	-0.431608	C	4.301296	-2.577314	3.374839
H	-5.896280	-1.391546	0.522872	H	3.709328	-2.706558	4.291372
H	-4.844341	-0.223379	-0.291339	H	4.852343	-3.515199	3.219184
H	-6.201305	-0.966586	-1.162834	H	5.045027	-1.797542	3.571389
C	-5.339889	-3.552425	-1.162114				
H	-6.081948	-3.365443	-1.951734	7 _{OR}			
H	-4.737631	-4.415906	-1.475299	C	1.700745	0.929816	3.924536
H	-5.904023	-3.851188	-0.266745	C	0.805080	-0.041460	4.385505
Zn	-1.804273	1.933502	0.239168	C	-0.143632	-0.604218	3.545675
O	1.150638	2.856842	1.526077	C	-0.254594	-0.183502	2.217263
C	0.109380	3.309383	2.081986	C	0.602266	0.856640	1.730950
O	-1.081117	3.052224	1.757780	C	1.585500	1.379165	2.621971
C	0.295060	4.246259	3.248531	H	2.449690	1.350877	4.589868
H	-0.423235	5.067856	3.177992	H	0.864179	-0.380945	5.417743
H	0.073003	3.702982	4.174924	H	-0.823249	-1.380144	3.888858
H	1.316938	4.628724	3.299223	H	2.206264	2.195021	2.254119
O	-2.608282	3.359460	-1.124909	O	-1.217577	-0.742759	1.491311
C	-3.725539	3.255247	-0.518138	C	-1.036663	-1.140946	0.142755
O	-3.853859	2.502561	0.481870	C	-2.138487	-1.192815	-0.615944
C	-4.910549	4.037887	-1.006950	Si	-3.982612	-1.085219	-0.256427
H	-5.704351	3.340787	-1.293200	C	-4.421221	-2.747066	0.573452
H	-5.303215	4.648784	-0.188609	H	-3.932738	-2.680076	1.562260
H	-4.650958	4.672247	-1.856411	C	-4.590322	0.323036	0.875523
H	-2.542864	-0.450403	1.591158	H	-5.687715	0.298442	0.756389
P	0.706100	3.525587	-1.510692	C	-4.826393	-0.933307	-1.968655
O	0.064704	5.053102	-0.733260	H	-4.805812	-1.956673	-2.383915
H	-0.998849	4.923507	-0.508918	Pd	2.027784	-0.007667	0.262087
H	0.620595	5.249286	0.189705	C	-6.288657	-0.492818	-1.884194
H	0.196339	5.898035	-1.420037	H	-6.369943	0.543435	-1.526958
C	2.416504	4.027378	-1.943764	H	-6.768620	-0.525655	-2.872551

H	-0.686832	-6.311125	0.790660	C	3.199971	5.245979	-1.347899
H	0.443445	-6.742966	-0.487706	H	2.156496	4.924133	-1.202789
H	1.050499	-6.435144	1.173780	C	3.735275	3.714912	1.312245
H	-1.939961	-1.624890	-1.606253	H	3.938090	4.700279	1.766823
P	3.501289	-1.552524	1.459342	C	6.102025	4.348848	-0.632180
C	4.366925	-2.834779	0.478860	H	6.202541	4.888002	-1.590205
H	3.645604	-3.602683	0.183934	Pd	1.459801	-0.949788	-1.464173
H	4.811433	-2.382731	-0.413667	C	6.548920	5.299303	0.480060
H	5.160740	-3.290892	1.082941	H	6.526385	4.805741	1.461213
C	4.903310	-0.509241	2.025625	H	7.582558	5.637282	0.318063
H	5.680913	-1.114186	2.508752	H	5.919266	6.194129	0.554404
H	5.332363	0.009680	1.160747	C	7.033378	3.136182	-0.689593
H	4.537201	0.242404	2.733478	H	8.087829	3.444118	-0.636965
C	3.044811	-2.486996	2.963353	H	6.855266	2.443170	0.146989
H	3.934758	-2.958328	3.398886	H	6.907645	2.568217	-1.619251
H	2.593039	-1.816925	3.700272	C	4.573203	2.674793	2.052236
H	2.319164	-3.255112	2.675846	H	5.642822	2.919912	2.059458
C	0.853842	1.520130	-0.558156	H	4.252828	2.577142	3.101588
C	0.191247	1.716987	0.571966	H	4.470718	1.686442	1.582707
O	-0.855935	2.589106	0.817506	C	2.249110	3.412810	1.493353
C	-0.786577	3.282117	2.009385	H	1.604727	4.159005	1.010267
C	0.141270	4.309834	2.152870	H	1.988938	2.438096	1.057198
C	-1.644883	2.937949	3.046722	C	1.980366	3.384735	2.561460
C	0.213830	4.996642	3.358952	H	3.458682	5.316807	-2.851623
H	0.800143	4.547118	1.318057	H	4.496824	5.613676	-3.063027
C	-1.564198	3.633162	4.249549	H	3.286709	4.352178	-3.344967
C	-2.357957	2.128697	2.897933	H	2.811102	6.064154	-3.332458
C	-0.634920	4.656770	4.410047	C	3.376525	6.621891	-0.710746
H	0.935395	5.801640	3.478391	H	2.690386	7.357277	-1.155438
H	-2.229807	3.368168	5.067668	H	3.191848	6.615708	0.372036
H	-0.574608	5.194813	5.352957	H	4.394552	7.005453	-0.871458
Si	0.663115	2.356459	-2.240625	Zn	3.054927	0.332083	-3.362857
C	2.350304	2.876900	-2.951188	O	2.959153	-2.555132	-1.662172
H	2.098364	3.729949	-3.602993	C	3.911340	-2.411240	-2.482166
C	-0.375936	1.248741	-3.383321	O	4.136079	-1.389856	-3.188226
H	-1.349547	1.202153	-2.865341	C	4.859800	-3.568396	-2.661169
C	-0.326007	3.975210	-1.900349	H	4.869773	-3.855331	-3.718336
H	-0.047011	4.273005	-0.876936	H	5.875839	-3.246137	-2.406552
C	3.102148	1.862307	-3.805822	H	4.576888	-4.421613	-2.041264
H	4.015834	2.311032	-4.222716	O	2.032429	0.090563	-5.209445
H	3.403395	0.997905	-3.204911	C	3.004189	0.687123	-5.786652
H	2.501592	1.502163	-4.651310	O	3.999307	1.083313	-5.130522
C	3.242725	3.391445	-1.820932	C	2.927499	0.905390	-7.269885
H	2.739706	4.147031	-1.199873	H	2.777477	-0.054980	-7.772804
H	3.532785	2.562190	-1.159230	H	2.057425	1.528106	-7.500984
H	4.165819	3.843054	-2.211602	H	3.833910	1.384726	-7.642729
C	-0.598989	1.875861	-4.759308	H	4.911412	1.782678	-1.878998
H	-1.289712	1.263262	-5.357315	P	0.297588	-1.926008	-3.222984
H	-1.024244	2.885944	-4.704853	C	1.327984	-2.891127	-4.382989
H	0.340770	1.947729	-5.325530	H	1.946325	-2.202740	-4.968723
C	0.126980	-0.181667	-3.522050	H	1.957958	-3.582686	-3.815971
H	0.233207	-0.669121	-2.546586	H	0.671287	-3.460054	-5.052508
H	-0.563921	-0.790197	-4.124904	C	-0.754391	-3.234349	-2.488219
H	1.105808	-0.224028	-4.019949	H	-1.267523	-3.800513	-3.275671
C	-1.837299	3.739745	-1.904550	H	-0.108786	-3.908265	-1.913061
H	-2.132587	2.890663	-1.278240	H	-1.500436	-2.809506	-1.809761
H	-2.370178	4.624039	-1.526961	C	-0.789754	-0.981164	-4.337005
H	-2.210313	3.552651	-2.921073	H	-1.322618	-1.676195	-4.997530
C	0.022718	5.135304	-2.833319	H	-1.505570	-0.380413	-3.770633
H	-0.148666	4.880393	-3.889115	H	-0.146766	-0.323421	-4.932395
H	-0.607652	6.008529	-2.611719	C	3.319414	-0.491436	0.411093
H	1.067106	5.456470	-2.739595	C	2.131563	-0.630658	0.749713
				O	4.531639	-0.302834	0.058231
				C	5.469584	-1.348849	0.076727
				C	5.218105	-2.564427	0.691465
				C	6.677011	-1.049326	-0.533042
				C	6.235940	-3.513453	0.698516
				H	4.246777	-2.769051	1.136610
				C	7.679214	-2.012309	-0.518181
				H	6.807221	-0.078438	-1.005091
				C	7.462814	-3.242211	0.100079
				H	6.062291	-4.474210	1.176695
				H	8.633709	-1.797396	-0.991437
				H	8.250905	-3.990469	0.113226
				Si	1.315161	-1.036671	2.394679
				C	1.612063	-2.906709	2.601305
				H	2.697576	-2.989466	2.787791
				C	-0.510871	-0.559625	2.469377
6' OR							
C	-2.254613	1.242126	-1.213051				
C	-1.861209	2.576344	-1.213806				
C	-0.516635	2.886438	-1.315410				
C	0.463909	1.886636	-1.414160				
C	0.085628	0.532214	-1.407996				
C	-1.282489	0.252285	-1.314691				
H	-3.303573	0.966432	-1.127899				
H	-2.596913	3.373445	-1.137463				
H	-0.173597	3.919120	-1.317006				
H	-1.615083	-0.784598	-1.301468				
O	1.723306	2.384769	-1.430584				
C	2.851472	1.714223	-1.865460				
C	4.017383	2.280885	-1.490425				
Si	4.246567	3.879092	-0.525294				

H	-0.797624	-0.712318	3.525064	C	5.648808	-3.026301	-3.296225
C	2.288049	-0.020426	3.681398	H	5.505421	-3.465934	-4.290231
H	2.397394	0.974438	3.213805	H	6.588257	-2.467875	-3.317605
C	0.884640	-3.456887	3.828320	H	5.695172	-3.827590	-2.554891
H	1.155500	-2.928019	4.751344	O	1.914190	0.222376	-5.262162
H	-0.205256	-3.377425	3.714195	C	2.678092	1.057641	-5.854893
H	1.113966	-4.520466	3.982052	O	3.653770	1.576055	-5.256220
C	1.291779	-3.735291	1.356337	C	2.382201	1.403932	-7.285049
H	0.221803	-3.690433	1.111549	H	2.404122	0.492654	-7.890850
H	1.848346	-3.398206	0.471433	H	1.369968	1.813606	-7.359156
H	1.536139	-4.794131	1.525256	H	3.104152	2.124646	-7.671952
C	3.688961	-0.577520	3.923511	H	4.842261	1.901097	-1.985270
H	4.276158	0.095491	4.563150	P	0.595272	-2.178681	-3.284750
H	3.650322	-1.551965	4.431693	C	1.473500	-2.906922	-4.716064
H	4.259525	-0.714470	2.994675	H	1.950815	-2.097368	-5.279963
C	1.550044	0.158477	5.007710	H	2.235381	-3.604318	-4.354162
H	1.388716	-0.802183	5.517364	H	0.766171	-3.437545	-5.365196
H	2.131618	0.788172	5.695059	C	-0.334463	-3.623531	-2.634843
H	0.568661	0.631325	4.880886	H	-0.915604	-4.101914	-3.433116
C	-0.688708	0.924729	2.142166	H	0.370607	-4.348635	-2.213733
H	-0.312269	1.166847	1.139574	H	-1.018435	-3.302240	-1.842023
H	-1.749773	1.209282	2.164861	C	-0.708901	-1.165303	-4.066372
H	-0.158499	1.568366	2.856329	H	-1.336567	-1.784416	-4.719456
C	-1.401980	-1.455062	1.609742	H	-1.330709	-0.700344	-3.293811
H	-2.412808	-1.032083	1.516406	H	-0.216614	-0.387270	-4.658500
H	-1.002463	-1.562232	0.593196	C	3.084297	-0.523278	0.092949
H	-1.500006	-2.462223	2.034455	C	1.937345	-0.407321	0.657929
				C	4.387993	-0.389002	0.094883
				C	5.226409	-1.495053	0.187786
TS' _{670R}				C	4.760212	-2.772445	0.465887
C	-1.954820	0.144473	-0.726200	C	6.576668	-1.224911	0.017551
C	-1.915025	1.482829	-1.119383	C	5.684708	-3.806090	0.569858
C	-0.691879	2.095003	-1.334987	H	3.693297	-2.959536	0.566844
C	0.512119	1.395114	-1.171520	C	7.486074	-2.270722	0.127092
C	0.483336	0.034593	-0.798449	H	6.888732	-0.204783	-0.192842
C	-0.767279	-0.554742	-0.561138	C	7.044955	-3.562382	0.402243
H	-2.905802	-0.351435	-0.541358	H	5.332182	-4.812680	0.781518
H	-2.834644	2.045874	-1.256687	H	8.546575	-2.070862	-0.004371
H	-0.621121	3.135870	-1.643561	H	7.759751	-4.376780	0.486907
H	-0.798777	-1.596549	-0.242201	Si	1.288614	-0.845754	2.396159
O	1.623170	2.135185	-1.352535	C	1.288898	-2.760163	2.453249
C	2.816365	1.621491	-1.849459	H	2.370174	-2.986301	2.517193
C	3.930833	2.296030	-1.517804	C	-0.317185	0.008981	2.958715
Si	4.150581	3.927375	-0.611662	H	-0.140905	0.031857	4.050025
C	3.718773	5.304407	-1.855155	C	2.600953	-0.159752	3.613773
H	2.628760	5.202961	-2.002750	H	2.377874	0.920047	3.657950
C	3.111934	4.176772	0.970609	C	0.618853	-3.361859	3.691384
H	3.606668	5.027277	1.471892	H	0.932354	-2.893797	4.629683
C	6.009017	4.013637	-0.145821	H	-0.473247	-3.276037	3.631496
H	6.514515	4.354071	-1.067062	H	0.845974	-4.434162	3.766743
Pd	1.979909	-1.183524	-1.559735	C	0.748301	-3.452278	1.202417
C	6.315732	5.026797	0.956925	H	-0.336438	-3.298144	1.103013
H	5.888025	4.707755	1.918130	H	1.222549	-3.094901	0.276636
H	7.399388	5.130453	1.110611	H	0.906293	-4.538785	1.259824
H	5.918059	6.026235	0.740321	C	4.061877	-0.320403	3.203853
C	6.598074	2.651008	0.223881	H	4.723563	0.003347	4.019438
H	7.660936	2.737165	0.493847	H	4.316351	-1.368908	2.987638
H	6.079236	2.200414	1.084443	H	4.318655	0.274274	2.322274
H	6.519596	1.933981	-0.602251	C	2.420658	-0.728972	5.024432
C	3.206219	2.969858	1.898614	H	2.747266	-1.777093	5.069140
H	4.244085	2.719066	2.158150	H	3.045115	-0.174000	5.737537
H	2.667880	3.149736	2.843138	H	1.388847	-0.681697	5.395775
H	2.761007	2.083797	1.420743	C	-0.379045	1.464245	2.488752
C	1.652114	4.565897	0.749664	H	-0.572901	1.530935	1.410849
H	1.544886	5.439857	0.094842	H	-1.189390	2.001411	3.000379
H	1.087269	3.742953	0.294144	H	0.551970	2.011315	2.687388
H	1.165893	4.810798	1.705778	C	-1.658964	-0.688912	2.754997
C	4.396059	5.088493	-3.206885	H	-2.451882	-0.144522	3.286627
H	5.491663	5.130643	-3.114604	H	-1.944709	-0.715639	1.699436
H	4.138349	4.119101	-3.650103	H	-1.663486	-1.717352	3.132252
H	4.109731	5.871599	-3.923458				
C	4.013617	6.708768	-1.331036				
H	3.651981	7.479094	-2.027282	7' _{OR}			
H	3.556720	6.909903	-0.352607	C	-1.403272	-0.484784	-1.166921
H	5.097199	6.864894	-1.224384	C	-1.158692	0.793767	-1.663563
Zn	3.094184	0.453443	-3.524341	C	0.060010	1.423297	-1.431427
C	3.585437	-2.511764	-2.258114	C	1.022985	0.811620	-0.629279
O	4.503487	-2.089077	-3.012585	C	0.803862	-0.492319	-0.107560
O	4.541928	-0.957839	-3.573693	C	-0.423969	-1.128520	-0.415804

H	-2.354563	-0.976704	-1.355417	C	4.561791	-6.538351	-0.282644
H	-1.923302	1.305163	-2.245312	H	2.486543	-6.786989	-0.802947
H	0.277810	2.413368	-1.829493	H	6.561280	-5.980285	0.297013
H	-0.603051	-2.115971	0.010580	H	4.818445	-7.576314	-0.478438
O	2.139828	1.475114	-0.277504	Si	1.906664	-0.892286	2.726188
C	3.120387	1.690047	-1.274828	C	2.128193	-2.636945	3.482726
C	3.693842	2.897613	-1.355791	H	3.176568	-2.903649	3.258175
Si	3.428396	4.610314	-0.640314	C	0.328335	-0.042657	3.382024
C	2.537754	5.585724	-2.020664	H	0.576210	0.179533	4.436438
H	1.520383	5.156714	-2.055759	C	3.375852	0.260455	3.129642
C	2.410411	4.726580	0.960632	H	2.933910	1.269052	3.093613
H	2.515545	5.774607	1.291462	C	1.943859	-2.668448	5.002202
C	5.177795	5.331710	-0.354870	H	2.629433	-2.000764	5.533286
H	5.509577	5.679834	-1.349569	H	0.921280	-2.383507	5.286929
Pd	1.861134	-1.703311	-1.787575	H	2.108048	-3.683555	5.390381
C	5.185904	6.534454	0.589097	C	1.230074	-3.701939	2.850610
H	4.903647	6.238802	1.609425	H	0.178400	-3.549341	3.128736
H	6.189463	6.978320	0.654047	H	1.278902	-3.704537	1.756476
H	4.494681	7.328155	0.278516	H	1.511539	-4.706150	3.197343
C	6.182912	4.282594	0.123781	C	4.502634	0.213087	2.099892
H	7.176651	4.729300	0.271909	H	5.288436	0.940118	2.353818
H	5.881027	3.842364	1.085075	H	4.971148	-0.780873	2.063183
C	6.291730	3.454297	-0.585001	H	4.147585	0.448768	1.089132
C	2.988647	3.821875	2.046221	C	3.937470	0.068072	4.537728
H	4.022645	4.083349	2.306368	H	4.416131	-0.915278	4.646635
H	2.395707	3.875302	2.972660	H	4.707763	0.822516	4.750414
C	2.990367	2.776439	1.708595	C	3.171080	0.157826	5.319003
C	0.923183	4.447051	0.758094	H	0.032486	1.289134	2.688925
H	0.463914	5.130710	0.032268	H	-0.345574	1.130660	1.668283
H	0.763045	3.419909	0.403545	H	-0.746337	1.846978	3.228080
C	0.368548	4.551803	1.702541	H	0.910203	1.943030	2.612780
C	3.178302	5.368121	-3.390500	C	-0.924133	-0.917423	3.367551
H	4.223554	5.710403	-3.403771	H	-1.795082	-0.362337	3.744455
H	3.176411	4.309995	-3.681855	H	-1.171687	-1.241908	2.346039
H	2.648657	5.933360	-4.170978	H	-0.819927	-1.818707	3.982738
C	2.419462	7.077572	-1.717985				
H	1.822129	7.596111	-2.481724	C ₆ H ₅ OC≡CSiMe ₃			
H	1.953329	7.277106	-0.743780	C	0.347028	-1.870913	-0.506870
H	3.410132	7.554501	-1.713092	C	0.313063	-0.613750	-1.100552
Zn	3.855030	0.259623	-2.551159	C	1.160959	0.400797	-0.665236
O	3.254672	-3.030300	-2.647622	C	2.037200	0.125552	0.372633
C	4.461921	-2.649424	-2.754099	C	2.092827	-1.120360	0.981898
O	4.892777	-1.493122	-2.530116	C	1.239008	-2.119624	0.533753
C	5.427586	-3.710886	-3.208282	H	-0.319393	-2.656307	-0.853736
H	5.241802	-3.922631	-4.267491	H	-0.380553	-0.413437	-1.913624
H	6.457692	-3.372752	-3.085575	H	1.149057	1.389675	-1.116679
H	5.253607	-4.635453	-2.648562	H	1.272678	-3.100202	1.002262
O	3.448416	0.434334	-4.651060	O	2.922912	1.076112	0.876323
C	4.507030	1.133639	-4.765684	C	2.926666	2.272736	0.373568
O	5.251212	1.355137	-3.775067	C	2.963444	3.407704	-0.068319
C	4.864506	1.724298	-6.100228	Si	3.038917	5.120243	-0.718055
H	4.222745	1.339038	-6.894768	H	2.800189	-1.282975	1.790486
H	4.757623	2.812918	-6.043572	C	3.062321	5.061964	-2.595892
H	5.914541	1.517340	-6.324876	H	3.111838	6.076110	-3.010782
H	4.488760	2.918203	-2.113334	H	3.929892	4.503447	-2.963785
P	0.857033	-1.498941	-4.047813	C	2.160230	4.581735	-2.991185
C	1.919215	-2.222998	-5.351568	H	1.533721	6.079719	-0.133209
H	2.789606	-1.568222	-5.475759	H	0.604462	5.614578	-0.480153
H	2.250974	-3.217194	-5.036876	H	1.496649	6.129533	0.960462
H	1.370496	-2.293670	-6.298812	H	1.560271	7.106672	-0.517766
C	-0.650945	-2.547125	-4.149545	C	4.604093	5.938725	-0.080702
H	-1.038485	-2.586560	-5.175232	H	5.497138	5.391910	-0.402147
H	-0.408520	-3.562826	-3.818385	H	4.681002	6.965382	-0.459079
C	-1.423094	-2.142088	-3.486402	H	4.611017	5.981308	1.013838
C	0.305203	0.069217	-4.817290				
H	-0.142197	-0.127841	-5.799642	2 _{OME}			
H	-0.428967	0.567734	-4.177020	C	5.055859	-0.761592	-0.267793
H	1.185097	0.710389	-4.934338	C	4.420778	-1.655313	-1.127776
C	2.556295	-1.924960	0.100446	C	3.157909	-2.146733	-0.815788
C	1.788638	-1.125447	0.845183	C	2.556343	-1.724774	0.360239
O	3.657190	-2.573433	0.519422	C	3.159389	-0.835740	1.234107
C	3.899963	-3.891896	0.215620	C	4.425560	-0.355347	0.905848
C	2.910922	-4.772311	-0.210144	H	6.045583	-0.383412	-0.512080
C	5.211523	-4.316471	0.400627	H	4.911702	-1.976668	-2.043039
C	3.253577	-6.095092	-0.462879	H	2.636842	-2.843446	-1.468384
H	1.895414	-4.414344	-0.367290	H	4.917634	0.348157	1.573878
C	5.537104	-5.644711	0.152451	O	1.294407	-2.237888	0.706142
H	5.952436	-3.593611	0.733543				

C	0.287867	-1.899264	-0.057163	P	0.309460	-1.874946	1.951747
C	-0.846695	-1.902520	-0.590952	C	-1.193357	-2.010991	2.996823
Si	-2.575189	-2.199595	-1.211610	H	-1.206846	-1.200919	3.733581
C	-2.616275	-3.920256	-1.967598	H	-2.070194	-1.914715	2.346832
H	-3.619992	-4.147518	-2.347198	H	-1.229442	-2.975933	3.518994
C	-3.732727	-2.064918	0.253469	C	0.170412	-3.383050	0.912411
H	-4.736875	-2.412102	-0.019384	H	0.088056	-4.287414	1.528628
C	-2.963730	-0.897021	-2.501929	H	-0.723772	-3.291257	0.283274
H	-3.954145	-1.066594	-2.941757	H	1.055083	-3.452379	0.268466
Pd	0.150187	0.012674	-1.064562	C	1.635608	-2.353333	3.132056
Zn	-1.020967	0.600605	1.130354	H	1.399887	-3.299993	3.634972
O	-2.897871	1.210256	0.336345	H	2.581460	-2.456834	2.589603
C	-2.544485	2.410232	0.530274	H	1.760566	-1.567043	3.883275
O	-1.415789	2.680306	1.043094	C	-1.171719	4.340003	1.233168
C	-3.478665	3.519708	0.144958	H	-0.500343	4.023412	2.039937
H	-3.002115	4.495492	0.256036	H	-0.579008	4.902752	0.503120
H	-3.815540	3.374036	-0.885770	H	-1.919639	5.019649	1.658677
H	-4.368418	3.475248	0.781089	C	-3.136640	3.328344	-0.959312
O	-1.371072	-0.740320	2.688467	H	-3.946724	3.967975	-0.588179
C	-0.198122	-0.532170	3.116727	H	-2.609963	3.873330	-1.750079
O	0.557238	0.313183	2.546232	H	-3.582635	2.426764	-1.396805
C	0.335783	-1.318969	4.276454	C	-2.899129	1.824209	1.715481
H	0.861459	-0.656752	4.969651	H	-3.446708	1.004500	1.232593
H	-0.460593	-1.859117	4.790847	H	-2.200154	1.389495	2.440490
H	1.067179	-2.041224	3.893667	H	-3.627442	2.436227	2.260983
H	2.613473	-0.500938	2.116152				
P	1.273264	2.061299	-1.133105	3 _{OMe}			
C	0.405534	3.529823	-1.807457	C	-5.366051	0.128195	0.027912
H	0.042067	3.327923	-2.819657	C	-5.445389	1.488993	0.306609
H	-0.449156	3.744487	-1.156328	C	-4.285643	2.254244	0.403102
C	1.070156	4.402786	-1.826905	C	-3.072116	1.612881	0.218370
H	1.879772	2.699446	0.474267	C	-2.936137	0.246879	-0.062812
H	2.501718	3.590861	0.320302	C	-4.122604	-0.480568	-0.159511
H	1.024900	2.954957	1.108604	H	-6.275906	-0.464814	-0.043523
C	2.465481	1.921940	0.976866	H	-6.414187	1.962433	0.449332
C	2.827492	2.011294	-2.110650	H	-4.318373	3.320670	0.611797
H	3.334059	2.985209	-2.101607	H	-4.084661	-1.547295	-0.382990
H	3.489909	1.255457	-1.670566	O	-1.905067	2.362473	0.328695
H	2.613296	1.722058	-3.144219	C	-0.830875	1.620055	0.069528
H	-2.353945	-4.684712	-1.228160	C	0.470366	1.730593	-0.029809
H	-1.912972	-4.001382	-2.803915	Si	1.560198	3.210199	-0.408075
H	-3.377081	-2.660221	1.101317	Pd	-0.954436	-0.291609	-0.470639
H	-3.806636	-1.020904	0.580768	Zn	1.608798	-0.002568	0.240480
H	-2.224459	-0.901723	-3.311791	O	2.749246	-1.581581	-0.609971
H	-2.964265	0.092215	-2.027706	C	3.790410	-0.916967	-0.317697
				O	3.692439	0.210594	0.253370
TS _{23OMe}				C	5.149884	-1.461426	-0.634736
C	5.219872	0.297103	0.037380	H	5.083020	-2.376476	-1.225142
C	5.261307	1.629504	-0.368162	H	5.730913	-0.704700	-1.169456
C	4.090870	2.288307	-0.733794	H	5.677995	-1.666943	0.301861
C	2.909432	1.570538	-0.679672	O	1.339188	-0.904584	2.153123
C	2.797033	0.223893	-0.317607	C	0.444065	-1.369880	2.854132
C	4.006313	-0.384692	0.056059	O	-0.825756	-1.417122	2.524618
H	6.139126	-0.210561	0.321844	C	0.714253	-1.979133	4.189841
H	6.207875	2.164360	-0.395715	H	0.536994	-3.058311	4.128456
H	4.088801	3.332654	-1.035069	H	1.746341	-1.793483	4.488638
H	3.991644	-1.442403	0.325869	H	0.017950	-1.579510	4.931919
O	1.730424	2.274740	-1.012484	H	-1.004558	-1.008307	1.631832
C	0.662545	1.761698	-0.466329	P	-0.601335	-2.542559	-1.191734
C	-0.614706	1.764828	-0.256252	C	0.428089	-2.784347	-2.690662
Si	-1.981377	2.845174	0.434652	H	0.015860	-2.200474	-3.519543
Pd	0.751013	0.062765	0.671030	H	1.438586	-2.422386	-2.468318
Zn	-1.339783	-0.211655	-0.807740	H	0.470059	-3.842905	-2.977455
O	-2.624239	-1.740794	-0.051117	C	0.195973	-3.716497	-0.022875
C	-3.570822	-1.156803	-0.656252	H	0.142959	-4.743818	-0.404666
O	-3.355073	-0.090283	-1.311871	H	1.248243	-3.431949	0.092447
C	-4.965233	-1.702582	-0.597358	H	-0.304251	-3.669375	0.951424
H	-5.008438	-2.618255	-0.005889	C	-2.144122	-3.441061	-1.623030
H	-5.627384	-0.945505	-0.164975	H	-1.927278	-4.443520	-2.013220
H	-5.322158	-1.895038	-1.613568	H	-2.769882	-3.529649	-0.727823
O	-0.348771	-1.190322	-2.271855	H	-2.702740	-2.869589	-2.371674
C	0.702828	-1.863182	-2.403634	C	0.432172	4.664933	-0.785900
O	1.794720	-1.701937	-1.770347	H	-0.207334	4.446139	-1.648758
C	0.678620	-3.004688	-3.381224	H	-0.221791	4.884771	0.065350
H	1.686617	-3.275713	-3.699926	H	1.013348	5.567185	-1.011878
H	0.225974	-3.869223	-2.881004	C	2.660402	3.569733	1.070911
H	0.049102	-2.754035	-4.238032	H	3.303386	4.437313	0.877941
H	1.995013	-0.755566	-1.039694	H	2.067470	3.780270	1.967932

H	3.310018	2.710631	1.278773	Si	1.568952	3.009609	-0.587162
C	2.630318	2.763059	-1.885436	Pd	-1.110566	-0.494122	-0.237363
H	3.236089	3.615256	-2.215539	Zn	1.606622	-0.196418	-0.152713
H	3.313993	1.950081	-1.608168	O	0.668114	1.163138	2.706326
H	2.016738	2.429041	-2.729977	C	1.503899	0.164180	2.858939
TS_{34OMe}				O	2.023472	-0.455845	1.929888
C	-5.466894	0.163480	-0.094534	C	1.763020	-0.178090	4.286995
C	-5.514259	1.551994	-0.166341	H	0.875892	-0.674742	4.694917
C	-4.337163	2.290952	-0.259681	H	2.619918	-0.847711	4.362630
C	-3.138515	1.597385	-0.279466	H	1.923295	0.730810	4.872396
C	-3.038983	0.201120	-0.213972	O	2.429348	-2.002992	-0.837763
C	-4.238429	-0.502231	-0.117420	C	3.495538	-1.369029	-1.118609
H	-6.390219	-0.407851	-0.019826	O	3.570410	-0.123260	-0.909557
H	-6.471628	2.067856	-0.147483	C	4.673494	-2.112328	-1.669209
H	-4.344745	3.376667	-0.314519	H	5.353813	-1.431978	-2.184587
H	-4.225158	-1.590525	-0.058543	H	5.212306	-2.578124	-0.836928
O	-1.953462	2.313735	-0.362031	H	4.343165	-2.911111	-2.337334
C	-0.902648	1.485091	-0.361264	H	0.481869	1.328000	1.740748
C	0.408382	1.576852	-0.359093	P	-0.926373	-2.877352	-0.165746
Si	1.516407	3.092894	-0.396420	C	0.180092	-3.575513	1.123935
Pd	-1.077262	-0.489199	-0.315729	H	1.207952	-3.267746	0.901236
Zn	1.618242	-0.128221	-0.198855	H	-0.101774	-3.184067	2.107182
O	0.066502	0.424091	2.765957	C	0.125746	-4.671389	1.139944
C	1.242201	-0.156141	2.853202	H	-2.496437	-3.777217	0.150733
O	1.907860	-0.532736	1.890430	H	-2.322246	-4.856459	0.245837
C	1.724709	-0.294329	4.257327	H	-2.962547	-3.398594	1.066606
H	0.894045	-0.492695	4.937887	C	-3.183773	-3.598106	-0.683246
H	2.480094	-1.078855	4.314894	H	-0.305469	-3.729541	-1.666467
H	2.183842	0.654266	4.558094	H	-0.319138	-4.818862	-1.532930
O	2.521991	-1.859065	-0.991691	H	-0.926859	-3.462098	-2.526851
C	3.596353	-1.191353	-1.109913	H	0.721493	-3.395958	-1.850163
O	3.634564	0.024635	-0.756667	C	2.209146	2.890820	-2.346952
C	4.833196	-1.841482	-1.649404	H	2.785041	1.966678	-2.477406
H	4.606492	-2.806757	-2.104773	H	1.383077	2.887556	-3.066683
H	5.313688	-1.178039	-2.373297	C	2.867337	3.735380	-2.584606
H	5.541270	-1.988875	-0.827158	H	0.594309	4.593284	-0.316851
H	-0.217860	0.523513	1.825009	H	-0.255278	4.658485	-1.004920
P	-0.802816	-2.861654	-0.225919	H	0.200576	4.644472	0.704745
C	0.329157	-3.527733	1.059964	H	1.234230	5.469671	-0.478224
H	1.345516	-3.173660	0.853403	C	3.010235	2.913171	0.618860
H	0.019950	-3.161997	2.045427	H	3.684699	3.767609	0.485484
C	0.322196	-4.625090	1.063328	H	2.660826	2.924392	1.659305
C	-2.335897	-3.818313	0.099998	H	3.597591	2.000341	0.452547
H	-2.127180	-4.894415	0.153211	TS_{45OMe}			
H	-2.781962	-3.485771	1.043266	C	-3.184166	3.856102	-0.831672
H	-3.054914	-3.631723	-0.705006	C	-2.132909	4.759129	-0.944496
C	-0.161534	-3.677330	-1.737388	C	-0.822659	4.352191	-0.702603
H	-0.112861	-4.765988	-1.607897	C	-0.597197	3.031554	-0.346125
H	-0.813908	-3.442170	-2.584304	C	-1.634097	2.100760	-0.220385
C	0.840640	-3.285421	-1.940666	C	-2.932173	2.529286	-0.472319
C	2.775409	2.922546	0.992865	H	-4.205172	4.179911	-1.021780
H	2.277274	2.786191	1.961373	H	-2.329329	5.791125	-1.225611
H	3.442758	2.069059	0.814621	H	0.015484	5.038589	-0.791682
C	3.399792	3.821509	1.064146	H	-3.765832	1.832791	-0.383977
C	0.443403	4.611711	-0.128561	O	0.682473	2.596403	-0.123747
H	-0.082225	4.555540	0.831421	C	0.735076	1.275105	0.204225
H	1.053264	5.523454	-0.133023	C	1.902484	0.591418	0.326448
H	-0.314622	4.700284	-0.914382	Si	3.586542	1.302965	-0.082098
C	2.414916	3.171570	-2.042006	Pd	-1.039100	0.283245	0.377357
H	3.074693	4.046838	-2.085668	Zn	1.336625	-1.257775	-0.319394
H	3.032757	2.275908	-2.178767	O	1.445441	-0.552692	2.703903
H	1.708305	3.234812	-2.876759	C	0.435334	-1.316316	2.510670
4_{OMe}				O	0.071630	-1.725921	1.374860
C	-5.484888	0.271397	-0.101640	C	-0.366434	-1.707240	3.708119
C	-5.493384	1.661113	-0.157318	H	-1.342080	-1.210167	3.628025
C	-4.293959	2.368273	-0.213356	H	-0.545353	-2.786059	3.699212
C	-3.116804	1.640314	-0.212202	H	0.120597	-1.401144	4.634814
C	-3.054754	0.242016	-0.161812	O	0.138340	-2.287312	-1.733016
C	-4.274834	-0.428483	-0.104876	C	1.012724	-3.205181	-1.701515
H	-6.424938	-0.275120	-0.054819	O	2.055013	-3.074583	-0.987479
H	-6.436427	2.202926	-0.156417	C	0.795639	-4.459148	-2.491797
H	-4.269557	3.454278	-0.256321	H	1.688800	-5.085415	-2.493624
H	-4.292932	-1.517303	-0.058529	H	-0.036098	-5.016201	-2.046648
O	-1.906723	2.324581	-0.255324	H	0.503206	-4.205789	-3.514434
C	-0.884476	1.467222	-0.256883	H	1.746283	-0.099981	1.726484
C	0.434820	1.545360	-0.247559	P	-2.986635	-1.123880	0.008423
				C	-2.701204	-2.910794	0.310983

H	-1.787876	-3.195160	-0.222947	H	-3.755847	0.508656	1.477932
H	-2.541850	-3.090916	1.379005	H	-3.362505	2.085170	0.745663
H	-3.546060	-3.513852	-0.044514	H	-5.036170	1.492725	0.741169
C	-4.643635	-0.869242	0.762774				
H	-5.373011	-1.579408	0.353670	6 _{OMe}			
H	-4.578442	-1.008250	1.846978	C	2.280256	3.113916	2.442111
H	-4.995009	0.150337	0.573361	C	1.183212	3.964984	2.369359
C	-3.346211	-1.117533	-1.788160	C	0.089901	3.627258	1.576871
H	-4.185033	-1.780118	-2.035356	C	0.126199	2.434907	0.868845
H	-3.568148	-0.098426	-2.121451	C	1.210290	1.550334	0.916830
H	-2.441064	-1.458102	-2.303574	C	2.286289	1.916283	1.723332
C	3.640963	1.798196	-1.898578	H	3.138275	3.379516	3.055943
H	3.423156	0.934524	-2.539740	H	1.174274	4.896338	2.930523
H	2.890278	2.568278	-2.109134	H	-0.784351	4.269369	1.499855
H	4.624527	2.188989	-2.186095	H	3.168869	1.280075	1.785547
C	3.996461	2.778532	1.012200	O	-0.946841	2.109349	0.081875
H	3.274631	3.588076	0.857089	C	-0.783760	0.954383	-0.619963
H	3.966010	2.499711	2.071892	C	-1.917459	0.433663	-1.191922
H	4.999102	3.166805	0.794981	Si	-3.653106	1.180117	-1.085393
C	4.824604	-0.084688	0.224397	Pd	1.022488	-0.012018	-0.334444
H	5.857226	0.227615	0.029272	Zn	-1.356002	-1.129315	0.421801
H	4.768532	-0.429616	1.264921	O	0.719698	-1.654657	-1.797830
H	4.611531	-0.947440	-0.421884	C	-0.041692	-2.634266	-1.606770
				O	-0.881323	-2.745797	-0.657991
5 _{OMe}				C	0.045572	-3.799206	-2.557309
C	2.266275	4.154134	0.278842	H	0.386568	-4.681367	-2.004101
C	1.011921	4.752811	0.296544	H	-0.948724	-4.035395	-2.947178
C	-0.121124	4.007877	-0.017253	H	0.735567	-3.590327	-3.377074
C	0.037607	2.669197	-0.338882	O	-0.905329	-1.385559	2.462471
C	1.278932	2.023518	-0.346923	C	-2.146247	-1.545896	2.663306
C	2.393663	2.799537	-0.037376	O	-2.967715	-1.478295	1.696212
H	3.153796	4.739112	0.510278	C	-2.664018	-1.819219	4.042118
H	0.910778	5.805574	0.548895	H	-1.860079	-1.789418	4.778807
H	-1.115505	4.447693	-0.020692	H	-3.433027	-1.082476	4.292357
H	3.389509	2.358187	-0.048922	H	-3.146042	-2.801683	4.056204
O	-1.074385	1.939002	-0.679875	H	-1.741186	-0.385248	-1.898190
C	-0.800065	0.666796	-1.056059	P	2.762626	-1.340758	0.627041
C	-1.883383	-0.173193	-1.190065	C	2.722702	-3.085479	0.067529
Si	-3.699604	0.328396	-0.995100	H	1.743792	-3.511073	0.318720
Pd	1.168199	0.088418	-0.873399	H	2.853461	-3.126800	-1.018137
Zn	-0.948621	-1.073010	0.642923	H	3.507566	-3.670022	0.562156
O	0.946909	-1.984055	-1.626419	C	4.530449	-0.905191	0.391329
C	0.469520	-2.936199	-0.965531	H	5.185245	-1.629775	0.890915
O	-0.166694	-2.828815	0.133582	H	4.752906	-0.892502	-0.681194
C	0.671288	-4.336469	-1.479775	H	4.733413	0.093755	0.792064
H	1.268859	-4.897123	-0.752304	C	2.585151	-1.535941	2.437973
H	-0.293520	-4.846309	-1.555340	H	3.316467	-2.250541	2.835425
H	1.175410	-4.332518	-2.447496	H	2.703981	-0.569937	2.937509
O	-0.398004	-0.220387	2.462148	H	1.565614	-1.883800	2.643246
C	-1.499890	-0.632140	2.940013	C	2.139743	1.224432	-3.028526
O	-2.299418	-1.306727	2.221051	C	2.799681	1.882059	-2.253884
C	-1.887285	-0.293217	4.345809	C	3.583397	2.717073	-1.357566
H	-1.050479	0.144477	4.891984	H	2.936897	3.262880	-0.658525
H	-2.713592	0.425740	4.312302	H	4.176228	3.450116	-1.917183
H	-2.257635	-1.186023	4.856729	H	4.279985	2.121757	-0.753115
H	-1.652702	-1.112155	-1.706578	C	1.339013	0.480111	-3.987588
P	3.252365	-0.567625	0.111394	H	0.339495	0.277397	-3.584670
C	3.444702	-2.385521	0.253213	H	1.792335	-0.489112	-4.222300
H	2.563155	-2.797652	0.758239	H	1.225952	1.040300	-4.923124
H	3.513958	-2.829284	-0.744933	C	-3.771929	2.688154	-2.204064
H	4.342880	-2.635323	0.830589	H	-3.045005	3.447314	-1.892441
C	4.898322	-0.072595	-0.534710	H	-3.565656	2.433587	-3.249670
H	5.695531	-0.430659	0.128258	H	-4.771777	3.136268	-2.155448
H	5.038603	-0.503452	-1.530949	C	-4.057502	1.652096	0.685702
H	4.969612	1.015921	-0.622091	H	-3.918007	0.787674	1.346803
C	3.301924	-0.051502	1.867085	H	-3.417074	2.467359	1.038352
H	4.160478	-0.492346	2.388647	H	-5.102869	1.974501	0.765858
H	3.350555	1.039404	1.935479	C	-4.810498	-0.186934	-1.658767
H	2.368045	-0.367007	2.346886	H	-5.858787	0.132059	-1.628587
C	-4.188995	1.463416	-2.412750	H	-4.585091	-0.500733	-2.685136
H	-3.565105	2.364377	-2.404041	H	-4.709932	-1.063480	-1.005527
H	-4.059130	0.972735	-3.383791				
H	-5.237172	1.774291	-2.326746	TS _{67OMe}			
C	-4.664996	-1.283737	-1.040577	C	0.082350	4.023922	-1.805276
H	-5.742391	-1.112643	-0.934155	C	0.902539	3.426553	-2.767514
H	-4.502750	-1.824316	-1.980792	C	1.419197	2.163289	-2.547779
H	-4.348904	-1.934389	-0.214822	C	1.134911	1.455159	-1.368676
C	-3.985840	1.189775	0.649369	C	0.296539	2.037622	-0.395562

C	-0.206747	3.328776	-0.643097	Zn	-0.181624	1.433154	0.469912
H	-0.319954	5.021932	-1.962099	O	2.511672	-0.309034	1.968937
H	1.143710	3.954663	-3.687018	C	2.058834	0.758660	2.482169
H	2.071311	1.680775	-3.272489	O	1.049294	1.398170	2.099556
H	-0.818050	3.801045	0.127297	C	2.831399	1.319975	3.647323
O	1.797390	0.290998	-1.249918	H	3.383884	2.201653	3.302835
C	1.379058	-0.805544	-0.491115	H	2.137601	1.658041	4.421381
C	2.379765	-1.542351	0.025422	H	3.536208	0.590727	4.050371
Si	4.206607	-1.138356	-0.065077	O	0.906097	2.540461	-0.993004
Pd	-0.707782	0.841967	0.961238	C	0.355306	3.602713	-0.548797
Zn	-0.502716	-1.615587	-0.446867	O	-0.443329	3.563309	0.420656
O	-1.669757	-0.392523	2.467687	C	0.709154	4.917181	-1.184703
C	-1.779058	-1.636244	2.276247	H	1.660265	5.265098	-0.765849
O	-1.387235	-2.270401	1.259983	H	0.846767	4.798470	-2.262428
C	-2.474889	-2.439757	3.345108	H	-0.055204	5.667293	-0.973523
H	-3.458880	-2.740162	2.967052	H	-3.079032	2.183237	0.675088
H	-1.916060	-3.358424	3.542376	P	2.991193	0.079693	-1.163713
H	-2.603919	-1.862002	4.261972	C	3.853178	1.491268	-0.375678
O	-2.046604	-1.635291	-1.887605	H	3.130356	2.304635	-0.257249
C	-1.717351	-2.834471	-2.183570	H	4.230155	1.180999	0.603578
O	-0.777103	-3.411211	-1.583954	H	4.690871	1.828428	-0.998136
C	-2.478301	-3.534194	-3.271916	C	4.384258	-1.097516	-1.410776
H	-2.324432	-3.004145	-4.217459	H	5.218013	-0.630514	-1.950091
H	-2.151165	-4.569946	-3.374480	H	4.735576	-1.435150	-0.428856
H	-3.549769	-3.496383	-3.053457	H	4.040902	-1.974344	-1.971412
H	2.074653	-2.465153	0.531471	C	2.697665	0.713927	-2.855931
P	-2.820178	1.101739	-0.138851	H	3.622982	1.134894	-3.268656
C	-4.056753	-0.214328	0.149294	H	2.349541	-0.092848	-3.507351
H	-3.702736	-1.134824	-0.326678	H	1.931203	1.492609	-2.788134
H	-4.158309	-0.371468	1.228445	C	0.317625	-2.259189	1.595580
H	-5.027270	0.073037	-0.272613	C	-0.533324	-2.851570	0.768013
C	-3.675734	2.578708	0.537046	C	-1.662097	-3.790477	1.039882
H	-4.675151	2.684938	0.097039	H	-2.616834	-3.307844	0.787194
H	-3.766713	2.475105	1.623495	H	-1.695306	-4.086455	2.093266
C	-3.095655	3.480963	0.318432	H	-1.581207	-4.697591	0.426742
C	-2.867037	1.370989	-1.944402	C	0.502180	-2.279893	3.061956
H	-3.882380	1.635407	-2.264625	H	0.208487	-1.316133	3.497394
H	-2.176536	2.177934	-2.213262	H	1.547643	-2.454051	3.338052
H	-2.555678	0.441316	-2.433503	C	-0.119645	-3.062284	3.519707
C	1.086564	0.952528	2.062613	H	-5.191695	-1.001009	1.197594
C	1.339778	2.003865	1.410189	H	-4.418807	-1.773721	1.106376
C	2.087498	3.267865	1.295950	H	-5.191353	-0.649237	2.235475
H	2.595982	3.351617	0.328151	C	-6.165220	-1.465489	0.996936
H	2.837097	3.294507	2.096321	H	-6.136941	1.763448	0.247308
H	1.430121	4.136524	1.408084	H	-7.152842	1.381796	0.089673
C	1.404509	-0.052564	3.083449	H	-6.087145	2.169935	1.264490
H	1.695615	-0.986491	2.582976	C	-5.978920	2.594230	-0.450530
H	0.534514	-0.257014	3.715389	H	-4.970735	-0.251185	-1.764516
H	2.242288	0.277115	3.710742	H	-5.972031	-0.650385	-1.968513
C	4.551110	0.634388	0.486168	H	-4.766687	0.537193	-2.498915
H	4.119770	1.347045	-0.227361	H	-4.244240	-1.057403	-1.920015
H	4.118851	0.837828	1.474842				
H	5.631168	0.818809	0.543790	TS _{78OMe}			
C	4.871272	-1.348928	-1.813703	C	0.555971	-3.929462	-1.864085
H	4.730896	-2.374044	-2.174090	C	0.312198	-3.063816	-2.933270
H	4.337690	-0.678581	-2.497948	C	-0.428964	-1.907734	-2.739202
H	5.941125	-1.112050	-1.867195	C	-0.961478	-1.613763	-1.483385
C	5.086622	-2.316925	1.114680	C	-0.766872	-2.496130	-0.390215
H	4.900495	-3.362416	0.841277	C	0.020084	-3.645662	-0.618279
H	6.171534	-2.158452	1.115173	H	1.149263	-4.828979	-2.010748
H	4.726912	-2.173657	2.141980	H	0.720657	-3.282560	-3.917477
				H	-0.607943	-1.200020	-3.544675
				H	0.176776	-4.327945	0.217174
7 _{OMe}				O	-1.668085	-0.466212	-1.360596
C	0.796703	-2.423865	-2.808045	C	-1.284540	0.454639	-0.381405
C	-0.042144	-1.414724	-3.266825	C	-2.247748	1.251244	0.117778
C	-0.982334	-0.825190	-2.423474	Si	-4.081379	1.137800	-0.264510
C	-1.131391	-1.295321	-1.123048	Pd	0.637088	-0.868120	0.750469
C	-0.293879	-2.330247	-0.623646	Zn	0.493561	1.603365	-0.193533
C	0.685166	-2.870303	-1.489349	O	1.515738	0.068104	2.586801
H	1.538748	-2.865132	-3.469637	C	1.490602	1.327529	2.607994
H	0.043115	-1.066158	-4.294195	O	1.085188	2.090902	1.681601
H	-1.631258	-0.019390	-2.760470	C	2.028885	2.011962	3.839795
H	1.306152	-3.686300	-1.122250	H	2.989151	2.476419	3.587915
O	-2.083314	-0.818418	-0.303864	H	1.354377	2.817409	4.142810
C	-1.987122	0.538673	0.094807	H	2.175836	1.304384	4.657623
C	-3.157680	1.157995	0.304222	O	2.021074	2.138043	-1.556757
Si	-4.849325	0.411042	-0.002711	C	1.443554	3.267080	-1.694830
Pd	1.411577	-1.110422	0.341767				

O	0.379925	3.524319	-1.072503	C	2.594251	1.312071	-2.736850
C	2.062422	4.286332	-2.604951	H	2.515313	0.462869	-3.419019
H	3.040804	4.574370	-2.207227	H	2.585346	2.236867	-3.333501
H	2.234471	3.843841	-3.590613	H	3.576577	1.235064	-2.258354
H	1.428514	5.169782	-2.693513	Zn	-1.557248	-1.182993	0.215227
H	-1.916647	2.000250	0.846777	O	0.718835	-2.834210	-0.816793
P	2.860834	-0.806873	-0.281109	C	-0.372172	-3.411446	-0.986902
C	4.057187	0.433838	0.339546	O	-1.520789	-2.913402	-0.724485
H	3.781676	1.414065	-0.061734	C	-0.389998	-4.815775	-1.535949
H	4.007600	0.458207	1.433431	H	0.620083	-5.166611	-1.753242
H	5.076884	0.180570	0.024499	H	-0.871360	-5.481923	-0.813216
C	3.636223	-2.384223	0.257629	H	-0.999271	-4.842146	-2.444955
H	4.679817	-2.451755	-0.074846	O	-2.584580	-1.430836	2.044954
H	3.597688	-2.443325	1.351177	C	-1.558881	-0.990464	2.641225
H	3.067321	-3.224786	-0.155810	O	-0.512723	-0.681551	1.989902
C	3.171633	-0.805081	-2.085101	C	-1.597264	-0.780199	4.125155
H	4.235307	-0.972399	-2.296172	H	-2.055430	0.197150	4.319094
H	2.576967	-1.595560	-2.555884	H	-2.218497	-1.539635	4.605004
C	2.863414	0.167047	-2.483310	H	-0.589699	-0.777216	4.546596
C	-1.068214	-1.377734	1.682420	C	-3.872180	2.973047	-1.224474
C	-1.522659	-2.357366	0.909410	H	-3.006336	3.623017	-1.046618
C	-2.629923	-3.328942	1.185232	H	-3.970086	2.831954	-2.307126
H	-3.396662	-3.272912	0.399810	C	-4.765332	3.502006	-0.869744
H	-3.111262	-3.128124	2.148222	H	-3.536833	1.663396	1.517530
H	-2.257953	-4.362283	1.201422	H	-3.642083	0.730670	2.082541
C	-1.506888	-0.770964	2.952588	H	-2.581925	2.128786	1.787604
H	-1.797760	0.275425	2.778779	H	-4.345000	2.340867	1.820421
H	-0.702920	-0.770956	3.696302	C	-5.106157	0.182781	-0.657601
H	-2.377984	-1.300020	3.366160	H	-6.047743	0.617730	-0.302939
C	-4.446971	1.670965	-2.029368	H	-5.218030	-0.034770	-1.726428
H	-4.140249	2.708729	-2.200548	H	-4.961360	-0.769727	-0.131448
H	-3.898440	1.038264	-2.736426				
H	-5.516874	1.589395	-2.256791	9 _{OMe}			
C	-4.655150	-0.638553	-0.011723	C	1.909283	-4.501576	0.720511
H	-4.172652	-1.300946	-0.740530	C	3.097922	-3.875587	1.092459
H	-4.387760	-0.989497	0.993559	C	3.397550	-2.608116	0.610924
H	-5.742054	-0.728714	-0.127378	C	2.502836	-1.971634	-0.241509
C	-4.966097	2.258011	0.962100	C	1.295299	-2.574194	-0.629460
H	-4.637744	3.298871	0.858442	C	1.022012	-3.855580	-0.129670
H	-6.053093	2.233237	0.821519	H	1.675015	-5.495921	1.091311
H	-4.754873	1.942717	1.991826	H	3.795625	-4.376600	1.758878
				H	4.315631	-2.088150	0.876236
8 _{OMe}				H	0.098210	-4.350844	-0.416622
C	2.790130	3.972932	0.691035	O	2.857235	-0.743605	-0.686789
C	1.650873	4.200105	1.463604	C	1.971886	0.076423	-1.365987
C	0.484792	3.500784	1.187694	C	2.351130	1.363279	-1.480583
C	0.480390	2.582152	0.147916	H	1.688867	2.024923	-2.035472
C	1.602146	2.320935	-0.641754	Pd	-0.248102	-0.571159	0.281216
C	2.763566	3.051473	-0.346955	P	-0.945973	-0.133238	2.437217
H	3.705333	4.522712	0.896625	C	-0.093076	-1.388217	3.475307
H	1.671347	4.922338	2.275332	H	0.990118	-1.288763	3.339784
H	-0.428916	3.646264	1.759058	H	-0.342147	-1.263058	4.537184
H	3.660561	2.892971	-0.940480	H	-0.382749	-2.391916	3.146519
O	-0.696572	1.921763	-0.065517	C	-0.438915	1.439263	3.225492
C	-0.875144	1.043780	-1.073306	H	-0.631572	1.404456	4.305417
C	-2.151220	0.445087	-1.058170	O	0.628724	1.610934	3.051901
H	-2.372424	-0.119942	-1.969317	H	-1.019462	2.253745	2.778443
Pd	1.361376	-0.602879	-0.797110	C	-2.689555	-0.289257	2.965149
P	2.946047	-0.941074	0.942180	H	-2.758031	-0.269599	4.060176
C	4.773204	-0.917099	0.724990	H	-3.266860	0.542444	2.548762
H	5.069695	0.055600	0.316073	H	-3.113186	-1.220791	2.579197
H	5.290717	-1.073212	1.680374	C	0.385360	-1.827497	-1.514665
H	5.079655	-1.694851	0.018625	C	0.729785	-0.527859	-1.874824
C	2.725517	0.294413	2.280317	Si	3.745287	2.088358	-0.471014
H	3.375767	0.077204	3.137876	C	0.010498	0.275267	-2.917824
H	2.945042	1.299345	1.899323	H	-0.952156	-0.152795	-3.198204
H	1.674193	0.259103	2.587654	H	-0.185772	1.294203	-2.569082
C	2.666779	-2.509576	1.849899	H	0.640311	0.352196	-3.814726
H	3.300022	-2.586096	2.743107	C	-0.784218	-2.568058	-2.096005
H	1.610042	-2.529899	2.139419	H	-1.465263	-1.910786	-2.640314
H	2.850799	-3.358564	1.184960	H	-0.439373	-3.362414	-2.772857
C	1.497562	1.315651	-1.704782	H	-1.373527	-3.045014	-1.302560
C	0.188311	0.787561	-2.010289	Zn	-2.300080	0.788593	-0.367797
Si	-3.652418	1.327445	-0.329134	O	-2.569898	2.454984	0.905371
C	-0.208563	0.199428	-3.341301	C	-1.822904	3.127279	0.125662
H	0.655699	0.061922	-3.994635	O	-1.385055	2.621891	-0.945557
H	-0.679636	-0.784615	-3.226991	C	-1.413130	4.515839	0.518319
H	-0.923816	0.848516	-3.866946	H	-0.487520	4.446638	1.103478

H	-1.205631	5.122856	-0.365263	O	0.236902	-0.981192	2.430882
H	-2.175362	4.985268	1.143864	C	1.450392	-1.235167	2.678216
O	-3.124842	-0.094439	-2.086175	C	2.381534	-1.309848	1.831706
C	-3.951225	-0.711614	-1.342647	C	1.816344	-1.437638	4.126575
O	-3.957315	-0.530078	-0.093123	H	2.667888	-2.115413	4.218539
C	-4.907355	-1.677686	-1.977717	H	2.115002	-0.467639	4.544015
H	-5.461109	-1.174520	-2.775647	H	0.960492	-1.801911	4.700549
H	-4.335482	-2.486089	-2.446901	O	2.437047	-2.981208	-0.961888
H	-5.598888	-2.093223	-1.243252	C	3.701239	-2.832209	-1.024978
C	3.816922	3.931480	-0.843565	O	4.242491	-1.754914	-0.661437
H	4.079001	4.110812	-1.892918	C	4.557624	-3.950149	-1.544436
H	2.848321	4.410224	-0.656309	H	3.967364	-4.846204	-1.743791
H	4.566295	4.435461	-0.221868	H	5.052300	-3.623524	-2.464609
C	3.291960	1.825286	1.344287	H	5.346380	-4.170769	-0.819369
H	4.024977	2.263109	2.032268	H	3.006620	1.764343	0.356473
H	2.313605	2.284725	1.540508	P	-0.729226	-2.895860	0.140110
H	3.209172	0.751383	1.560718	C	0.277832	-3.924605	1.263781
C	5.421307	1.311449	-0.830733	H	1.334196	-3.787150	1.022234
H	5.687119	1.415249	-1.888817	H	0.088590	-3.623469	2.298308
H	6.208062	1.793916	-0.237831	H	0.002637	-4.977997	1.132351
H	5.414505	0.242809	-0.589448	C	-2.420138	-3.284780	0.734314
P _{OMe}				H	-2.609591	-4.363267	0.663518
				H	-2.487547	-2.972423	1.783219
C	-0.625638	-0.896588	0.362231	H	-3.184153	-2.744634	0.166473
C	-0.594618	-0.519843	1.703882	C	-0.569325	-3.749579	-1.461411
C	0.612986	-0.470514	2.385284	H	-0.897197	-4.790808	-1.352861
C	1.785764	-0.799225	1.715300	H	-1.167311	-3.248057	-2.226378
C	1.788854	-1.184371	0.369792	H	0.489355	-3.721241	-1.743634
C	0.553718	-1.224865	-0.291423	C	-0.814067	1.615783	1.080636
H	-1.570439	-0.934957	-0.173681	C	-1.810764	1.691837	0.349590
H	-1.515252	-0.262456	2.221952	O	-2.830235	1.773696	-0.426188
H	0.677221	-0.181900	3.431998	C	-3.941998	0.961934	-0.149666
H	0.518515	-1.519061	-1.337427	C	-4.012649	0.171497	0.986384
O	2.931274	-0.731527	2.429685	C	-4.945445	0.989106	-1.105363
C	4.165880	-0.997372	1.873401	C	-5.137985	-0.632421	1.155601
C	5.218356	-0.827887	2.699987	H	-3.200333	0.169828	1.711297
H	6.203338	-1.039270	2.289156	C	-6.056768	0.177720	-0.919861
C	3.064715	-1.520925	-0.255105	H	-4.821847	1.616170	-1.984231
C	4.207055	-1.430152	0.477500	C	-6.154999	-0.636777	0.207365
C	3.014069	-1.947224	-1.688668	H	-5.211950	-1.261803	0.2039739
H	3.993341	-2.184678	-2.104449	H	-6.849493	0.179058	-1.663656
H	2.379373	-2.834952	-1.807665	H	-7.026961	-1.270441	0.347361
C	2.573918	-1.158430	-2.312404	Si	-0.062369	2.335392	2.638017
C	5.575451	-1.741248	-0.043009	C	-0.978683	1.522275	4.060496
H	6.219988	-0.854427	0.008437	H	-0.855842	0.434057	4.002950
H	6.054126	-2.514177	0.571274	H	-0.592373	1.872846	5.025662
H	5.573062	-2.091011	-1.075826	H	-2.048848	1.759510	4.019503
Si	5.082787	-0.251398	4.471402	C	1.791645	2.126592	2.819581
C	6.840233	-0.057669	5.121992	H	2.171767	1.151905	2.497419
H	6.841010	0.265411	6.169841	H	2.322685	2.895350	2.246066
H	7.391438	-1.004125	5.065978	C	2.050031	2.265633	3.878267
H	7.397121	0.688798	4.543144	H	-0.442228	4.175446	2.573253
C	4.192559	1.405213	4.588803	H	-0.089394	4.673553	3.484847
H	4.145892	1.747965	5.629984	H	0.055212	4.651844	1.718697
H	4.706821	2.175604	4.002941	H	-1.519306	4.357387	2.481464
H	3.167491	1.322814	4.209756	C	2.997541	4.835217	-0.068628
C	4.165470	-1.505549	5.537970	H	2.471590	4.864882	0.895493
H	4.668217	-2.479299	5.531177	H	4.040385	4.559802	0.131079
H	4.110701	-1.161860	6.578573	H	2.993160	5.853635	-0.475870
H	3.141727	-1.653453	5.175922	C	0.376982	4.119513	-1.476166
6 _{ORMe}				H	-0.138526	3.462558	-2.187070
				H	-0.165879	4.067545	-0.524434
C	-2.619626	-0.597181	-3.350432	H	0.309527	5.149908	-1.848377
C	-1.831488	0.181151	-4.192044	C	3.037264	3.717260	-2.934400
C	-0.623997	0.677754	-3.731922	H	2.959899	4.726542	-3.358028
C	-0.177226	0.410236	-2.430043	H	4.099892	3.461162	-2.857637
C	-0.960347	-0.376161	-1.567121	H	2.573718	3.014730	-3.636786
C	-2.175257	-0.863407	-2.057628	TS _{6⁷ORMe}			
H	-3.578735	-0.988175	-3.684301				
H	-2.157423	0.406336	-5.204925	C	-2.120679	-1.936742	-3.010212
H	0.010689	1.304271	-4.356020	C	-1.775680	-0.923812	-3.912518
H	-2.826050	-1.448724	-1.407192	C	-0.980562	0.130722	-3.508203
O	0.981475	1.028851	-2.117616	C	-0.499168	0.212694	-2.189180
C	1.704554	0.811082	-0.950127	C	-0.833209	-0.802535	-1.265196
C	2.348381	1.906841	-0.504977	C	-1.650539	-1.863227	-1.710751
Si	2.181835	3.617080	-1.259892	H	-2.759848	-2.760607	-3.318582
Pd	-0.386915	-0.607850	0.356074	H	-2.141060	-0.956903	-4.936588
Zn	2.316292	-1.000164	-0.192144	H	-0.713338	0.937868	-4.187335

H	-1.948872	-2.624402	-0.989265	C	0.994708	0.613914	-3.309492
O	0.178244	1.339470	-1.931391	C	0.148867	0.629058	-2.194536
C	0.978074	1.593964	-0.805735	C	-0.564697	-0.554234	-1.836348
C	0.868246	2.849023	-0.336310	C	-0.391785	-1.710989	-2.644472
Si	-0.329273	4.153627	-0.952095	H	0.549620	-2.597052	-4.359623
Pd	0.233878	-1.074241	0.471305	H	1.770829	-0.511539	-4.954434
Zn	2.538041	0.441981	-0.128160	H	1.526312	1.530150	-3.551597
O	1.214628	-1.330566	2.391480	H	-0.972512	-2.596472	-2.386339
C	2.278925	-0.696904	2.637997	O	-0.018262	1.792016	-1.560269
O	2.930830	0.009709	1.821658	C	0.365993	1.996622	-0.210469
C	2.787319	-0.752589	4.055579	C	-0.288954	2.972022	0.432701
H	3.876189	-0.671197	4.080560	Si	-1.724603	3.986344	-0.217154
H	2.375915	0.111218	4.593864	Pd	0.622883	-1.211558	-0.042059
H	2.449112	-1.659951	4.561036	Zn	2.055981	1.135952	0.592832
O	3.844157	-0.801387	-1.241791	O	1.092251	-1.805446	1.966604
C	4.712831	0.135556	-1.210507	C	1.754094	-1.011186	2.696975
O	4.479873	1.213210	-0.609728	O	2.242538	0.092716	2.342301
C	6.018197	-0.075995	-1.921723	C	1.928557	-1.422982	4.134422
H	6.468753	-1.018533	-1.596946	H	2.870485	-1.040415	4.533757
H	5.831925	-0.161798	-2.997322	H	1.110609	-0.972038	4.711030
H	6.702429	0.753161	-1.735250	H	1.864394	-2.507888	4.244939
H	1.560943	3.113594	0.469806	O	3.910016	0.860003	-0.416271
P	1.397401	-2.940239	-0.426927	C	4.349977	1.892016	0.193066
C	2.970826	-3.407128	0.376081	O	3.627845	2.518178	1.009569
H	3.724797	-2.652208	0.133612	C	5.754050	2.343595	-0.089549
H	2.818170	-3.443878	1.459668	H	6.450282	1.528191	0.130391
C	3.304396	-4.388923	0.018434	H	5.854560	2.572143	-1.155303
C	0.390588	-4.455419	-0.182372	H	6.011618	3.222523	0.503434
H	0.935269	-5.340016	-0.535264	H	0.075431	3.178337	1.443920
H	0.162904	-4.571563	0.882475	P	2.773223	-2.213620	-0.679395
-O	5.49793	-4.374880	-0.736091	C	4.068744	-2.243904	0.615838
C	1.774131	-2.969724	-2.213124	H	4.406491	-1.218595	0.795337
H	2.166078	-3.952051	-2.504238	H	3.654434	-2.659883	1.539727
H	0.862886	-2.756940	-2.783262	H	4.913574	-2.862782	0.289965
C	2.526681	-2.199261	-2.414028	C	2.435929	-4.006268	-0.901867
C	-1.181260	0.331896	1.159545	C	3.360934	-4.569402	-1.078288
C	-1.980918	0.239710	0.178019	H	1.947447	-4.386961	0.002309
O	-3.103180	0.426060	-0.452885	H	1.757667	-4.154503	-1.749277
C	-4.168338	-0.450482	-0.220489	C	3.748336	-1.789545	-2.168923
C	-4.239066	-1.253741	0.907773	H	4.608867	-2.463849	-2.262512
C	-5.161235	-0.439446	-1.188192	H	3.126584	-1.874202	-3.065177
C	-5.356344	-2.070252	1.063389	H	4.093845	-0.756160	-2.057144
H	-3.433088	-1.242836	1.638742	C	-1.332523	-0.679543	0.409342
C	-6.269963	-1.257134	-1.013118	C	-1.697321	-0.524352	-0.857156
H	-5.038320	0.200140	-2.058246	O	-2.914544	-0.355778	-1.467165
C	-6.370615	-2.073606	0.111587	C	-4.039517	-0.969859	-0.969512
H	-5.430004	-2.706738	1.941867	C	-4.017798	-2.269752	-0.470765
H	-7.057628	-1.260242	-1.762318	C	-5.232001	-0.261968	-1.070176
H	-7.238918	-2.713723	0.244158	C	-5.208296	-2.850683	-0.047846
Si	-1.178225	1.174582	2.834678	H	-3.075158	-2.808099	-0.395852
C	-1.312042	-0.187315	4.116999	C	-6.415493	-0.858069	-0.650189
H	-0.481229	-0.892032	3.990709	C	-5.204832	0.749741	-1.468133
H	-1.280237	0.226480	5.132338	C	-6.409117	-2.150164	-0.132289
H	-2.253350	-0.740210	4.010135	H	-5.194854	-3.863751	0.348310
C	0.364187	2.209691	3.080759	H	-7.348165	-0.303312	-0.721412
H	1.281017	1.692632	2.774951	H	-7.335259	-2.610696	0.202015
H	0.298828	3.132301	2.491709	Si	-2.026519	-0.558280	2.148534
H	0.458541	2.487781	4.138385	C	-1.930074	-2.243814	2.975173
C	-2.697512	2.284232	2.849498	H	-0.906946	-2.633717	2.946563
H	-2.867736	2.721615	3.840612	H	-2.254419	-2.172284	4.021278
H	-2.576261	3.108862	2.134992	H	-2.592135	-2.959792	2.472188
H	-3.597972	1.724213	2.566404	C	-1.085073	0.756364	3.110814
C	-0.342447	5.547713	0.319035	H	0.003225	0.722166	3.000870
H	-0.742300	5.194168	1.278830	H	-1.412286	1.745881	2.764400
H	0.666512	5.936208	0.501964	H	-1.332234	0.675141	4.177932
H	-0.969417	6.384648	-0.011447	C	-3.817787	0.028630	2.177148
C	-2.086864	3.489509	-1.117157	H	-4.090790	0.193872	3.228709
H	-2.156179	2.758617	-1.931982	H	-3.939844	0.986255	1.655708
H	-2.425613	2.991861	-0.199041	H	-4.525284	-0.689560	1.750505
H	-2.785514	4.307985	-1.333220	C	-2.410880	4.959997	1.242746
C	0.203464	4.809965	-2.634642	H	-2.763778	4.273649	2.023742
H	-0.494126	5.569075	-3.009814	H	-1.647321	5.607911	1.689138
H	1.204531	5.253290	-2.596975	H	-3.257262	5.591003	0.946867
H	0.230753	3.983739	-3.355248	C	-3.086706	2.873487	-0.891367
				H	-2.740137	2.293180	-1.753821
				H	-3.415577	2.156571	-0.127288
				H	-3.958075	3.466810	-1.197984
				C	-1.150334	5.149480	-1.581492
7ORMe							
C	0.436214	-1.703777	-3.750452				
C	1.118584	-0.527494	-4.083398				

H	-1.982189	5.736506	-1.989435	C	-4.278821	-1.538369	0.018408
H	-0.388028	5.845807	-1.214799	C	-5.532212	0.319149	-0.895035
H	-0.707776	4.568523	-2.398967	C	-5.466261	-2.079585	0.504879
TS _{78ORMe}				H	-3.328067	-2.035688	0.201926
				C	-6.707096	-0.235269	-0.406927
C	-0.858075	-2.234161	-3.635321	H	-5.521751	1.262126	-1.436144
C	0.162054	-1.477481	-4.222686	C	-6.681797	-1.435721	0.300089
C	0.589907	-0.301986	-3.628253	H	-5.432549	-3.019181	1.052689
C	-0.007406	0.154582	-2.450785	H	-7.650096	0.280049	-0.574493
C	-1.066015	-0.574735	-1.852676	H	-7.601839	-1.864243	0.688858
C	-1.460151	-1.783510	-2.475600	8 _{ORMe}			
H	-1.192054	-3.158608	-4.099754				
H	0.634571	-1.818394	-5.141206	C	2.324734	-1.224411	3.779748
H	1.395441	0.294338	-4.049064	C	1.282624	-0.547253	4.416373
H	-2.291607	-2.334631	-2.036655	C	0.421964	0.255384	3.680342
O	0.461803	1.306598	-1.935168	C	0.615234	0.363896	2.310003
C	0.830626	1.370894	-0.589282	C	1.630844	-0.318880	1.646232
C	0.736264	2.571370	0.007470	C	2.496226	-1.113309	2.407331
Si	-0.016705	4.121257	-0.746978	H	3.004999	-1.842674	4.359955
Pd	0.261126	-1.023619	0.136926	H	1.143802	-0.641677	5.490169
Zn	2.452110	0.447463	0.444895	H	-0.396245	0.802289	4.142033
O	0.592603	-1.593358	2.295612	H	3.304826	-1.638163	1.903253
C	1.449271	-0.903107	2.908847	O	-0.243430	1.175687	1.622885
O	2.243259	-0.058451	2.395994	C	-0.202366	1.325144	0.274734
C	1.509358	-1.059337	4.407235	C	-1.340745	2.006324	-0.208624
H	2.531504	-0.930322	4.770576	H	-1.254421	2.278867	-1.265248
H	0.895214	-0.265717	4.851822	Pd	0.212011	-1.252548	-0.761854
H	1.099153	-2.022459	4.719007	P	0.097786	-3.442522	0.143178
O	4.251781	-0.336469	-0.343553	C	1.532566	-4.588061	0.077720
C	4.826187	0.748242	0.006757	H	2.395086	-4.101987	0.547697
O	4.174040	1.665483	0.570192	H	1.317703	-5.527102	0.603611
C	6.295933	0.901268	-0.249162	H	1.789679	-4.806914	-0.963229
H	6.842801	0.202452	0.392404	C	-0.286807	-3.430539	1.935748
H	6.523218	0.633632	-1.284911	H	-0.454281	-4.448200	2.311918
H	6.625983	1.919432	-0.037721	H	0.545189	-2.972051	2.483419
H	1.082652	2.619975	1.045130	H	-1.180694	-2.814595	2.087404
P	1.927066	-2.711528	-0.406813	C	-1.269931	-4.462079	-0.527778
C	3.205942	-3.139065	0.832216	H	-1.340213	-5.431381	-0.018426
H	3.953916	-2.339020	0.856925	H	-2.202381	-3.903430	-0.391174
H	2.736191	-3.236792	1.816166	H	-1.124814	-4.610454	-1.601918
H	3.689719	-4.086088	0.563233	C	1.720547	-0.169351	0.193290
C	0.936046	-4.253978	-0.488318	C	0.900966	0.807812	-0.492615
H	1.574020	-5.129526	-0.663200	Si	-2.210979	3.334325	0.815472
H	0.397519	-4.378607	0.457906	Zn	-2.567237	0.261786	-0.369317
H	0.203220	-4.170063	-1.298580	O	-1.360995	-1.770547	-2.355002
C	2.865729	-2.734900	-1.975131	C	-2.382245	-1.204671	-2.793152
H	3.397943	-3.687079	-2.092401	O	-3.049759	-0.297624	-2.189835
H	2.177431	-2.593616	-2.815132	C	-2.881332	-1.567383	-0.168036
H	3.586209	-1.910419	-1.950852	H	-2.453587	-2.513696	-4.503989
C	-1.464128	0.024609	0.472660	H	-3.973460	-1.605966	-4.182915
C	-1.945137	-0.039411	-0.763906	H	-2.572627	-0.775667	-4.861452
C	1.008286	4.751180	-2.192559	O	-4.311855	0.188587	0.819398
H	2.031136	4.985705	-1.877371	C	-3.729137	-0.664479	1.550677
H	1.063952	3.995889	-2.984282	O	-2.561048	-1.074729	1.264425
H	0.567440	5.660498	-2.619254	C	-4.402165	-1.150546	2.798788
C	-1.765212	3.720280	-1.317180	H	-4.228421	-0.408950	3.588031
H	-1.755388	2.979567	-2.124694	H	-5.481282	-1.226644	2.647784
H	-2.348982	3.298250	-0.488646	H	-3.986399	-2.106381	3.124621
H	-2.285116	4.616395	-1.677373	C	-0.938691	4.657012	1.249253
C	-0.080624	5.425616	0.609097	H	-0.121036	4.221067	1.836924
H	0.919104	5.634066	1.007861	H	-0.501588	5.100145	0.346248
H	-0.494591	6.368205	0.231517	H	-1.382755	5.466335	1.841303
H	-0.712276	5.097700	1.444195	C	-3.007416	2.695688	2.393635
Si	-2.094567	0.593237	2.149106	H	-3.877645	2.073704	2.154603
C	-3.702808	1.554987	1.937354	H	-2.303771	2.094902	2.981658
H	-4.555373	0.890321	1.754129	H	-3.340145	3.537475	3.013252
H	-3.903954	2.123667	2.854554	C	-3.536528	4.023291	-0.324622
H	-3.650281	2.267831	1.105653	H	-4.089733	4.845526	0.143179
C	-0.842457	1.750497	2.942704	H	-3.102210	4.398917	-1.259601
H	0.183440	1.363966	2.926535	H	-4.259686	3.237180	-0.578944
H	-0.840467	2.718087	2.424453	Si	1.258977	1.565894	-2.210324
H	-1.127655	1.931823	3.987442	C	1.352697	3.440148	-2.010750
C	-2.403308	-0.896165	3.250484	H	1.706447	3.894750	-2.944659
H	-2.702064	-0.563649	4.252909	H	0.381757	3.888374	-1.769439
H	-3.214152	-1.518401	2.852224	H	2.059731	3.716033	-1.217955
H	-1.498425	-1.507636	3.334153	C	-0.064926	1.116828	-3.474362
O	-3.215583	0.278960	-1.208658	H	0.149223	1.652281	-4.408978
C	-4.319366	-0.329791	-0.673533	H	-0.010939	0.038970	-3.677233

H	-1.096585	1.343784	-3.182144	C	2.566050	-0.215489	-3.559061
C	2.871995	0.969748	-2.962806	H	2.595807	-0.777049	-4.500977
H	2.881844	1.301268	-4.009692	H	2.358399	0.834095	-3.804388
H	3.756982	1.389298	-2.473353	H	3.558971	-0.271750	-3.098469
H	2.952853	-0.122509	-2.951879	C	1.671300	-2.605229	-1.792553
O	2.947940	-0.543131	-0.345025	H	2.746211	-2.697200	-1.601619
C	4.053162	0.231008	-0.094369	H	1.135268	-2.830607	-0.863984
C	4.012353	1.487090	0.507450	H	1.377308	-3.355352	-2.537066
C	5.264128	-0.307234	-0.527404	C	-0.346876	-1.028384	-3.480385
C	5.199136	2.199985	0.663861	H	-0.412503	-0.207326	-4.203896
H	3.069985	1.914746	0.841154	H	-0.274677	-1.967345	-4.044413
C	6.436018	0.416890	-0.365115	H	-1.279514	-1.076397	-2.909800
H	5.254475	-1.285707	-1.002001	O	2.714151	-0.883106	0.301495
C	6.411427	1.675751	0.232090	C	4.052162	-0.756461	0.007711
H	5.166102	3.181169	1.132229	C	4.846049	-1.852418	0.338152
H	7.376987	-0.005604	-0.710158	C	4.603517	0.368644	-0.600145
H	7.330274	2.242321	0.358352	C	6.205137	-1.819349	0.057377
				H	4.374761	-2.713666	0.805964
9 _{ORMe}				C	5.969244	0.384283	-0.873083
C	2.705069	2.123037	3.300041	H	3.978799	1.218481	-0.867309
C	2.107330	3.346688	2.995061	C	6.774284	-0.700993	-0.547616
C	1.469341	3.541864	1.774753	H	6.824063	-2.675986	0.313697
C	1.429612	2.499759	0.855632	H	6.402094	1.261697	-1.347912
C	2.023144	1.262492	1.147154	H	7.838835	-0.677290	-0.764971
C	2.663511	1.085205	2.379081				
H	3.204824	1.982545	4.254713	P _{ORMe}			
H	2.139670	4.160725	3.715209	C	-1.285789	4.103185	-0.719573
H	1.000467	4.487507	1.511825	C	0.040354	4.463673	-0.477135
H	3.122092	0.122542	2.596065	C	1.015966	3.491843	-0.299691
O	0.831211	2.717169	-0.335647	C	0.652748	2.151706	-0.363796
C	0.404234	1.648416	-1.139424	C	-0.670409	1.768452	-0.604521
C	-0.607770	1.935775	-1.971257	C	-1.636975	2.762979	-0.786677
H	-0.955853	1.122720	-2.602133	H	-2.042961	4.869793	-0.860226
Pd	-0.159962	-0.231960	0.970953	H	0.317286	5.513949	-0.425635
P	-1.667914	-0.442803	2.715623	H	2.057288	3.742675	-0.111407
C	-0.624040	-0.145995	4.199870	H	-2.664604	2.468310	-0.985671
H	-0.105292	0.813627	4.091083	O	1.627051	1.233536	-0.187016
H	-1.239263	-0.129470	5.108877	C	1.380265	-0.134796	-0.180502
C	0.129321	-0.935510	4.284824	C	2.448245	-0.888940	0.149592
H	-2.929384	0.874952	2.865669	H	2.299085	-1.966907	0.154594
H	-3.415975	0.826515	3.848313	C	-0.929570	0.343964	-0.681988
H	-2.460157	1.856226	2.736834	C	0.031518	-0.595418	-0.510767
C	-3.681868	0.728867	2.083367	Si	4.139224	-0.215532	0.573941
C	-2.607174	-1.942157	3.175341	C	5.241026	-1.703810	0.920835
H	-2.970314	-1.849376	4.206352	H	4.855655	-2.295642	1.759817
H	-3.456872	-2.051707	2.493661	H	5.301904	-2.363560	0.046931
H	-1.976403	-2.828557	3.066589	H	6.261225	-1.392439	1.174536
C	1.904890	0.216932	0.131531	C	4.853051	0.777491	-0.858260
C	1.104857	0.359531	-0.987842	H	5.838527	1.184095	-0.599502
Si	-1.730840	3.414828	-1.775738	H	4.967805	0.159154	-1.755716
Zn	-2.008964	-1.613552	-0.160196	H	4.191904	1.614956	-1.108455
O	-3.987696	-1.060382	0.327797	C	4.086709	0.884845	2.102964
C	-4.000086	-0.266121	-0.665016	H	3.656085	0.356886	2.961324
O	-2.991255	-0.153742	-1.416688	H	5.098759	1.206614	2.379118
C	-5.214796	0.579605	-0.918011	H	3.484464	1.782804	1.923206
H	-5.023615	1.591974	-0.538519	Si	-0.296154	-2.469734	-0.658707
H	-5.400887	0.666400	-1.991796	C	-0.235742	-3.221591	1.066510
H	-6.089444	0.172368	-0.407346	H	-0.313675	-4.314233	1.008578
O	-1.495200	-3.150950	-1.461536	H	0.690257	-2.973755	1.596729
C	-1.504897	-3.975051	-0.492163	H	-1.077298	-2.860951	1.670319
O	-1.771350	-3.590008	0.679634	C	-1.966568	-2.867594	-1.420548
C	-1.167834	-5.411397	-0.764687	H	-2.803727	-2.607616	-0.764346
H	-1.751876	-5.774711	-1.614841	H	-2.117725	-2.357839	-2.377824
H	-0.111466	-5.478876	-1.047729	H	-2.004588	-3.950014	-1.601061
H	-1.348176	-6.032125	0.114375	C	1.019898	-3.230737	-1.780615
C	-3.165803	3.137516	-2.957681	H	1.876399	-3.630749	-1.227489
H	-2.864099	3.295798	-3.999628	H	0.577773	-4.058377	-2.348290
H	-3.502774	2.097472	-2.859644	H	1.405342	-2.499597	-2.500051
H	-4.013097	3.800836	-2.747106	O	-2.218922	-0.005746	-1.008194
C	-2.353332	3.382048	0.007433	C	-3.162789	-0.061811	-0.014024
H	-3.141751	4.120528	0.197482	C	-4.476259	-0.254335	-0.438861
H	-2.748718	2.380673	0.224915	C	-2.858458	0.036239	1.340960
H	-1.525897	3.566827	0.705362	C	-5.491741	-0.345632	0.502715
C	-0.882133	5.060526	-2.113991	H	-4.669543	-0.336310	-1.505919
H	-0.495521	5.109308	-3.138162	C	-3.891054	-0.054355	2.271321
H	-1.579781	5.895951	-1.978177	H	-1.830119	0.180182	1.663395
H	-0.038851	5.203997	-1.428549	C	-5.205778	-0.244267	1.862693
Si	1.213061	-0.902674	-2.441772	H	-6.515918	-0.497758	0.170017

H	-3.655929	0.025462	3.330242	C	2.359937	-1.500745	-1.726479
H	-6.003563	-0.314283	2.597386	H	2.618679	-2.111407	-2.604681
				H	2.249869	-2.178417	-0.868750
C ₆ H ₅ CH ₂ C≡CSiPr ₃				H	1.369056	-1.052640	-1.907568
C	-0.820256	-1.578448	-0.922837	C	3.049001	-1.175490	2.106904
C	-0.527327	-0.454268	-1.686353	H	2.949810	-1.965904	1.352205
C	0.584473	0.328955	-1.387907	H	3.507589	-1.624918	2.998365
C	1.416208	-0.007340	-0.322097	H	2.029859	-0.872437	2.386945
C	1.114447	-1.135855	0.441911	C	3.927056	1.099002	2.708579
C	0.005420	-1.917886	0.145580	H	4.588828	1.932267	2.439898
H	-1.690796	-2.186980	-1.156596	H	2.929915	1.515903	2.912772
H	-1.168850	-0.180311	-2.521109	H	4.294704	0.676099	3.653584
H	0.811420	1.214888	-1.980981	C	3.106312	3.107145	-1.544688
H	-0.218582	-2.792501	0.752377	H	3.221047	2.538256	-2.478791
C	2.715044	2.114255	-0.576673	H	2.031051	3.192264	-1.341148
C	2.732366	3.214910	-1.098836	H	3.494089	4.117093	-1.738312
Si	2.675530	4.881215	-1.880023	C	5.356573	2.404683	-0.663775
C	1.122406	5.731719	-1.197449	H	5.761539	3.416050	-0.806762
H	1.291986	5.817070	-0.111089	H	5.918801	1.935996	0.155032
C	4.248198	5.807383	-1.361748	H	5.576014	1.840924	-1.581411
H	4.233198	6.780631	-1.880538	Zn	-0.827141	-1.627818	0.841682
C	2.546147	4.675858	-3.769497	O	-1.236796	-3.300865	-0.452998
H	1.462928	4.614232	-3.973436	C	-0.074179	-3.719915	-0.175908
C	3.095197	5.891465	-4.518073	O	0.650403	-3.111705	0.666761
H	4.181984	5.982598	-4.384750	C	0.472591	-4.913143	-0.901742
H	2.912026	5.805039	-5.597947	H	0.881029	-4.567205	-1.860044
H	2.647062	6.835792	-4.183399	H	1.279202	-5.382525	-0.335380
C	3.188857	3.389185	-4.284063	H	-0.321814	-5.631113	-1.117945
H	3.060686	3.291396	-5.371228	O	-0.708029	-0.977105	2.863535
H	4.269135	3.371553	-4.082261	C	-1.971504	-1.042099	2.920722
H	2.760047	2.499314	-3.808666	O	-2.651787	-1.373076	1.902936
C	5.504222	5.049021	-1.788260	C	-2.679630	-0.665017	4.189691
H	5.558244	4.905868	-2.875060	H	-3.595751	-1.248306	4.305816
H	6.414696	5.581699	-1.479959	H	-2.024422	-0.792285	5.053550
H	5.534426	4.052953	-1.325078	H	-2.966070	0.392927	4.129165
C	4.263178	6.061355	0.144427	H	-3.143230	1.043195	1.539776
H	3.414726	6.673616	0.474797	P	-2.102126	-0.517124	-2.085212
H	4.224370	5.114728	0.701812	C	-1.648783	-1.782020	-3.332366
H	5.182623	6.580177	0.449570	H	-0.808681	-1.423802	-3.936641
C	-0.121895	4.872928	-1.414036	H	-1.349753	-2.690914	-2.798459
H	-0.335631	4.745175	-2.485306	H	-2.499106	-2.005534	-3.989127
H	-0.009404	3.872393	-0.978091	C	-3.604429	-1.237040	-1.325050
H	-1.010581	5.338923	-0.966152	H	-4.361402	-1.432680	-2.095179
C	0.925736	7.132806	-1.772713	H	-3.344048	-2.172196	-0.818827
H	0.063877	7.635931	-1.312950	H	-4.006389	-0.541245	-0.580923
H	1.801687	7.778155	-1.622404	C	-2.807648	0.831719	-3.112227
H	0.728916	7.090042	-2.853706	H	-3.615713	0.459687	-3.755401
H	1.758604	-1.400842	1.280638	H	-3.197069	1.613833	-2.449833
C	2.657463	0.790951	0.022243	H	-2.021135	1.270228	-3.734901
H	3.548336	0.219400	-0.282451	C	-0.657539	2.164583	1.793397
H	2.733645	0.882271	1.115865	H	-0.973733	1.428660	2.546770
				H	-0.174641	2.989478	2.338564
2 _{CH2}				TS _{23CH2}			
C	-3.996569	3.623676	-0.505953	C	4.630109	2.946431	0.037967
C	-2.788179	4.316502	-0.502457	C	3.976626	4.063360	-0.474012
C	-1.719127	3.846006	0.251860	C	2.676976	3.946787	-0.960536
C	-1.841104	2.678515	1.005634	C	2.035099	2.711569	-0.937004
C	-3.048348	1.980145	0.988433	C	2.670983	1.555091	-0.426967
C	-4.122292	2.454304	0.238648	C	3.977804	1.715978	0.055815
H	-4.838319	3.996738	-1.085166	H	5.646843	3.037300	0.416338
H	-2.682022	5.231637	-1.080763	H	4.477878	5.029000	-0.494002
H	-0.772210	4.387055	0.256335	H	2.163713	4.825068	-1.353438
H	-5.061881	1.904766	0.239312	H	4.510990	0.838230	0.431391
C	0.350268	1.520109	0.946274	C	-0.053476	1.449441	-0.740111
C	1.355644	1.054339	0.375256	C	-1.050776	0.722117	-0.369470
Si	3.152376	0.718509	0.006320	Si	-2.803014	1.210981	0.122868
C	3.854334	2.440518	-0.392258	C	-2.658860	3.020714	0.702502
H	3.676269	3.035283	0.519522	H	-2.296809	3.575798	-0.180550
C	3.861295	0.026781	1.623059	C	-3.886250	1.104873	-1.432234
H	4.889261	-0.304188	1.399038	H	-4.904989	1.389738	-1.119196
C	3.433683	-0.444506	-1.476240	C	-3.461144	0.134240	1.550521
H	3.463274	0.225084	-2.353719	H	-3.1110836	0.645398	2.464137
Pd	-0.357856	0.299953	-0.774294	H	1.075485	0.302426	0.542125
C	4.800508	-1.126579	-1.357216	C	-4.991897	0.118365	1.574319
H	4.804518	-1.847295	-0.527995	H	-5.393130	-0.419361	0.704315
H	5.035160	-1.688135	-2.271757	H	-5.363269	-0.398491	2.469835
H	5.624510	-0.422651	-1.184844	H	-5.432818	1.122737	1.568948

C	-2.926870	-1.294276	1.584710	C	2.940176	-1.300067	-1.813683
H	-3.318325	-1.838132	2.456261	H	3.404010	-1.835427	-2.654430
H	-3.227078	-1.854529	0.687849	H	3.019761	-1.953333	-0.933233
H	-1.830253	-1.324118	1.650697	H	1.874369	-1.178211	-2.057005
C	-3.930344	-0.312823	-1.997626	C	3.612951	-0.441308	2.056315
H	-4.254176	-1.058373	-1.260514	H	3.933387	-1.238794	1.374792
H	-4.612087	-0.375929	-2.857002	H	4.199673	-0.536429	2.980808
H	-2.939417	-0.631448	-2.348736	H	2.568510	-0.658491	2.324381
C	-3.420878	2.089092	-2.504023	C	3.242929	1.999278	2.458488
H	-3.449446	3.132356	-2.164221	H	3.385515	3.030071	2.109752
H	-2.389848	1.867944	-2.817519	H	2.169074	1.858727	2.650966
H	-4.049440	2.018552	-3.402453	H	3.756915	1.903786	3.425176
C	-1.641330	3.208529	1.826807	C	2.198940	3.171881	-2.107632
H	-1.920136	2.629434	2.719069	H	2.720773	2.680765	-2.940664
H	-0.630871	2.892401	1.538272	H	1.174415	2.778235	-2.090891
H	-1.587763	4.262212	2.134670	H	2.146091	4.241534	-2.355412
C	-4.010344	3.609426	1.108631	C	4.371502	3.463587	-0.892567
H	-3.920638	4.680059	1.339088	H	4.391631	4.524826	-1.177973
H	-4.774744	3.505632	0.327236	H	4.927959	3.366259	0.048393
H	-4.395188	3.122726	2.016131	H	4.930542	2.917708	-1.666065
Zn	-0.414592	-1.389206	-0.626448	Zn	0.526935	-1.341293	0.374139
O	-0.332644	-3.320073	0.273229	O	0.079433	-3.349738	-0.223712
C	-1.348726	-3.618722	-0.421634	C	1.130178	-3.708866	0.386311
O	-1.867685	-2.765221	-1.204555	O	1.872662	-2.847375	0.946776
C	-1.986022	-4.967762	-0.283796	C	1.515519	-5.156030	0.454802
H	-2.832256	-4.877203	0.407686	H	0.793714	-5.786087	-0.067173
H	-2.379665	-5.304643	-1.245515	H	2.510317	-5.285179	0.017349
H	-1.281359	-5.694469	0.124434	H	1.587035	-5.459797	1.503592
O	0.967838	-1.636316	-2.123271	O	-0.549436	-1.474017	2.236715
C	2.193310	-1.520532	-2.342050	C	-1.586019	-1.140079	2.806494
O	2.981034	-0.642477	-1.849814	O	-2.487098	-0.320731	2.325617
C	2.855960	-2.517511	-3.250778	C	-1.942645	-1.651898	4.165064
H	3.668529	-2.051947	-3.812592	H	-2.909173	-2.162911	4.120961
H	3.291844	-3.306937	-2.626667	H	-1.171516	-2.331902	4.526897
H	2.124006	-2.974008	-3.919543	H	-2.058434	-0.809000	4.853038
H	2.591512	0.210415	-1.152915	H	-2.235724	0.057273	1.433531
P	2.034668	-1.281492	2.008801	P	-2.423236	-1.493511	-1.750639
C	1.073987	-2.378698	3.124359	C	-1.531253	-2.555262	-2.955894
H	0.462990	-1.771818	3.800971	H	-1.069143	-1.925182	-3.723230
H	0.411142	-2.999717	2.511899	H	-0.745456	-3.101103	-2.422984
H	1.739826	-3.020812	3.715415	H	-2.213893	-3.267657	-3.437209
C	3.057618	-2.503811	1.094619	C	-3.229657	-2.748196	-0.681384
H	3.651160	-3.123941	1.778286	H	-3.851491	-3.434122	-1.270624
H	2.388697	-3.148521	0.512190	H	-2.445873	-3.319504	-0.170448
H	3.720357	-1.970841	0.402954	H	-3.853468	-2.242870	0.064869
C	3.259547	-0.554243	3.170526	C	-3.824473	-0.892806	-2.775442
H	3.789377	-1.334187	3.732221	H	-4.347701	-1.725872	-3.262021
H	3.980287	0.047392	2.606338	H	-4.528039	-0.333582	-2.150490
H	2.744958	0.109403	3.872894	H	-3.442356	-0.208459	-3.539901
C	0.623960	2.552619	-1.446531	C	-0.420099	2.935349	0.498209
H	0.617256	2.332487	-2.527607	H	-0.040396	3.243747	1.485848
H	0.022104	3.469541	-1.332255	H	0.045634	3.628987	-0.223737
3_{CH2}				TS_{34CH2}			
C	-4.699862	2.962329	0.326281	C	-5.306692	2.231434	-0.065755
C	-4.029883	4.119413	0.711525	C	-4.840930	3.516086	0.196264
C	-2.639630	4.126594	0.764517	C	-3.472395	3.738475	0.298360
C	-1.920793	2.980940	0.426449	C	-2.576759	2.681945	0.135940
C	-2.578207	1.800842	0.010145	C	-3.022583	1.369963	-0.140977
C	-3.976892	1.820688	-0.017496	C	-4.406119	1.180062	-0.230538
H	-5.788421	2.947838	0.297348	H	-6.377336	2.045949	-0.143084
H	-4.589497	5.013152	0.980332	H	-5.540563	4.339730	0.324443
H	-2.112366	5.028175	1.079421	H	-3.098249	4.741589	0.509431
H	-4.523148	0.917070	-0.297811	H	-4.804610	0.187089	-0.436160
C	0.037878	1.553580	0.170692	C	-0.394949	1.592488	0.032175
C	1.036336	0.723602	0.043720	C	0.724536	0.926612	-0.031005
Si	2.859529	1.132085	-0.210233	Si	2.513358	1.387283	-0.466434
C	2.936646	2.947864	-0.788091	C	2.835732	0.678371	-2.207571
H	2.418437	3.527882	-0.005068	H	2.145589	1.237149	-2.861838
C	3.748535	0.957744	1.461693	C	2.686273	3.282897	-0.566956
H	4.817129	1.149399	1.265307	H	3.765144	3.453318	-0.725036
C	3.631634	0.039743	-1.574846	C	3.735517	0.697078	0.823030
H	3.516282	0.639916	-2.493395	H	3.976225	-0.324686	0.492408
Pd	-1.275490	0.256180	-0.625710	Pd	-1.481955	-0.045642	-0.423603
C	5.129210	-0.174673	-1.345016	C	5.036383	1.502047	0.870944
H	5.308530	-0.786299	-0.450404	H	4.872472	2.515275	1.262819
H	5.584485	-0.703756	-2.193767	H	5.765219	1.018431	1.535747
H	5.678949	0.765966	-1.212600	H	5.511604	1.606683	-0.112244

C	3.131194	0.589680	2.222734	C	3.215189	0.473966	2.190751
H	3.884845	0.250989	2.947295	H	3.988715	0.116682	2.884707
H	2.742624	1.554256	2.581496	H	2.847258	1.434395	2.581107
H	2.309745	-0.135513	2.258332	H	2.393377	-0.249854	2.240461
C	2.307038	3.981123	0.737773	C	2.382217	3.912833	0.772561
H	2.920870	3.640617	1.581218	H	2.982625	3.539561	1.612270
H	2.435779	5.069526	0.656103	H	2.540101	4.998841	0.714116
H	1.259425	3.800162	1.009338	H	1.328333	3.754964	1.035614
C	1.946817	3.879993	-1.762914	C	2.035550	3.860500	-1.735526
H	2.366770	3.538951	-2.716891	H	2.466549	3.534359	-2.689761
H	0.882566	3.608499	-1.768281	H	0.969297	3.599081	-1.764135
H	2.003052	4.977620	-1.754087	H	2.102426	4.957044	-1.703213
C	2.520199	-0.807019	-2.368316	C	2.461318	-0.833681	-2.391884
H	3.116615	-1.424209	-1.681347	H	3.057867	-1.468290	-1.720494
H	1.456096	-1.024589	-2.192239	H	1.396202	-1.029643	-2.198292
H	2.744830	-1.144368	-3.390111	H	2.661530	-1.169444	-3.419229
C	4.268134	0.954640	-2.665533	C	4.245304	0.887765	-2.702671
H	4.419184	0.628044	-3.703814	H	4.372709	0.568813	-3.746502
H	4.536517	2.018035	-2.615843	H	4.543693	1.942811	-2.646273
H	4.989984	0.400312	-2.048649	H	4.960873	0.307587	-2.102650
Zn	0.674839	-1.294234	0.274744	Zn	0.663599	-1.293878	0.303383
O	-0.634494	0.445996	2.962592	O	-0.295095	0.624767	2.978940
C	-0.456006	-0.842336	3.162544	C	-0.425046	-0.673403	3.150410
O	-0.002296	-1.613566	2.321037	O	-0.039743	-1.516927	2.343434
C	-0.858291	-1.278548	4.530083	C	-1.107356	-1.030544	4.425819
H	-0.646464	-2.339043	4.664897	H	-2.182579	-0.863924	4.296221
H	-0.324144	-0.684927	5.277931	H	-0.933420	-2.080046	4.664253
H	-1.926466	-1.084987	4.669489	H	-0.770967	-0.380833	5.237249
O	0.864556	-3.351813	-0.248948	O	0.760633	-3.346525	-0.248411
C	2.059783	-3.307639	0.169638	C	1.960926	-3.362284	0.161069
O	2.537483	-2.227958	0.630403	O	2.489607	-2.312285	0.632235
C	2.935796	-4.519848	0.079291	C	2.777516	-4.613338	0.047349
H	3.600729	-4.401573	-0.784093	H	3.431807	-4.719094	0.915898
H	3.565899	-4.598596	0.968503	H	2.138523	-5.490868	-0.065705
H	2.342327	-5.425619	-0.056186	H	3.417428	-4.529137	-0.838573
H	-0.420586	0.675122	2.028939	H	0.062539	0.815346	2.079025
P	-2.367982	-2.126220	-1.127949	P	-2.409292	-2.142441	-1.034167
C	-2.499783	-3.487104	0.097107	C	-2.420617	-3.524490	0.177997
H	-1.494930	-3.778500	0.416343	H	-1.387071	-3.795838	0.421887
H	-3.060523	-3.137799	0.970478	H	-2.934941	-3.208344	1.091720
H	-3.007936	-4.357571	-0.336967	H	-2.935801	-4.398608	-0.240667
C	-4.088035	-2.073942	-1.775180	C	-4.172424	-2.126593	-1.554695
H	-4.361869	-3.036173	-2.226182	H	-4.467653	-3.104720	-1.955168
H	-4.779707	-1.858233	-0.954148	H	-4.804108	-1.891333	-0.691351
H	-4.182285	-1.277544	-2.520394	H	-4.329714	-1.354809	-2.315107
C	-1.495909	-2.954050	-2.516751	C	-1.611923	-2.938879	-2.485456
H	-2.034560	-3.852000	-2.845503	H	-2.163018	-3.834480	-2.800121
H	-1.408488	-2.256667	-3.356564	H	-1.571756	-2.227574	-3.316923
H	-0.492319	-3.236347	-2.181988	H	-0.590836	-3.222134	-2.206161
C	-1.096521	2.889720	0.270028	C	-1.047368	2.895828	0.222436
H	-0.714436	3.661956	-0.418360	H	-0.795937	3.259003	1.234909
H	-0.837735	3.253483	1.280369	H	-0.633332	3.653763	-0.463121
4_{CH2}				TS_{45CH2}			
C	-5.266805	2.326347	-0.162364	C	3.897785	3.885072	0.537168
C	-4.775895	3.607427	0.069578	C	2.900188	4.834981	0.733225
C	-3.404188	3.803587	0.185552	C	1.567293	4.494244	0.526536
C	-2.529931	2.723626	0.067462	C	1.226671	3.202498	0.127627
C	-3.002311	1.415341	-0.179520	C	2.229542	2.238663	-0.056823
C	-4.387396	1.251167	-0.285022	C	3.562661	2.589187	0.143635
H	-6.340196	2.162809	-0.250325	H	4.942374	4.149959	0.690938
H	-5.458732	4.449610	0.163231	H	3.161259	5.843658	1.045973
H	-3.011254	4.804227	0.372887	H	0.784805	5.238780	0.674615
H	-4.801780	0.260551	-0.469676	H	4.357830	1.859292	-0.009468
C	-0.375497	1.577980	0.009935	C	-0.163674	1.289097	-0.449304
C	0.745832	0.904245	-0.009952	C	-1.146892	0.363660	-0.535616
Si	2.535519	1.337949	-0.471928	Si	-2.987019	0.608385	-0.094908
C	2.813097	0.642992	-2.226422	C	-3.084700	1.561247	1.560429
H	2.125944	1.223651	-2.864946	H	-2.738480	2.585553	1.343195
C	2.752083	3.229733	-0.543202	C	-3.901895	1.571310	-1.462615
H	3.835176	3.377243	-0.691651	H	-4.962359	1.554950	-1.158183
C	3.776280	0.601340	0.775525	C	-3.834571	-1.096065	0.131137
H	3.991658	-0.417297	0.418874	H	-3.637374	-1.383841	1.177964
Pd	-1.495689	-0.039716	-0.404248	Pd	1.622173	0.362688	-0.583213
C	5.092013	1.383193	0.802585	C	-5.352355	-0.998506	-0.054823
H	4.953094	2.395598	1.206232	H	-5.612729	-0.798599	-1.103509
H	5.825183	0.880794	1.448384	H	-5.835802	-1.946988	0.217187
H	5.549430	1.487916	-0.189068	H	-5.814261	-0.210289	0.550805

C	-3.301428	-2.225835	-0.750909	C	-3.204910	-2.611025	0.040192
H	-3.906342	-3.133234	-0.613915	H	-3.724577	-3.461421	0.503676
H	-3.327432	-1.973043	-1.819379	H	-3.098013	-2.847848	-1.029267
H	-2.270939	-2.515251	-0.511742	H	-2.199237	-2.577451	0.477455
C	-3.782315	0.876021	-2.818447	C	-3.542362	-0.772078	-3.248304
H	-4.170236	-0.150247	-2.802093	H	-3.961183	-1.710556	-2.863207
H	-4.335887	1.423188	-3.594714	H	-3.927967	-0.635299	-4.268332
H	-2.733920	0.822972	-3.143647	H	-2.454595	-0.904149	-3.333417
C	-3.469979	3.029018	-1.584850	C	-3.334456	1.710965	-2.987164
H	-3.510748	3.569709	-0.629919	H	-3.630548	2.609769	-2.431027
H	-2.441797	3.097352	-1.966493	H	-2.234979	1.688535	-3.020289
H	-4.106440	3.571223	-2.297954	H	-3.684023	1.835709	-4.021542
C	-2.165600	0.972149	2.631382	C	-3.322023	1.746791	1.875632
H	-2.441010	-0.065474	2.869249	H	-3.894102	0.977281	2.412148
H	-1.110455	0.967994	2.322862	H	-2.265244	1.500777	2.031278
H	-2.230812	1.547576	3.565568	H	-3.526163	2.707579	2.369084
C	-4.511586	1.675054	2.096181	C	-5.206978	2.119965	0.286557
H	-4.542877	2.299666	2.999996	H	-5.438058	3.074440	0.779551
H	-5.202134	2.120140	1.367331	H	-5.553880	2.193884	-0.751670
H	-4.909267	0.690327	2.376535	H	-5.813437	1.351809	0.786200
Zn	-0.334991	-1.348504	0.441473	Zn	0.003794	-0.747968	1.131350
O	-0.639947	-1.192066	-2.612693	O	1.069610	-2.142784	-1.343043
C	0.056124	-2.198954	-2.282609	C	0.661482	-2.955853	-0.482109
O	0.267180	-2.567860	-1.089049	O	0.369312	-2.662144	0.725183
C	0.723530	-2.973508	-3.379380	C	0.489613	-4.399504	-0.868275
H	1.756994	-2.611794	-3.463521	H	1.047247	-5.031262	-0.169043
H	0.759209	-4.036958	-3.130084	H	-0.566729	-4.672585	-0.768087
H	0.224661	-2.810059	-4.336360	H	0.823231	-4.579175	-1.891626
O	0.862177	-1.803466	2.125280	O	0.713951	0.125368	2.878105
C	-0.177918	-2.291766	2.661983	C	-0.411771	-0.119254	3.414224
O	-1.274574	-2.315224	2.021954	O	-1.323320	-0.703010	2.753525
C	-0.138440	-2.805400	4.067355	C	-0.689201	0.303219	4.823779
H	0.885942	-3.004775	4.386210	H	0.188397	0.758746	5.284499
H	-0.568592	-2.040476	4.723890	H	-1.520130	1.017508	4.817341
H	-0.756331	-3.701647	4.160509	H	-1.017184	-0.562618	5.406225
H	-0.912881	-0.470267	-1.593473	H	-1.185264	-1.095107	-1.111878
P	3.487455	-1.176515	-0.188643	P	3.863464	-0.911900	-0.353813
C	3.201287	-2.988490	-0.079845	C	3.863971	-2.726296	-0.072865
H	2.435653	-3.174656	0.681491	H	3.116563	-2.964147	0.692712
H	2.834638	-3.383254	-1.031871	H	3.595210	-3.248806	-0.996267
H	4.130265	-3.500331	0.202245	H	4.848899	-3.065488	0.270689
C	5.001765	-1.109331	-1.230239	C	5.372671	-0.717352	-1.384946
H	5.797498	-1.737465	-0.810514	H	6.239518	-1.163671	-0.882332
H	4.765246	-1.460583	-2.240269	H	5.218415	-1.218161	-2.345861
H	5.361677	-0.078377	-1.308568	H	5.581394	0.338616	-1.581177
C	4.135881	-0.847908	1.495524	C	4.396184	-0.304342	1.292090
H	4.989210	-1.497994	1.727044	H	5.312762	-0.806410	1.625512
H	4.433258	0.201066	1.591798	H	4.556392	0.777664	1.260128
H	3.321177	-1.040709	2.202494	H	3.588115	-0.494735	2.008711
C	-0.170968	2.760018	-0.153031	C	-0.340396	2.168007	-0.239481
H	-0.572859	3.279905	-1.038771	H	-0.782853	2.277846	0.765814
H	-0.874662	2.995008	0.662414	H	-1.020536	2.707385	-0.919780
5_{CH2}				10_{CH2}			
C	3.600268	3.819768	-0.457242	C	-3.828663	3.192017	0.154310
C	2.529139	4.658767	-0.169166	C	-2.842911	4.173517	0.174050
C	1.247516	4.128863	-0.085565	C	-1.502050	3.809379	0.105812
C	1.026543	2.764592	-0.275030	C	-1.137223	2.466781	0.018225
C	2.106228	1.904705	-0.538089	C	-2.131478	1.471078	0.002002
C	3.387255	2.454971	-0.638722	C	-3.472164	1.846263	0.068675
H	4.606428	4.225368	-0.545038	H	-4.879672	3.470941	0.206359
H	2.690923	5.724146	-0.020426	H	-3.119554	5.223475	0.243027
H	0.399147	4.781928	0.121116	H	-0.727289	4.576474	0.120299
H	4.242838	1.826496	-0.879759	H	-4.257615	1.090513	0.057614
C	-0.281253	0.709713	-0.635161	C	0.244677	0.485417	-0.096697
C	-1.385527	-0.078763	-0.745132	C	1.224449	-0.422844	-0.113435
Si	-3.255785	0.226139	-0.578438	Si	3.094128	-0.181104	-0.024124
C	-3.715152	1.797469	0.400732	C	3.578589	1.436560	-0.906173
H	-3.159670	2.620300	-0.078430	C	3.046156	2.241926	-0.373242
C	-3.885065	0.427618	-2.366634	C	3.586851	-0.101738	1.816221
H	-4.983613	0.509086	-2.306928	H	4.687004	-0.034180	1.854791
C	-3.993833	-1.319447	0.265976	C	3.966777	-1.651018	-0.884410
H	-3.950153	-1.102617	1.347134	H	4.065316	-1.343476	-1.939893
Pd	1.662733	-0.035356	-0.850978	P	-1.523287	-0.461285	-0.100516
C	-5.457721	-1.532368	-0.127906	C	5.376445	-1.900175	-0.342153
H	-5.546842	-1.801314	-1.189925	H	5.348920	-2.256644	0.696949
H	-5.903770	-2.354344	0.448841	H	5.890313	-2.673583	-0.930235
H	-6.081008	-0.643985	0.032525	H	6.007974	-1.003055	-0.359885

C	3.163545	-2.951561	-0.864162	H	0.858878	3.779616	-4.713932
H	3.728882	-3.768172	-1.335605	C	1.769778	6.232695	-3.930869
H	2.933209	-3.273340	0.161906	H	0.995700	6.293681	-4.707867
H	2.212768	-2.859171	-1.401750	H	1.737610	7.170166	-3.360796
C	3.154784	-1.363648	2.562596	H	2.739161	6.197631	-4.446218
H	3.601537	-2.275346	2.145526	H	2.962763	-1.791214	0.650790
H	3.437715	-1.315329	3.623697	C	3.221133	0.665045	-0.262213
H	2.062657	-1.483978	2.524636	O	4.305297	0.134079	-0.087977
C	3.004796	1.131482	2.503973				
H	3.328000	2.070357	2.035563	2 _{co}			
H	1.905603	1.106211	2.479902	C	4.349908	-3.349970	-0.962488
H	3.301216	1.173803	3.561600	C	3.146337	-3.295474	-1.662374
C	3.121690	1.451168	-2.364323	C	1.980915	-2.912644	-1.008639
H	3.664347	0.699030	-2.954283	C	2.013365	-2.619648	0.357355
H	2.051243	1.236053	-2.473311	C	3.217218	-2.697811	1.060554
H	3.320415	2.425029	-2.833669	C	4.385518	-3.047717	0.397346
C	5.076512	1.729022	-0.824320	H	5.263775	-3.633361	-1.479829
H	5.314032	2.706549	-1.267164	H	3.117541	-3.550787	-2.719727
H	5.455344	1.735142	0.205886	H	1.038569	-2.848458	-1.552726
H	5.654864	0.980552	-1.384495	H	5.326961	-3.086922	0.939521
H	0.894741	-1.479855	-0.116459	C	-0.288756	-1.574884	0.367503
Pd	-3.537109	-1.814823	-0.083709	C	-1.386254	-1.110004	-0.015992
C	-3.426091	-3.651542	-0.163191	Si	-3.221328	-0.767130	-0.165570
H	-2.934403	-3.953953	-1.093346	C	-3.599637	0.525348	-1.511724
H	-2.829942	-4.024916	0.675549	H	-3.762918	-0.064439	-2.430684
H	-4.423137	-4.107832	-0.122710	C	-3.960697	-2.446971	-0.653597
C	-4.593277	-1.604728	1.406303	H	-3.719519	-3.125327	0.181153
H	-5.535929	-2.158368	1.310682	C	-3.762930	-0.225080	1.564512
H	-4.049320	-1.969229	2.283735	H	-4.838060	0.012323	1.484732
H	-4.806825	-0.542809	1.565316	Pd	0.212958	0.040337	-1.006555
C	-4.725573	-1.488238	-1.447332	C	-3.588645	-1.349002	2.584738
H	-5.649597	-2.065762	-1.318919	H	-2.532654	-1.642250	2.671379
H	-4.965624	-0.420911	-1.485964	H	-3.908678	-1.018820	3.582148
H	-4.260756	-1.759263	-2.400776	H	-4.169595	-2.245294	2.332227
C	0.274958	1.989197	-0.065817	C	-3.013125	1.027318	2.021725
H	0.772265	2.379808	-0.969664	H	-3.431950	1.409816	2.962145
H	0.877347	2.351904	0.784521	H	-1.957143	0.799121	2.223012
				H	-3.035780	1.845820	1.290853
C ₆ H ₅ C(O)C≡CSi ⁱ Pr ₃				C	-3.325564	-3.008266	-1.923883
C	-0.419248	-1.432614	0.480681	H	-2.240094	-3.134623	-1.822206
C	-0.475502	-0.133247	-0.014944	H	-3.752728	-3.987572	-2.180038
C	0.699615	0.564268	-0.264646	H	-3.502844	-2.348692	-2.785668
C	1.935639	-0.040281	-0.020255	C	-5.479988	-2.367057	-0.796957
C	1.986193	-1.347328	0.472708	H	-5.970927	-1.991005	0.110433
C	0.812033	-2.040281	0.723503	H	-5.762095	-1.702762	-1.626365
H	-1.340092	-1.976587	0.679444	H	-5.909309	-3.353692	-1.018778
H	-1.437459	0.336717	-0.204694	C	-2.491082	1.537597	-1.798414
H	0.667235	1.581940	-0.652157	H	-2.203157	2.111985	-0.907378
H	0.850744	-3.056000	1.109685	H	-1.576617	1.050260	-2.180323
C	3.126157	2.042775	-0.712586	H	-2.816179	2.256428	-2.565118
C	3.026191	3.202074	-1.080149	C	-4.906408	1.259898	-1.194651
Si	2.797974	4.965552	-1.601436	H	-5.191568	1.918197	-2.026403
C	1.568122	4.995875	-3.053700	H	-5.747779	0.578630	-1.013878
H	0.571784	5.069425	-2.584439	H	-4.797357	1.893715	-0.304467
C	2.080393	5.853841	-0.086578	Zn	0.727166	1.456244	1.102304
H	2.861451	5.795238	0.689050	C	-0.664826	3.009223	0.696425
C	4.504192	5.647605	-2.061863	C	0.314830	3.757917	0.414552
H	4.345869	6.672238	-2.439099	O	1.507911	3.331692	0.506525
C	5.413100	5.712598	-0.835300	C	0.059030	5.150691	-0.081168
H	5.539080	4.717678	-0.385226	H	0.953355	5.770155	0.009332
H	6.414621	6.072521	-1.107816	H	-0.224756	5.094066	-1.139149
H	5.024798	6.382267	-0.057985	H	-0.778723	5.598817	0.458208
C	5.159278	4.818081	-3.166383	O	0.389439	0.813182	3.039509
H	6.155773	5.208957	-3.413427	C	1.554868	0.309432	3.063134
H	5.288952	3.774325	-2.848470	O	2.299846	0.372154	2.038304
H	4.571417	4.810074	-4.093178	C	2.040417	-0.382170	4.299005
C	0.830859	5.153545	0.442257	H	3.129321	-0.326470	4.368831
H	1.030979	4.111164	0.719024	H	1.571408	0.043175	5.188603
H	0.435320	5.665828	1.329969	H	1.744961	-1.434819	4.224284
H	0.026935	5.150686	-0.308182	H	3.214776	-2.455235	2.120111
C	1.796822	7.325410	-0.384337	P	2.115524	1.017075	-1.964509
H	2.682920	7.861095	-0.750358	C	2.017914	2.694237	-2.698305
H	1.010206	7.427960	-1.145559	H	1.144343	2.763642	-3.355312
H	1.442323	7.851323	0.512571	H	1.915186	3.416926	-1.883513
C	1.594562	3.723857	-3.899778	H	2.924402	2.922886	-3.272557
H	2.579259	3.570383	-4.362822	C	3.627011	1.107140	-0.936483
H	1.374819	2.828508	-3.306242	H	4.497319	1.372805	-1.549885
				H	3.485916	1.861573	-0.155008

H	3.788883	0.136452	-0.452099	C	-3.657173	-1.328761	-2.725493
C	2.692382	0.012845	-3.391750	H	-4.134624	-2.225863	-3.139564
H	3.590609	0.454954	-3.841789	H	-4.373076	-0.788848	-2.096634
H	2.926018	-0.998725	-3.041281	H	-3.362369	-0.665649	-3.545103
H	1.903557	-0.052023	-4.148235	C	-0.705273	2.845316	0.416927
C	0.794331	-2.231036	1.106701	O	-0.055271	3.875340	0.456449
O	0.680441	-2.395970	2.309147				
TS_{23co}				3_{co}			
C	-4.918437	2.557714	0.167432	C	-4.595705	3.091123	0.270193
C	-4.313183	3.815083	0.218304	C	-3.872493	4.245796	0.580182
C	-2.935594	3.906856	0.338211	C	-2.488228	4.193814	0.608942
C	-2.173235	2.737797	0.407422	C	-1.846450	2.988841	0.310626
C	-2.752168	1.449747	0.382316	C	-2.548347	1.819297	-0.036099
C	-4.148214	1.401547	0.251846	C	-3.944540	1.893797	-0.025077
H	-6.000395	2.484791	0.069467	H	-5.684452	3.128602	0.258331
H	-4.919782	4.715574	0.155422	H	-4.395211	5.171735	0.808691
H	-2.424298	4.867664	0.358227	H	-1.883253	5.061297	0.869915
H	-4.647302	0.430453	0.257321	H	-4.544377	1.009590	-0.250240
C	-0.024431	1.535354	0.224578	C	0.044815	1.460251	0.094076
C	1.005909	0.776249	0.127059	C	1.051338	0.641590	-0.012716
Si	2.841514	1.191092	-0.164654	Si	2.895862	1.015933	-0.276585
C	2.820541	2.832659	-1.117332	C	3.043775	2.771303	-0.980621
H	2.222990	3.519053	-0.497236	H	2.574913	3.428802	-0.233596
C	3.596441	1.431627	1.559843	C	3.714714	0.906111	1.433728
H	4.688007	1.494797	1.405483	H	4.802504	0.954174	1.255658
C	3.694658	-0.121726	-1.255019	C	3.644987	-0.190852	-1.561775
H	4.314850	0.509371	-1.917100	H	3.719642	0.428091	-2.471789
Pd	-1.206125	0.108458	-0.651685	Pd	-1.335129	0.181098	-0.632311
C	4.638514	-1.075086	-0.525365	C	5.062112	-0.621696	-1.180131
C	4.086629	-1.734274	0.155169	H	5.054151	-1.251500	-0.280077
H	5.174238	-1.711034	-1.245266	H	5.522529	-1.212485	-1.984414
H	5.395597	-0.543244	0.064384	H	5.725417	0.229476	-0.978924
C	2.729632	-0.892598	-2.157483	C	2.803115	-1.413349	-1.916818
H	3.285328	-1.501137	-2.885046	H	3.258007	-1.972136	-2.747095
H	2.092949	-1.585668	-1.589153	H	2.741350	-2.107097	-1.066263
H	2.053585	-0.234770	-2.719184	H	1.781765	-1.146565	-2.225933
C	3.306982	0.269878	2.509975	C	3.399889	-0.406356	2.147054
H	3.611442	-0.706307	2.117155	H	3.620455	-1.299095	1.548882
H	3.814818	0.421820	3.472321	H	3.960041	-0.488884	3.088913
H	2.229918	0.209721	2.729721	H	2.333006	-0.457011	2.413986
C	3.112370	2.743108	2.179987	C	3.308521	2.092075	2.308180
H	3.375367	3.623361	1.581865	H	3.593391	3.058594	1.875844
H	2.019009	2.746237	2.293606	H	2.219759	2.118076	2.455415
H	3.542853	2.880038	3.181445	H	3.772307	2.021770	3.302135
C	2.139378	2.719829	-2.479667	C	2.283019	2.943303	-2.293604
H	2.695022	2.054019	-3.156062	H	2.708395	2.321742	-3.095111
H	1.113784	2.335317	-2.400944	H	1.222860	2.677429	-2.199322
H	2.087304	3.700777	-2.971767	H	2.332277	3.984822	-2.639922
C	4.233511	3.397615	-1.266677	C	4.510256	3.168067	-1.153740
H	4.215309	4.364712	-1.788013	H	4.596140	4.202797	-1.513757
H	4.732113	3.558001	-0.301846	H	5.081584	3.100100	-0.218585
H	4.874988	2.730964	-1.861277	H	5.015447	2.532924	-1.896274
Zn	0.507769	-1.325994	0.623086	Zn	0.509878	-1.415929	0.360881
O	0.664450	-3.277710	-0.225887	O	-0.009835	-3.428036	-0.143216
C	1.751317	-3.408091	0.413707	C	1.060475	-3.794915	0.428963
O	2.165021	-2.475640	1.167973	O	1.851968	-2.933159	0.916655
C	2.592000	-4.633267	0.233099	C	1.407153	-5.248579	0.539405
H	3.392652	-4.390365	-0.477146	H	0.657183	-5.875673	0.055026
H	3.064169	-4.915714	1.176852	H	2.389396	-5.420908	0.089117
H	2.005001	-5.459221	-0.172026	H	1.490462	-5.517385	1.596944
O	-0.685031	-1.533338	2.238197	O	-0.485928	-1.480650	2.267525
C	-1.877348	-1.347152	2.583665	C	-1.493056	-1.105059	2.862589
O	-2.705803	-0.532002	2.068579	O	-2.416933	-0.322340	2.359855
C	-2.402160	-2.191303	3.712010	C	-1.782946	-1.508790	4.271146
H	-3.370663	-1.832462	4.063331	H	-2.768583	-1.980452	4.323770
H	-2.504210	-3.222345	3.354761	H	-1.013996	-2.190721	4.633752
H	-1.675504	-2.205990	4.528648	H	-1.821447	-0.615331	4.901937
H	-2.430167	0.281892	1.200076	H	-2.190649	-0.022478	1.434759
P	-2.179684	-1.758744	-1.722576	P	-2.533906	-1.591064	-1.667088
C	-1.215318	-2.810492	-2.873631	C	-1.668710	-2.700028	-2.846873
H	-0.803187	-2.193035	-3.678494	H	-1.214704	-2.100782	-3.643218
H	-0.386838	-3.254257	-2.310378	H	-0.877950	-3.230905	-2.305919
H	-1.837898	-3.604213	-3.305984	H	-2.362514	-3.424980	-3.291749
C	-2.859386	-3.004406	-0.556872	C	-3.332630	-2.792320	-0.533995
H	-3.480020	-3.745116	-1.076373	H	-3.967523	-3.499005	-1.083202
H	-2.023898	-3.517142	-0.067086	H	-2.545808	-3.345729	-0.009284
H	-3.453902	-2.493510	0.209581	H	-3.941646	-2.250208	0.198633
				C	-3.950675	-1.010711	-2.681604

H	-4.487927	-1.854341	-3.133360	H	-1.717269	-2.171333	-3.379629
H	-4.639552	-0.432936	-2.056845	H	-0.687601	-3.174531	-2.323212
H	-3.582857	-0.349660	-3.472937	H	-1.010458	2.860290	0.179963
C	-0.384821	2.869031	0.391488	O	-0.391144	3.883313	0.417570
O	0.408500	3.746186	0.684606				
TS_{34co}				4_{co}			
C	-5.189525	2.424743	-0.091079	C	-5.174551	2.488200	-0.228897
C	-4.658049	3.702423	0.107257	C	-4.629016	3.758618	-0.022297
C	-3.285356	3.856223	0.187998	C	-3.257680	3.889990	0.104306
C	-2.463176	2.731658	0.056305	C	-2.450407	2.750923	0.006989
C	-2.968325	1.435871	-0.159859	C	-2.969087	1.461858	-0.216690
C	-4.360833	1.310809	-0.213426	C	-4.360835	1.359902	-0.313934
H	-6.270067	2.298151	-0.153178	H	-6.254245	2.378821	-0.327403
H	-5.318927	4.560550	0.205451	H	-5.278312	4.628326	0.046409
H	-2.822518	4.826706	0.362297	H	-2.783716	4.853151	0.289544
H	-4.821086	0.335110	-0.364597	H	-4.832491	0.391616	-0.472520
C	-0.338618	1.518146	0.025369	C	-0.341710	1.508011	0.018522
C	0.789217	0.866002	-0.013609	C	0.786343	0.854363	-0.015322
Si	2.602177	1.268203	-0.464253	Si	2.600894	1.251079	-0.472265
C	2.781680	0.604393	-2.245167	C	2.749077	0.651117	-2.278473
H	2.098988	1.231346	-2.842728	H	2.069264	1.312311	-2.841702
C	2.986995	3.126770	-0.482818	C	2.995931	3.107333	-0.418910
H	4.060646	3.138031	-0.747035	H	4.070984	3.129707	-0.675491
C	3.771224	0.380878	0.750969	C	3.781720	0.310223	0.691981
H	3.881120	-0.647981	0.377426	H	3.860715	-0.711678	0.292265
Pd	-1.511316	-0.075895	-0.400183	Pd	-1.529189	-0.077474	-0.389872
C	5.163844	1.015926	0.783125	C	5.183821	0.924694	0.697559
H	5.142048	2.028092	1.208395	H	5.186621	1.935826	1.126173
H	5.841106	0.420180	1.410353	H	5.865431	0.316158	1.307631
H	5.622108	1.089438	-0.211008	H	5.621678	0.994451	-0.306147
C	3.200235	0.286553	2.166514	C	3.250698	0.186831	2.120829
H	3.932328	-0.162098	2.852223	H	4.006033	-0.268695	2.776261
H	2.928104	1.271124	2.573140	H	2.982990	1.159965	2.557098
C	2.306319	-0.348238	2.206427	H	2.365907	-0.459846	2.173066
C	2.834556	3.794786	0.882879	C	2.834386	3.718340	0.972418
H	3.439718	3.307934	1.658211	H	3.447153	3.209170	1.727337
H	3.150256	4.846434	0.835539	H	3.135121	4.775376	0.967402
H	1.786687	3.788163	1.201928	H	1.786556	3.684834	1.290798
C	2.236451	3.903973	-1.561893	C	2.250436	3.924848	-1.471143
H	2.395740	3.489232	-2.565345	H	2.426347	3.556380	-2.489621
H	1.159586	3.923854	-1.358382	H	1.171095	3.924232	-1.281328
H	2.573493	4.949745	-1.584104	H	2.575907	4.974096	-1.442733
C	2.365529	-0.851528	-2.440263	C	2.305261	-0.789050	-2.523541
H	2.944984	-1.528141	-1.796011	H	2.886963	-1.500601	-1.919517
H	1.295595	-1.009487	-2.237316	H	1.237500	-0.936843	-2.302470
H	2.536571	-1.170597	-3.478190	H	2.448446	-1.067161	-3.577293
C	4.205712	0.809938	-2.761934	C	4.170162	0.854370	-2.804171
H	4.284174	0.532076	-3.822111	H	4.231219	0.624291	-3.876860
H	4.545091	1.849451	-2.669425	H	4.530729	1.882011	-2.668328
H	4.916497	0.175987	-2.212518	H	4.875137	0.183454	-2.292682
Zn	0.670426	-1.356390	0.261005	Zn	0.666890	-1.361740	0.246051
O	-0.596661	0.371363	2.996726	O	-0.361381	0.442042	3.027731
C	-0.480701	-0.929849	3.145694	C	-0.339450	-0.865293	3.165548
O	-0.036474	-1.687319	2.286026	O	0.059661	-1.645111	2.303386
C	-0.957225	-1.406632	4.474905	C	-0.849880	-1.317482	4.490615
H	-2.049871	-1.335237	4.502055	H	-1.909981	-1.056365	4.572748
H	-0.654665	-2.441503	4.634681	H	-0.720932	-2.394475	4.596350
H	-0.571588	-0.760551	5.267813	H	-0.325837	-0.786188	5.290171
O	0.670558	-3.394631	-0.367291	O	0.604648	-3.407267	-0.377636
C	1.857477	-3.487248	0.070843	C	1.825255	-3.499037	-0.049874
O	2.434971	-2.473895	0.563477	O	2.436561	-2.491937	0.416610
C	2.563860	-4.807689	0.029041	C	2.568358	-4.784514	-0.247792
H	2.314760	-5.343570	-0.890003	H	3.240219	-4.964519	0.594932
H	3.643202	-4.673563	0.119117	H	1.880390	-5.621293	-0.379547
H	2.215906	-5.416155	0.870828	H	3.188692	-4.691846	-1.146412
H	-0.348095	0.640947	2.084234	H	-0.080124	0.704130	2.122289
P	-2.478003	-2.139857	-1.071500	P	-2.547379	-2.163643	-0.928562
C	-2.514355	-3.558292	0.094673	C	-2.535219	-3.479333	0.353447
H	-1.485386	-3.870273	0.302850	H	-1.503868	-3.810765	0.510995
H	-2.994447	-3.253865	1.030745	H	-2.929795	-3.076705	1.292407
C	-3.069217	-4.400374	-0.338411	H	-3.147430	-4.334414	0.039553
H	-4.245364	-2.052090	-1.570524	C	-4.341276	-2.096062	-1.327589
H	-4.573952	-3.003700	-2.007403	H	-4.701812	-3.082890	-1.644752
H	-4.861666	-1.835006	-0.691410	H	-4.900838	-1.783375	-0.439524
H	-4.386482	-1.246190	-2.298055	H	-4.521004	-1.368922	-2.126157
C	-1.720294	-2.899385	-2.561712	C	-1.896512	-3.057084	-2.394253
H	-2.271847	-3.794961	-2.874932	H	-2.489435	-3.957154	-2.601546
				H	-1.926157	-2.397541	-3.267783

H	-0.859006	-3.344754	-2.194677	C	0.298926	2.501256	-0.274293
C	-1.002219	2.854124	0.186260	O	1.335000	3.096500	-0.512468
O	-0.378688	3.859513	0.482441				
TS_{45co}				5_{co}			
C	-3.630380	3.981489	-0.710850	C	3.358577	3.734596	-1.241527
C	-2.561793	4.817196	-1.045330	C	2.274528	4.559125	-0.941243
C	-1.264964	4.347325	-0.918436	C	1.070953	3.983548	-0.568845
C	-1.048638	3.045614	-0.459931	C	0.962771	2.593892	-0.497236
C	-2.109088	2.194578	-0.134012	C	2.048928	1.748504	-0.766960
C	-3.410937	2.680717	-0.260422	C	3.252034	2.347043	-1.149239
H	-4.650785	4.350264	-0.803487	H	4.304299	4.176810	-1.550860
H	-2.750853	5.828362	-1.397592	H	2.375202	5.639779	-1.006965
H	-0.399524	4.963249	-1.159096	H	0.192466	4.581145	-0.331319
H	-4.266657	2.055293	-0.005969	H	4.125809	1.746353	-1.397252
C	0.261530	1.077660	0.252890	C	-0.256287	0.468597	-0.391373
C	1.312479	0.240775	0.409650	C	-1.340135	-0.315656	-0.607879
Si	3.159250	0.433082	0.009453	Si	-3.230561	-0.145803	-0.804743
C	3.385689	1.080180	-1.768597	C	-4.017973	1.547800	-0.461232
H	3.072214	2.132181	-1.735037	H	-3.280396	2.283630	-0.810857
C	4.083433	1.476740	1.310446	C	-3.486225	-0.579774	-2.646582
H	5.150242	1.294856	1.092616	H	-4.572934	-0.495486	-2.816717
C	3.908424	-1.346936	0.051489	C	-3.952277	-1.464686	0.371122
H	3.771935	-1.733040	-0.974759	H	-4.018696	-0.953758	1.345947
Pd	-1.649906	0.335886	0.513807	Pd	1.708359	-0.238609	-0.578708
C	5.413972	-1.325457	0.333960	C	-5.368864	-1.852698	-0.058186
H	5.614592	-1.026266	1.372164	H	-5.365601	-2.371783	-1.027068
H	5.850742	-2.325139	0.200204	H	-5.830187	-2.534278	0.670123
H	5.966161	-0.636596	-0.315748	H	-6.033065	-0.984318	-0.156797
C	3.258851	-2.356353	0.998194	C	-3.098549	-2.714732	0.583586
H	3.794133	-3.315903	0.961765	H	-3.621230	-3.428297	1.236196
H	3.271730	-2.018051	2.042621	H	-2.883410	-3.241461	-0.357313
H	2.216087	-2.592541	0.746835	H	-2.139102	-2.489851	1.067098
C	3.798785	0.969398	2.724993	C	-3.052963	-1.989903	-3.038980
H	4.047987	-0.091464	2.858750	H	-3.589744	-2.766478	-2.479952
H	4.375140	1.537270	3.469166	H	-3.233592	-2.172686	-4.107865
H	2.736156	1.090958	2.978809	H	-1.977358	-2.141735	-2.869920
C	3.839716	2.980175	1.239658	C	-2.779775	0.452178	-3.526888
H	4.027618	3.393374	0.242028	H	-3.082675	1.482422	-3.300549
H	2.800437	3.222300	1.491062	H	-1.689641	0.397866	-3.394942
H	4.488778	3.507307	1.953939	H	-2.985525	0.274669	-4.591820
C	2.471939	0.347158	-2.750705	C	-4.227899	1.785252	1.033921
H	2.695948	-0.730326	-2.788939	H	-5.038892	1.154204	1.425025
H	1.409058	0.460317	-2.494050	H	-3.325829	1.574671	1.620279
H	2.597781	0.730396	-3.773243	H	-4.513655	2.829325	1.222542
C	4.835545	1.023925	-2.245501	C	-5.325144	1.773498	-1.223253
H	4.940670	1.490379	-3.235423	H	-5.736639	2.765083	-0.988135
H	5.519358	1.547736	-1.563945	H	-5.199685	1.723329	-2.311927
H	5.190687	-0.011517	-2.344520	H	-6.096843	1.040359	-0.947987
Zn	0.365007	-1.458962	-0.349746	Zn	0.109615	-0.437395	1.617725
O	0.721240	-0.960397	2.682091	O	1.184685	-2.400880	-0.456301
C	-0.388206	-1.554907	2.493310	C	0.820360	-2.965076	0.602397
O	-0.804808	-1.912592	1.350074	O	0.510398	-2.369299	0.686338
C	-1.263112	-1.813086	3.676536	C	0.726226	-4.465964	0.627205
H	-2.163213	-1.193790	3.567377	H	-0.318289	-4.755442	0.785222
H	-1.582641	-2.859169	3.680594	H	1.092106	-4.902568	-0.303709
H	-0.757985	-1.559245	4.609402	H	1.293484	-4.852615	1.479658
O	-0.999560	-2.012246	-1.886425	O	0.573208	1.094347	2.911287
C	-0.204247	-2.961504	-2.150665	C	-0.633705	1.066999	3.314842
O	0.865945	-3.103634	-1.476911	O	-1.423831	0.168724	2.895053
C	-0.496685	-3.919698	-3.262769	C	-1.137601	2.133002	4.233909
H	-0.323173	-4.944988	-2.925339	H	-1.896341	1.731056	4.908944
H	-1.518700	-3.801581	-3.625901	H	-0.318223	2.590531	4.791114
H	0.201855	-3.728390	-4.083864	H	-1.611617	2.903598	3.614489
H	1.070339	-0.522798	1.648652	H	-1.078738	-1.370774	-0.780084
P	-3.781369	-0.849198	0.187977	P	4.005809	-0.962427	-0.504010
C	-3.670455	-2.680027	0.272316	C	4.196532	-2.699638	0.051941
H	-2.824140	-2.997762	-0.346944	H	3.739820	-2.811232	1.041840
H	-3.483917	-3.002531	1.301405	H	3.678854	-3.369224	-0.641214
H	-4.594118	-3.143993	-0.095836	H	5.256809	-2.973258	0.113153
C	-5.347253	-0.537212	1.104484	C	5.050806	-0.945634	-2.014384
H	-6.171459	-1.132525	0.691485	H	6.064245	-1.302204	-1.792245
H	-5.212088	-0.800375	2.159134	H	4.597970	-1.598152	-2.767614
H	-5.616602	0.522946	1.053890	H	5.110117	0.063996	-2.433297
C	-4.287935	-0.620490	-1.560549	C	5.037442	-0.081414	0.730408
H	-5.197752	-1.188646	-1.791851	H	6.060333	-0.477213	0.747931
H	-4.452854	0.441405	-1.770295	H	5.060906	0.990641	0.514434
H	-3.462761	-0.971197	-2.190863	H	4.582620	-0.210792	1.718341
				C	-0.319275	1.956752	-0.165418

O	-1.299992	2.554105	0.248472	Si	2.929861	4.854257	-1.787401
10 _{co}				C	1.772962	4.680450	-3.291115
C	-3.823003	3.200558	-0.043260	H	0.753939	4.661824	-2.865669
C	-2.824444	4.174119	0.021628	C	2.083299	5.832690	-0.398706
C	-1.494347	3.785250	0.077442	H	2.836362	5.908732	0.403027
C	-1.178005	2.426897	0.061654	C	4.602782	5.624867	-2.238181
C	-2.169874	1.442026	-0.003568	H	4.383659	6.615062	-2.672823
C	-3.503686	1.842356	-0.052268	C	5.465431	5.823492	-0.992993
H	-4.868019	3.504024	-0.085635	H	5.651269	4.866288	-0.485632
H	-3.092374	5.227990	0.029640	H	6.444836	6.246588	-1.255716
H	-0.680926	4.507228	0.135926	H	5.000602	6.499650	-0.264783
H	-4.308242	1.108524	-0.099961	C	5.348993	4.793102	-3.280534
C	0.199632	0.430490	0.031446	H	6.332453	5.229908	-3.502853
C	1.215732	-0.432006	-0.055578	H	5.519831	3.769730	-2.918400
Si	3.113525	-0.252131	-0.043190	H	4.800591	4.719486	-4.228268
C	3.718904	1.279099	-0.982109	C	0.875886	5.084114	0.160773
H	3.357102	2.139597	-0.404148	H	1.154771	4.101971	0.561042
C	3.641443	-0.203198	1.785510	H	0.395805	5.651815	0.969876
H	4.741897	-0.280837	1.792316	C	0.110278	4.923320	-0.612833
C	3.826454	-1.812999	-0.904380	H	1.694532	7.243417	-0.835897
H	3.972440	-1.504642	-1.954261	H	2.543414	7.810204	-1.241805
Pd	-1.585932	-0.504757	-0.000226	H	0.914687	7.213425	-1.610383
C	5.197403	-2.204685	-0.346847	C	1.285203	7.821384	0.004023
H	5.117003	-2.569897	0.686010	H	1.973925	3.384896	-4.075363
H	5.642713	-3.017290	-0.938185	H	2.983993	3.327227	-4.503618
H	5.912816	-1.373389	-0.342964	H	1.841463	2.494988	-3.450056
C	2.908926	-3.033887	-0.909868	C	1.264679	3.320670	-4.912425
H	3.402501	-3.892263	-1.387717	H	1.874523	5.889285	-4.224091
H	2.643391	-3.347231	0.110853	H	1.130043	5.826867	-5.029463
H	1.975266	-2.851947	-1.455063	H	1.721126	6.845128	-3.707007
C	3.071868	-1.387979	2.565515	H	2.861925	5.933739	-4.704114
H	3.351978	-2.357536	2.131313	H	2.395093	-2.013621	0.669173
H	3.419524	-1.382191	3.608224	S	3.489613	0.448739	-0.104298
H	1.973686	-1.342574	2.592309	2 _s			
C	3.247862	1.111115	2.454656	C	4.416586	-3.136048	-0.890113
H	3.693797	1.982680	1.960143	C	3.269068	-3.921017	-0.981895
H	2.159361	1.254046	2.431772	C	2.174593	-3.649719	-0.167684
C	3.561843	1.124672	3.508193	C	2.231305	-2.580647	0.724969
C	3.108001	1.365451	-2.378292	C	3.366513	-1.776808	0.809966
H	3.390274	0.502034	-2.999124	C	4.462944	-2.066852	0.000032
H	2.012973	1.405734	-2.344571	H	5.277915	-3.359677	-1.515698
C	3.456545	2.264321	-2.906043	H	3.230731	-4.754881	-1.678855
C	5.244259	1.333526	-1.055657	H	1.276202	-4.262109	-0.217568
H	5.578992	2.263210	-1.536948	H	5.355455	-1.447658	0.063830
H	5.715887	1.291889	-0.064297	C	-0.253529	-1.513353	0.754255
H	5.650158	0.504596	-1.653409	C	-1.324941	-1.070234	0.264434
H	0.900660	-1.493035	-0.091233	Si	-3.143678	-0.873721	-0.097147
P	-3.621740	-1.830476	-0.078679	C	-3.512656	0.310125	-1.548915
C	-3.502306	-3.667843	-0.086256	H	-3.666436	-0.360168	-2.412143
H	-2.907946	-3.997340	-0.944528	C	-3.725431	-2.620537	-0.567970
H	-3.005312	-4.011576	0.826432	C	-3.512122	-3.244984	0.315512
H	-4.497353	-4.126503	-0.144850	C	-3.894966	-0.294245	1.544367
C	-4.812938	-1.567215	1.295356	H	-4.939231	-0.013096	1.326864
H	-5.733656	-2.143371	1.139454	Pd	0.300943	-0.142997	-0.834721
H	-4.350522	-1.874625	2.238721	C	-3.901275	-1.419093	2.577526
H	-5.059381	-0.503484	1.376274	H	-2.881541	-1.786507	2.765761
C	-4.675535	-1.549644	-1.557787	H	-4.294793	-1.064265	3.539919
H	-5.609838	-2.121970	-1.496993	H	-4.511449	-2.276217	2.265133
H	-4.906727	-0.483753	-1.653428	C	-3.157049	0.930504	2.088474
H	-4.124857	-1.852634	-2.454098	H	-3.684715	1.351799	2.954929
C	0.202456	1.924514	0.121125	H	-2.147822	0.659226	2.430628
O	1.201398	2.614708	0.244295	H	-3.032205	1.733882	1.350677
C ₆ H ₅ SC≡CSi _i Pr ₃				C	-2.929092	-3.178245	-1.745199
C	-0.800158	-1.138987	-0.098562	H	-1.852022	-3.200410	-1.534531
C	-0.567158	0.153539	-0.555792	H	-3.245443	-4.201503	-1.991664
C	0.721418	0.677695	-0.577365	H	-3.075707	-2.573350	-2.651994
C	1.782012	-0.106818	-0.134589	C	-5.226561	-2.665891	-0.845787
C	1.559787	-1.405562	0.325074	H	-5.818408	-2.282906	-0.003688
C	0.268016	-1.916051	0.340497	H	-5.486279	-2.068410	-1.731398
H	-1.810270	-1.540512	-0.084172	H	-5.564439	-3.692075	-1.046422
H	-1.396387	0.767419	-0.900197	C	-2.407854	1.298017	-1.918133
H	0.902634	1.689873	-0.934645	H	-2.170824	1.967118	-1.079598
H	0.097130	-2.928122	0.700125	H	-1.474218	0.783111	-2.201478
C	3.357221	2.021033	-0.692986	H	-2.714658	1.921596	-2.771507
C	3.248556	3.162636	-1.122719	C	-4.823764	1.065094	-1.312218
				H	-5.104062	1.642813	-2.203716
				H	-5.666224	0.402925	-1.074705

H	-4.722702	1.779439	-0.484334	O	0.611516	3.301317	0.118555
Zn	0.607433	1.672134	0.952449	C	1.638514	3.535689	-0.587671
O	-0.997207	3.019375	0.671896	O	2.070444	2.668047	-1.405067
C	-0.218198	3.776568	0.021276	C	2.384618	4.823276	-0.412288
O	1.011277	3.493093	-0.097119	H	3.069271	4.707457	0.436526
C	-0.778005	4.987164	-0.664682	H	2.974766	5.055806	-1.300571
H	0.005811	5.714733	-0.883992	H	1.696836	5.638343	-0.176197
H	-1.229600	4.662223	-1.610815	O	-0.922209	1.698246	-2.210494
H	-1.569369	5.437163	-0.060935	C	-2.170245	1.775355	-2.274864
O	0.507686	1.071217	2.946458	O	-3.010166	1.104340	-1.586962
C	1.766488	0.934501	2.958838	C	-2.763939	2.769892	-3.231944
O	2.454748	1.180354	1.921137	H	-2.736495	3.758771	-2.760151
C	2.447194	0.434695	4.198336	H	-2.155698	2.822836	-4.137901
H	3.466212	0.822536	4.263791	H	-3.800276	2.523668	-3.469124
H	1.872585	0.697851	5.088671	H	-2.673204	0.183168	-0.929199
H	2.500508	-0.659634	4.142009	P	-1.520375	1.422391	2.229235
H	3.379949	-0.916219	1.478971	C	-0.258645	2.297663	3.237961
P	2.052043	0.856691	-2.019698	H	0.372037	1.570211	3.760827
C	1.530192	2.151553	-3.208462	H	0.369034	2.892827	2.565369
H	0.747335	1.757173	-3.865075	H	-0.733824	2.960698	3.972442
H	1.124739	2.991947	-2.634707	C	-2.445421	2.833825	1.507379
H	2.374622	2.500017	-3.816288	H	-2.860314	3.487254	2.285544
C	3.457755	1.652455	-1.160601	H	-1.750351	3.408929	0.883688
H	4.244233	1.917305	-1.878405	H	-3.252202	2.451968	0.871034
H	3.098594	2.551968	-0.651535	C	-2.669718	0.817365	3.529672
H	3.854031	0.972227	-0.400294	H	-3.005561	1.637631	4.176807
C	2.898165	-0.368689	-3.093303	H	-3.537544	0.344863	3.057925
H	3.677875	0.106813	-3.702473	H	-2.165186	0.061015	4.139788
H	3.350646	-1.139792	-2.457694	S	-0.944501	-2.464129	-1.760685
H	2.166687	-0.850525	-3.750180				
S	0.844231	-2.263252	1.827511	3s			
TS_{23s}				C	5.089615	-2.218888	-0.116765
C	-4.932054	-2.263262	0.437161	C	4.677568	-3.426515	0.435804
C	-4.551644	-3.425835	-0.227713	C	3.337839	-3.618822	0.754847
C	-3.333320	-3.476175	-0.897518	C	2.428010	-2.589527	0.515822
C	-2.518580	-2.346446	-0.894251	C	2.796864	-1.353508	-0.064591
C	-2.859853	-1.136764	-0.251653	C	4.156883	-1.212518	-0.364718
C	-4.095391	-1.151350	0.418375	H	6.140130	-2.057444	-0.352063
H	-5.886672	-2.223613	0.958206	H	5.396794	-4.220737	0.623480
H	-5.200072	-4.299176	-0.222350	H	3.009757	-4.563079	1.187202
H	-3.021114	-4.390078	-1.400370	H	4.508136	-0.271334	-0.791475
H	-4.428958	-0.232505	0.907153	C	0.092443	-1.385057	0.377230
C	-0.083103	-1.332811	-0.849492	C	-1.003698	-0.697594	0.140572
C	1.003884	-0.702685	-0.493752	Si	-2.707452	-1.361107	-0.301399
Si	2.635225	-1.404828	0.131549	C	-2.440650	-3.094729	-1.037227
C	2.240062	-3.165397	0.744074	H	-1.924902	-3.677118	-0.255323
H	1.862011	-3.700430	-0.143897	C	-3.704245	-1.481231	1.314733
C	3.823866	-1.471922	-1.348754	H	-4.727527	-1.785865	1.037614
H	4.771705	-1.888224	-0.966354	C	-3.565939	-0.265469	-1.609100
C	3.326774	-0.358068	1.565466	H	-3.313487	-0.746621	-2.569351
H	2.836453	-0.765163	2.467600	Pd	1.213346	-0.062576	-0.619850
Pd	-0.995887	-0.174347	0.574128	C	-5.088259	-0.296821	-1.460080
C	4.837694	-0.553418	1.715042	H	-5.404831	0.194572	-0.529917
H	5.375807	-0.119632	0.861033	H	-5.575261	0.237333	-2.287822
H	5.209453	-0.049446	2.617758	H	-5.492808	-1.317154	-1.444895
H	5.131135	-1.607945	1.783118	C	-3.071924	1.176205	-1.677425
C	2.998765	1.129736	1.492145	H	-3.561230	1.722174	-2.496647
H	3.399099	1.664872	2.365932	H	-3.294432	1.723736	-0.750474
H	3.434849	1.594432	0.596515	H	-1.987956	1.228980	-1.855988
H	1.915917	1.307824	1.472728	C	-3.779644	-0.140339	2.041510
C	4.102206	-0.083648	-1.922231	H	-4.176785	0.669495	1.415865
H	4.517158	0.610116	-1.180018	H	-4.414585	-0.208857	2.935897
H	4.814407	-0.137475	-2.757285	H	-2.783438	0.176662	2.384981
H	3.185181	0.379953	-2.310431	C	-3.116209	-2.547886	2.237078
C	3.293523	-2.398206	-2.441478	H	-3.126318	-3.549049	1.787619
H	3.151754	-3.429176	-2.093503	H	-2.072548	-2.311707	2.493197
H	2.325914	-2.039928	-2.822617	H	-3.672863	-2.604262	3.183008
H	3.980370	-2.431528	-3.298442	C	-1.536867	-3.074573	-2.268535
C	1.147682	-3.199377	1.812173	H	-1.997785	-2.515393	-3.095592
H	1.436546	-2.615116	2.698294	H	-0.561560	-2.615687	-2.061829
H	0.191769	-2.795931	1.453391	H	-1.354379	-4.093550	-2.637386
H	0.966968	-4.228779	2.152340	C	-3.768259	-3.782364	-1.354582
C	3.485350	-3.898376	1.245278	H	-3.606786	-4.800646	-1.735157
H	3.256060	-4.947125	1.479647	H	-4.425439	-3.860841	-0.478296
H	4.307443	-3.898142	0.517299	H	-4.320389	-3.237043	-2.133954
H	3.862359	-3.443747	2.172557	Zn	-0.712524	1.361348	0.523649
Zn	0.534188	1.388943	-0.825307	O	-0.503725	3.379192	-0.117999
				C	-1.543023	3.649060	0.558639

O	-2.164054	2.731061	1.171523	H	0.737517	2.119598	4.746848
C	-2.038040	5.060497	0.652805	H	0.470520	0.431089	5.285662
H	-1.508512	5.713912	-0.042346	H	2.051748	0.901944	4.673813
H	-3.113957	5.087101	0.459447	O	-0.824060	3.343267	-0.026801
H	-1.886722	5.419668	1.675977	C	-2.017213	3.353961	0.403046
O	0.451886	1.564058	2.306424	O	-2.554453	2.286319	0.823309
C	1.488829	1.238839	2.881316	C	-2.817121	4.620233	0.375746
O	2.446467	0.511199	2.365048	H	-3.485936	4.588297	-0.492080
C	1.775154	1.649695	4.289276	H	-3.442928	4.691221	1.268528
H	2.762682	2.116040	4.347189	H	-2.169048	5.493800	0.286370
H	1.004889	2.332786	4.647095	H	0.581016	-0.776460	1.970657
H	1.804908	0.756894	4.922028	P	2.263067	2.230322	-1.233428
H	2.246855	0.193177	1.439131	C	2.504395	3.522747	0.044773
P	2.024710	1.768631	-1.899166	H	1.535796	3.745185	0.504394
C	0.904993	2.703367	-3.015397	H	3.185633	3.144305	0.814546
H	0.448815	2.017723	-3.737217	H	2.920879	4.439130	-0.392091
H	0.116100	3.161639	-2.410586	C	3.906469	2.215880	-2.059314
H	1.452067	3.486185	-3.556526	H	4.121303	3.197273	-2.500333
C	2.724578	3.117144	-0.868491	H	4.689861	1.978311	-1.333059
H	3.191503	3.893364	-1.488264	H	3.925074	1.450812	-2.841971
H	1.907884	3.561949	-0.286149	C	1.255937	3.116085	-2.489321
H	3.472247	2.701912	-0.182788	H	1.770066	4.021986	-2.835157
C	3.408040	1.381592	-3.045153	H	1.073784	2.456349	-3.344243
H	3.760198	2.288130	-3.553511	H	0.297477	3.393521	-2.038293
H	4.239192	0.928519	-2.496203	S	1.048319	-3.059783	0.128548
H	3.065634	0.658515	-3.792524				
S	0.730204	-2.843591	1.017993	4s			
TS ₃₄₈				C	5.429449	-1.896372	-0.183253
C	5.406502	-1.785760	0.023660	C	5.070372	-3.224189	0.011524
C	5.075579	-3.125333	0.188893	C	3.725150	-3.563456	0.105817
C	3.738720	-3.507907	0.195997	C	2.760675	-2.561764	0.006409
C	2.750109	-2.537901	0.032142	C	3.080449	-1.200838	-0.198995
C	3.044328	-1.169861	-0.166935	C	4.445520	-0.912670	-0.289972
C	4.401117	-0.835329	-0.154996	H	6.480157	-1.619662	-0.252495
H	6.450119	-1.476190	0.034441	H	5.831381	-3.997300	0.092291
H	5.853061	-3.874652	0.320936	H	3.432699	-4.601646	0.257415
H	3.470989	-4.554255	0.336929	H	4.763248	0.116863	-0.444333
H	4.690123	0.208358	-0.276453	C	0.367968	-1.461032	-0.033211
C	0.333800	-1.489343	-0.071549	C	-0.791381	-0.826420	-0.018753
C	-0.816433	-0.849616	-0.103870	Si	-2.555249	-1.325467	-0.515135
Si	-2.605442	-1.313270	-0.516452	C	-2.819000	-0.645498	-2.277145
C	-2.990278	-0.506370	-2.201134	H	-2.094261	-1.201480	-2.895777
H	-2.323362	-1.023662	-2.911120	C	-2.734587	-3.220387	-0.556462
C	-2.771315	-3.202055	-0.693015	H	-3.812268	-3.379181	-0.733607
H	-3.844816	-3.368338	-0.891226	C	-3.837225	-0.604916	0.702998
C	-3.782496	-0.679460	0.844651	H	-4.056397	0.413458	0.348402
H	-4.018295	0.362903	0.579684	Pd	1.493198	0.145289	-0.400544
Pd	1.437621	0.123097	-0.497835	C	-5.147568	-1.396772	0.689389
C	-5.095112	-1.465737	0.882882	H	-5.012284	-2.413501	1.082886
H	-4.938004	-2.500875	1.215560	H	-5.898964	-0.907000	1.323983
H	-5.799268	-1.007845	1.591185	H	-5.581229	-1.490758	-0.314147
H	-5.595746	-1.510338	-0.092002	C	-3.318358	-0.479445	2.134658
C	-3.142071	-0.660480	2.233018	H	-4.114867	-0.131735	2.807214
H	-3.875333	-0.364519	2.996288	H	-2.951368	-1.437020	2.531979
H	-2.746234	-1.645159	2.520868	C	-2.505262	0.252045	2.212209
H	-2.316511	0.058947	2.295001	H	-2.398300	-3.871838	0.784671
C	-2.427015	-3.947374	0.595838	H	-3.062297	-3.526121	1.587383
H	-3.086819	-3.663702	1.425438	H	-2.493996	-4.965106	0.727681
H	-2.518910	-5.033844	0.458535	H	-1.368891	-3.659323	1.104984
H	-1.396418	-3.754418	0.924224	C	-1.977854	-3.871601	-1.711582
C	-1.987166	-3.751501	-1.883049	H	-2.329081	-3.512101	-2.686695
H	-2.332408	-3.331151	-2.835692	H	-0.899251	-3.676447	-1.657950
H	-0.913912	-3.535961	-1.796854	H	-2.107653	-4.962891	-1.698016
H	-2.091265	-4.843572	-1.949634	C	-2.510055	0.842245	-2.426486
C	-2.668985	0.984907	-2.269975	H	-3.150279	1.455501	-1.775197
H	-3.243762	1.557802	-1.527728	H	-1.460106	1.070600	-2.192270
H	-1.599733	1.181293	-2.102998	H	-2.684726	1.177494	-3.458637
H	-2.915864	1.393807	-3.260067	C	-4.227763	-0.937888	-2.792375
C	-4.437116	-0.745004	-2.632923	H	-4.337598	-0.626457	-3.840567
H	-4.614509	-0.359171	-3.646498	H	-4.490978	-2.002382	-2.739548
H	-4.714563	-1.807200	-2.635169	H	-4.978171	-0.380257	-2.213998
H	-5.136101	-0.220574	-1.965618	Zn	-0.775378	1.300488	0.377027
Zn	-0.762158	1.261871	0.406874	O	0.183420	-0.652059	2.971836
O	0.804011	-0.573436	2.907084	C	0.315943	0.637420	3.179738
C	0.562112	0.688725	3.179528	O	-0.037904	1.509154	2.385069
O	0.044885	1.481893	2.395153	C	0.964224	0.958468	4.482315
C	0.977082	1.073241	4.558829	H	2.044812	0.815682	4.369913
				H	0.768026	1.995635	4.755310

H	0.622387	0.273444	5.261573	C	-0.406596	-2.652969	2.435156
O	-0.868160	3.333452	-0.219423	O	-1.487399	-2.577175	1.772120
C	-2.073115	3.362504	0.181651	C	-0.412600	-3.328257	3.770989
O	-2.601749	2.329078	0.683348	H	0.598668	-3.596054	4.081656
C	-2.882378	4.611395	0.011199	H	-0.832806	-2.631905	4.505561
H	-3.693637	4.649414	0.740607	H	-1.058539	-4.209051	3.747369
H	-2.247487	5.496602	0.087824	H	-0.932461	-0.288271	-1.646414
H	-3.324362	4.600239	-0.991913	P	3.366857	-1.409667	-0.157009
H	-0.155554	-0.828270	2.060145	C	2.968825	-3.200431	-0.224793
P	2.338768	2.299700	-1.004792	H	2.187038	-3.414038	0.511844
C	2.280321	3.651766	0.237693	H	2.582924	-3.469414	-1.212588
H	1.234252	3.861970	0.485924	H	3.863109	-3.794326	0.002906
H	2.809520	3.341324	1.144678	C	4.873303	-1.342005	-1.208734
H	2.748266	4.561193	-0.160517	H	5.629958	-2.052816	-0.854036
C	4.094397	2.402380	-1.542924	H	4.604877	-1.592850	-2.240406
H	4.310988	3.400467	-1.944065	H	5.300954	-0.334476	-1.209362
H	4.754672	2.216838	-0.689179	C	4.034262	-1.264466	1.544288
H	4.298646	1.647983	-2.309485	H	4.851049	-1.976949	1.715189
C	1.484866	3.067578	-2.437273	H	4.388301	-0.244339	1.725698
H	1.971290	4.006375	-2.731195	H	3.211065	-1.472929	2.237245
H	1.493410	2.373272	-3.283779	S	-0.114168	2.955302	0.137325
H	0.448697	3.272373	-2.149471				
S	1.053084	-3.039128	0.165877	5 _s			
TS _{45s}				C	4.010819	3.555542	-0.359429
C	4.384399	3.451358	0.504255	C	3.060507	4.498889	0.009108
C	3.550411	4.538466	0.734738	C	1.724812	4.127884	0.094408
C	2.171432	4.392463	0.623330	C	1.348985	2.810773	-0.171892
C	1.637704	3.151808	0.277560	C	2.294976	1.823364	-0.502333
C	2.463054	2.037832	0.038431	C	3.624708	2.238864	-0.609278
C	3.838654	2.212061	0.165124	H	5.057275	3.836804	-0.456532
H	5.463767	3.562581	0.584480	H	3.352098	5.525774	0.216445
H	3.970130	5.505207	1.002795	H	0.966492	4.863994	0.356476
H	1.514403	5.240195	0.810106	H	4.394085	1.531657	-0.911057
H	4.508085	1.371175	-0.014610	C	-0.252474	0.747994	-0.711719
C	-0.108859	1.276362	-0.311041	C	-1.384212	-0.036698	-0.752663
C	-1.134307	0.401026	-0.494546	Si	-3.242026	0.297169	-0.513622
Si	-2.968767	0.694281	-0.052070	C	-3.623407	1.759271	0.646845
C	-3.011254	1.484988	1.684289	H	-3.152814	2.643958	0.188601
H	-2.578368	2.492016	1.564790	C	-3.911542	0.703867	-2.251291
C	-3.805125	1.838860	-1.325398	H	-5.009265	0.760818	-2.515679
H	-4.871500	1.836534	-1.040828	C	-4.017114	-1.308222	0.176938
C	-3.904150	-0.976796	-0.007239	H	-3.974223	-1.193519	1.274118
H	-3.734937	-1.382788	1.004760	Pd	1.668888	-0.053510	-0.893926
Pd	1.606606	0.251510	-0.431727	C	-5.484483	-1.455566	-0.235357
C	-5.411873	-0.771348	-0.187619	H	-5.575715	-1.634050	-1.316012
H	-5.648888	-0.450240	-1.211483	H	-5.946405	-2.315077	0.269779
H	-5.952468	-1.712257	-0.015447	C	-6.091183	-0.572669	-0.000020
H	-5.831922	-0.022726	0.494203	H	-3.259217	-2.590199	-0.172594
C	-3.428992	-2.036326	-1.002973	H	-3.806434	-3.470012	0.194321
H	-4.088863	-2.914497	-0.967716	H	-3.145362	-2.717317	-1.260138
H	-3.425114	-1.669140	-2.037942	C	-2.258782	-2.634102	0.275386
H	-2.420939	-2.415072	-0.793246	H	-3.574169	-0.378975	3.274142
C	-3.688791	1.286809	-2.745309	H	-3.960741	-1.365427	-2.986502
H	-4.121863	0.283321	-2.843539	H	-3.995451	-0.136800	-4.259825
H	-4.203663	1.937914	-3.465857	C	-2.487151	-0.473262	-3.404979
H	-2.637869	1.222718	-3.059715	H	-3.395691	2.061137	-2.727970
C	-3.308096	3.280556	-1.279457	H	-3.705144	2.882837	-2.069644
H	-3.381032	3.723901	-0.277648	H	-2.296832	2.073454	-2.773231
H	-2.257524	3.346887	-1.594345	H	-3.762937	2.291753	-3.737900
H	-3.887580	3.916134	-1.963780	C	-3.061490	1.599691	2.057467
C	-2.148972	0.725063	2.692375	H	-3.433169	0.687727	2.543742
H	-2.497796	-0.310102	2.822238	H	-1.965851	1.544976	2.059650
H	-1.092944	0.687155	2.390007	H	-3.350222	2.453368	2.687408
H	-2.185713	1.205181	3.680346	C	-5.129735	2.022222	0.715064
C	-4.431857	1.650402	2.222842	H	-5.338605	2.936507	1.287368
H	-4.428699	2.189827	3.180383	H	-5.589540	2.142483	-0.274656
H	-5.083781	2.207297	1.536458	H	-5.651321	1.202628	1.228977
H	-4.900192	0.674053	2.409485	Zn	-0.195552	-0.885994	1.012370
Zn	-0.502134	-1.454307	0.334996	O	0.985651	-2.074660	-1.542898
O	-0.671340	-0.946521	-2.716345	C	0.549463	-2.950602	-0.759212
C	-0.032161	-2.011408	-2.465574	O	0.245449	-2.752551	0.463250
O	0.117519	-2.511440	-1.310432	C	0.359048	-4.351767	-1.271183
C	0.644625	-2.701653	-3.612517	H	0.879687	-5.052948	-0.610659
H	1.696721	-2.386939	-3.618936	H	-0.705322	-4.607600	-1.226427
H	0.619518	-3.785734	-3.476267	H	0.720577	-4.452938	-2.295741
H	0.195791	-2.414483	-4.565135	O	0.668496	-0.141033	2.746106
O	0.655920	-2.129247	1.983309	C	-0.401299	-0.448675	3.360178
				O	-1.354787	-1.010878	2.741829

C	-0.565479	-0.112482	4.809193	H	0.908517	-2.662861	4.908228
H	0.365284	0.258826	5.240176	H	0.717952	-4.275491	4.231531
H	-1.341599	0.656753	4.894381	H	-1.439419	-0.472074	-1.261633
H	-0.920327	-0.989897	5.356701	P	3.570455	-0.501215	-1.077240
H	-1.211816	-0.996570	-1.259173	C	3.555168	-2.076779	-2.015434
P	3.743100	-1.099749	-0.239904	H	3.036492	-2.842425	-1.426439
C	3.604828	-2.910180	0.026323	H	3.020025	-1.937867	-2.960165
H	2.757753	-3.121990	0.688476	H	4.580069	-2.413347	-2.214026
H	3.439541	-3.414421	-0.931331	C	4.694742	0.519652	-2.111211
H	4.525272	-3.294023	0.482746	H	5.672590	0.035058	-2.223223
C	5.320510	-1.033713	-1.182321	H	4.242530	0.650153	-3.100331
H	6.113614	-1.547380	-0.624834	H	4.834321	1.512977	-1.673625
H	5.180320	-1.534018	-2.145722	C	4.580863	-0.964402	0.376292
H	5.637390	-0.004868	-1.374797	H	5.518160	-1.443116	0.067033
C	4.205611	-0.520338	1.434192	H	4.800834	-0.084481	0.987430
H	5.061116	-1.083595	1.826635	H	3.987621	-1.655993	0.986721
H	4.443420	0.547179	1.407913	C	0.713113	2.252886	-2.768609
H	3.339117	-0.648446	2.094682	C	0.727923	3.038280	-1.844518
S	-0.364967	2.407317	-0.144538	C	0.723052	4.005281	-0.757753
				H	0.105170	3.657998	0.080447
6s				H	0.325233	4.970257	-1.092505
C	3.530089	3.019403	2.003115	H	1.732209	4.170843	-0.360917
C	2.613131	3.341269	2.996858	C	0.650128	1.351156	-3.909069
C	1.352613	2.759543	2.980590	H	-0.262000	0.742405	-3.874596
C	1.013544	1.839197	1.984314	H	1.486666	0.641714	-3.910735
C	1.941126	1.463217	0.992620	H	0.660985	1.906544	-4.854131
C	3.187898	2.093353	1.018354	S	-0.649024	1.250755	1.928011
H	4.512560	3.486566	1.987503				
H	2.869121	4.057738	3.773967	TS _{67s}			
H	0.612579	3.036321	3.729963	C	2.569540	3.945763	1.386408
H	3.918691	1.886979	0.238682	C	1.798757	3.756364	2.536458
C	-0.548827	0.420066	0.354482	C	0.814551	2.783426	2.558049
C	-1.659336	-0.001514	-0.298034	C	0.557941	1.968661	1.438889
Si	-3.510089	0.275276	-0.045690	C	1.368811	2.122375	0.297281
C	-3.987623	0.331918	1.789963	C	2.351845	3.128591	0.288692
H	-3.464444	1.198149	2.228178	H	3.331811	4.720783	1.351472
C	-3.911098	1.919460	-0.918985	H	1.961781	4.375485	3.415467
H	-5.009260	1.964927	-1.012456	H	0.205664	2.645340	3.450672
C	-4.420279	-1.182692	-0.892804	H	2.935150	3.277435	-0.621139
H	4.646165	-1.889499	-0.076360	C	-0.868280	-0.287428	0.362601
Pd	1.363824	0.242340	-0.500466	C	-2.039213	-0.674603	-0.190224
C	-5.750784	-0.753153	-1.514143	Si	-3.843726	-0.142525	0.037531
H	-5.593425	-0.074100	-2.363760	C	-4.315878	-0.396251	1.866595
H	-6.303844	-1.622176	-1.897546	C	-3.777855	0.393504	2.418732
H	-6.406000	-0.236752	-0.800358	C	-4.244247	1.656064	-0.480123
C	-3.576898	-1.939843	-1.919805	H	-5.339948	1.654487	-0.610616
H	-4.159151	-2.750455	-2.381037	C	-4.884852	-1.328554	-1.059545
H	-3.241486	-1.283311	-2.738266	H	-5.048884	-2.221230	-0.430406
H	-2.682256	-2.391289	-1.470442	Pd	1.688936	0.552776	-1.015480
C	-3.303118	1.973736	-2.322276	C	-6.256191	-0.755290	-1.420877
H	-3.553270	1.091150	-2.928234	H	-6.158125	0.093636	-2.112391
H	-3.654930	2.858677	-2.870824	H	-6.874645	-1.508294	-1.929456
H	-2.205459	2.044250	-2.270891	H	-6.819910	-0.401445	-0.549310
C	-3.441362	3.118598	-0.099199	C	-4.188590	-1.794959	-2.340241
H	-3.933675	3.177557	0.879813	H	-4.861893	-2.421806	-2.942527
H	-2.358054	3.065344	0.082265	H	-3.891700	-0.947000	-2.975623
H	-3.638560	4.061929	-0.628091	H	-3.288279	-2.387965	-2.144616
C	-3.539030	-0.924662	2.535458	C	-3.611518	2.001416	-1.825667
H	-4.006604	-1.827093	2.116238	H	-3.919814	1.310732	-2.622505
H	-2.452395	-1.077784	2.508763	H	-3.881064	3.018490	-2.148568
H	-3.833552	-0.879310	3.593214	H	-2.515650	1.952636	-1.752902
C	-5.492966	0.545895	1.951942	C	-3.915020	2.730873	0.551987
H	-5.771976	0.619019	3.012191	H	-4.366565	2.526998	1.531232
H	-5.845812	1.459087	1.454007	H	-2.832215	2.810526	0.711123
H	-6.058194	-0.299336	1.533078	H	-4.278021	3.714361	0.218719
Zn	0.175569	-1.726463	0.713280	C	-3.837437	-1.748283	2.392810
O	0.681779	-1.099074	-2.157317	H	-4.305356	-2.578221	1.842878
C	0.242293	-2.270409	-2.033976	H	-2.750780	-1.869860	2.303213
O	0.005026	-2.856629	-0.932097	H	-4.104952	-1.878235	3.451012
C	-0.032556	-3.058333	-3.286410	C	-5.812049	-0.221406	2.121224
H	0.573876	-3.970332	-3.278548	H	-6.043456	-0.284145	3.193955
H	-1.081688	-3.372746	-3.296547	H	-6.195101	0.741549	1.757654
H	0.189745	-2.469100	-4.178778	H	-6.389091	-1.015151	1.625767
O	1.775599	-2.450133	1.930833	Zn	0.651026	-1.656530	0.401731
C	0.885705	-2.724982	2.785028	O	2.056708	-0.999588	-2.503381
O	-0.342569	-2.493656	2.536513	C	1.772025	-2.209464	-2.285322
C	1.248780	-3.326872	4.107798	O	1.272569	-2.680696	-1.225527
H	2.325058	-3.485865	4.187360	C	2.084300	-3.201517	-3.376455

H	2.880021	-3.868979	-3.027227	H	-6.400930	-2.288639	-1.900598
H	1.207969	-3.827752	-3.566002	H	-6.233933	-1.969809	-0.166060
H	2.402848	-2.703097	-4.293459	H	-6.840202	-0.707146	-1.252230
O	1.965663	-1.891839	2.049628	Zn	0.470578	1.287125	-0.451555
C	1.234367	-2.858244	2.451120	O	2.043392	0.404138	2.514808
O	0.238723	-3.236089	1.782272	C	1.334335	1.458514	2.484885
C	1.588844	-3.536592	3.742450	O	0.721918	1.912788	1.491154
H	1.571064	-2.803265	4.554710	C	1.203395	2.202229	3.787948
H	0.894610	-4.349302	3.961049	H	1.171429	3.279040	3.606652
H	2.610581	-3.924315	3.682622	H	0.248277	1.916598	4.245264
H	-1.940165	-1.565650	-0.827080	H	2.008889	1.944293	4.478094
P	3.782064	-0.013852	0.008526	O	2.080079	1.884648	-1.663943
C	4.367358	-1.745152	-0.078485	C	1.533129	3.032147	-1.814998
H	3.720549	-2.366585	0.548145	O	0.439543	3.303016	-1.266697
H	4.321468	-2.090990	-1.116470	C	2.250172	4.043318	-2.663638
H	5.402649	-1.809373	0.277920	H	3.278131	4.158935	-2.302177
C	5.088685	0.866920	-0.932087	H	2.312938	3.674361	-3.692583
H	6.084776	0.625959	-0.540002	H	1.736391	5.005738	-2.649543
H	5.029947	0.570630	-1.985241	H	-2.140163	1.705687	0.217793
H	4.930382	1.948246	-0.863796	P	4.087123	0.334807	0.083388
C	4.110164	0.464480	1.738571	C	4.277431	2.047744	0.708737
H	5.152174	0.243797	2.000881	H	3.580184	2.697825	0.171975
H	3.918907	1.534704	1.868643	H	4.042833	2.070198	1.777828
H	3.435450	-0.108626	2.381143	H	5.304500	2.401742	0.557526
C	0.074075	1.357581	-2.108950	C	5.402468	-0.538645	1.030672
C	0.131336	2.401686	-1.405930	H	6.378427	-0.048432	0.923375
C	-0.278590	3.787461	-1.129004	H	5.123706	-0.559685	2.090478
H	-0.667187	3.895223	-0.108902	H	5.480899	-1.573591	0.676870
H	-1.073377	4.054707	-1.837376	C	4.846251	0.454643	-1.580897
H	0.553031	4.489420	-1.250920	H	5.840077	0.913414	-1.506653
C	-0.510049	0.532088	-3.173922	H	4.944064	-0.539696	-2.027679
H	-1.000996	-0.339537	-2.718657	H	4.189939	1.068200	-2.205053
H	0.265562	0.163920	-3.851979	C	0.497671	-1.928131	1.609107
H	-1.260647	1.096920	-3.740541	C	0.155122	-2.766385	0.636734
S	-0.909049	0.992021	1.602862	C	-0.835158	-3.884944	0.613364
				H	-1.616527	-3.697372	-0.135306
7_s				H	-1.318144	-4.013923	1.587364
C	3.133585	-2.638787	-1.744169	H	-0.340249	-4.828322	0.345531
C	2.569889	-2.073035	-2.868680	C	-0.038326	-1.665747	2.962054
C	1.230228	-1.654471	-2.853368	H	-0.592022	-0.715060	2.969185
C	0.437532	-1.823673	-1.729866	H	0.754204	-1.589026	3.713654
C	0.986274	-2.452541	-0.572657	H	-0.741487	-2.456905	3.260004
C	2.352303	-2.822415	-0.587510	S	-1.268359	-1.313259	-1.768639
H	4.173751	-2.959866	-1.745607				
H	3.165702	-1.928355	-3.767110	TS_{78s}			
H	0.796148	-1.175456	-3.728215	C	3.213561	-3.471468	-1.422405
H	2.746301	-3.392406	0.253320	C	2.731992	-2.962214	-2.629115
C	-1.207807	0.194771	-0.789010	C	1.528254	-2.271853	-2.664263
C	-2.334575	0.755141	-0.302592	C	0.756045	-2.107709	-1.508094
Si	-4.129238	0.232226	-0.098614	C	1.202545	-2.669975	-0.280132
C	-4.691428	-1.023151	-1.414639	C	2.461382	-3.316606	-0.267910
H	-4.001487	-1.880123	-1.332392	H	4.165808	-3.996049	-1.387520
C	-4.211452	-0.567109	1.635851	H	3.310713	-3.080949	-3.542763
H	-5.270923	-0.753865	1.877310	H	1.172322	-1.831675	-3.593884
C	-5.256932	1.778321	-0.173382	H	2.801455	-3.741608	0.675999
H	-5.593526	1.833901	-1.223052	C	-0.751553	-0.118164	-0.290953
Pd	2.016204	-0.843036	0.805928	C	-1.904215	0.284327	0.284915
C	-6.501435	1.642022	0.705778	Si	-3.728919	-0.076588	-0.081539
H	-6.234774	1.622792	1.771855	C	-4.045974	0.021119	-1.953891
H	-7.178913	2.496066	0.563257	H	-3.515539	-0.825973	-2.419356
H	-7.075583	0.729871	0.499290	C	-4.210479	-1.791831	0.609041
C	-4.534632	3.087381	0.143838	H	-5.293279	-1.760943	0.810554
H	-5.225370	3.940657	0.082317	C	-4.765885	1.309096	0.752383
H	-4.121061	3.084821	1.162900	H	-5.078828	1.954382	-0.086114
H	-3.704514	3.282118	-0.544516	Pd	1.778307	-0.606278	0.719554
C	-3.626823	0.354983	2.705080	C	-6.037736	0.785005	1.419263
H	-4.159556	1.312960	2.770066	H	-5.804047	0.138983	2.277486
H	-3.662981	-0.112580	3.700250	H	-6.647887	1.615156	1.802368
H	-2.572177	0.585223	2.489263	H	-6.668894	0.204348	0.734094
C	-3.471979	-1.901239	1.629790	C	-3.985485	2.189964	1.726642
H	-3.930876	-2.628856	0.946772	H	-4.639798	2.953039	2.171360
H	-2.427609	-1.764850	1.309358	H	-3.566789	1.604669	2.559445
H	-3.451385	-2.356088	2.632871	H	-3.154688	2.714863	1.238184
C	-4.574869	-0.452848	-2.827664	C	-3.477085	-2.044537	1.925191
H	-5.273380	0.383296	-2.974376	H	-3.648025	-1.251374	2.667507
H	-3.567141	-0.079514	-3.048929	H	-3.781506	-2.998563	2.381194
H	-4.822042	-1.211074	-3.584164	H	-2.394137	-2.089758	1.745158
C	-6.112000	-1.526259	-1.163233	C	-3.949610	-2.937743	-0.366433

H	-4.551583	-2.856825	-1.280186	H	2.486265	-3.010852	1.675322
H	-2.896021	-2.964531	-0.674665	H	3.776281	-3.436713	0.539187
H	-4.183545	-3.907941	0.096853	C	2.003891	1.482906	-1.539948
C	-3.490364	1.316628	-2.543543	C	0.638006	1.041860	-1.752875
H	-3.949384	2.200087	-2.076303	Si	-3.267260	0.858469	-0.036664
H	-2.407102	1.408900	-2.396566	C	-4.403551	-0.675511	-0.089958
H	-3.694293	1.381324	-3.621814	C	-3.229170	1.568780	1.738149
C	-5.537912	-0.121223	-2.254993	C	-3.932140	2.226527	-1.195771
H	-5.732889	-0.098854	-3.336362	H	-4.227694	-1.188240	0.871484
H	-5.957134	-1.058299	-1.863591	C	-4.088735	-1.677481	-1.201622
H	-6.112523	0.704692	-1.811113	C	-5.884054	-0.290142	-0.166476
Zn	0.432856	1.598964	-0.062479	H	-2.581964	2.459043	1.692825
O	2.275070	0.610027	2.507377	C	-2.654893	0.613936	2.782960
C	1.709890	1.730375	2.620119	C	-4.612623	2.038704	2.194927
O	0.922113	2.263782	1.784971	H	-4.937823	2.481485	-0.820842
C	2.016379	2.541536	3.853803	C	-3.060234	3.478582	-1.132620
H	2.614436	3.411580	3.560115	C	-4.077620	1.765199	-2.644006
H	1.086724	2.924627	4.283706	H	-4.164696	-1.220955	-2.198949
H	2.567305	1.955337	4.591207	H	-3.091242	-2.125223	-1.123980
O	1.369354	2.789094	-1.527467	H	-4.803412	-2.511700	-1.177152
C	0.334269	3.536053	-1.542434	H	-6.519930	-1.182318	-0.082546
O	-0.643544	3.293833	-0.788463	H	-6.194952	0.407708	0.619887
C	0.278606	4.691502	-2.497787	H	-6.123660	0.180744	-1.130189
H	-0.285666	5.517682	-2.059344	H	-1.606517	0.354035	2.588658
H	1.282200	5.014781	-2.781559	H	-2.699044	1.065184	3.784994
H	-0.250226	4.371052	-3.402265	H	-3.224052	-0.324930	2.819785
H	-1.773073	1.032760	1.080748	H	-5.097865	2.717328	1.481580
P	3.618977	0.510599	-0.481959	H	-5.286467	1.186301	2.357584
C	4.132963	2.157198	0.138066	H	-4.541213	2.569661	3.154450
H	3.403666	2.905209	-0.187899	H	-2.034468	3.259837	-1.467121
H	4.167204	2.129747	1.232613	H	-3.448913	4.269403	-1.789895
H	5.123652	2.420807	-0.252235	H	-2.991328	3.896580	-0.120325
C	5.119487	-0.490998	-0.130900	H	-4.458886	2.575562	-3.281323
H	6.020035	-0.018729	-0.543618	H	-3.108047	1.460252	-3.063746
H	5.229415	-0.599633	0.953902	H	-4.761191	0.913906	-2.750872
H	4.997793	-1.487793	-0.567788	C	0.089192	0.739683	-3.131456
C	3.693534	0.724655	-2.297511	H	0.805189	0.988435	-3.916535
H	4.667775	1.126250	-2.602666	H	-0.185819	-0.314544	-3.263366
H	3.530922	-0.243519	-2.781494	C	-0.813367	1.338234	-3.320574
H	2.898334	1.416868	-2.593368	H	2.950612	1.439278	-2.719493
C	0.471820	-1.748708	1.749271	H	2.713224	0.620938	-3.402240
C	0.344261	-2.804265	0.958634	H	2.938652	2.380308	-3.291340
C	-0.438477	-4.065730	1.149249	H	3.978302	1.267359	-2.382839
H	-1.192930	-4.173159	0.355781	Zn	-0.892270	-1.512790	0.105560
H	-0.956216	-4.079251	2.114290	O	1.455797	-2.766424	-1.210769
H	0.216380	-4.946340	1.095122	C	0.402861	-3.331384	-1.567511
C	-0.089341	-1.322286	3.044639	O	-0.776170	-2.930477	-1.280937
H	-0.717528	-0.429316	2.906883	C	0.479346	-4.591766	-2.391065
H	0.705709	-1.059943	3.750988	H	1.514074	-4.850642	-2.621164
H	-0.713478	-2.111610	3.488859	H	0.001428	-5.410655	-1.844208
S	-0.781977	-1.254260	-1.678910	H	-0.088445	-4.456452	-3.317016
8s				O	-1.995620	-2.409508	1.690730
C	3.980359	3.974855	0.531822	C	-0.973986	-2.263154	2.418440
C	3.119880	4.212402	1.602122	O	0.082620	-1.724232	1.954117
C	1.892730	3.571861	1.634986	C	-1.016112	-2.680799	3.857746
C	1.531799	2.687275	0.615433	H	-1.437417	-1.853158	4.440997
C	2.381076	2.420519	-0.470202	H	-1.669142	-3.546719	3.986206
C	3.611381	3.106579	-0.482700	H	-0.013187	-2.889937	4.235442
H	4.942730	4.478503	0.481573	S	-0.014746	1.891450	0.826747
H	3.400075	4.895684	2.399566	9s			
H	1.199067	3.749179	2.455593	C	1.660556	4.852832	0.625988
H	4.300847	2.960242	-1.308391	C	0.367195	5.191293	1.013768
C	-0.322505	1.037453	-0.676561	C	-0.700431	4.430579	0.559914
C	-1.569668	0.347836	-0.720735	C	-0.486324	3.339953	-0.283812
H	-1.740862	-0.065601	-1.723613	C	0.812515	2.976863	-0.693660
Pd	1.892514	-0.521482	-0.826876	C	1.873140	3.766441	-0.209138
P	3.533141	-1.034615	0.806617	H	2.509697	5.435405	0.974671
C	5.326566	-0.699584	0.574948	H	0.189496	6.040373	1.669017
H	5.463893	0.368301	0.368990	H	-1.718800	4.675162	0.856554
H	5.901670	-0.964893	1.471507	H	2.892358	3.518609	-0.490017
H	5.708553	-1.268467	-0.278602	C	-1.245069	0.880337	-1.231873
C	3.195606	-0.131564	2.367443	C	-2.027347	-0.209661	-1.069973
H	3.890297	-0.429194	3.163748	H	-1.576927	-1.132676	-1.439785
H	3.282567	0.947757	2.192801	Pd	1.146173	0.515164	0.271319
H	2.165723	-0.356344	2.666454	P	1.876364	-0.071471	2.383786
C	3.512728	-2.777713	1.371614	C	1.746353	1.494574	3.339133
H	4.198221	-2.940788	2.213106	H	0.720198	1.875410	3.271879

H	2.017226	1.346200	4.392621	H	-4.326412	0.774021	0.037770
H	2.410750	2.242161	2.892326	C	0.253318	0.461493	-0.020887
C	0.935714	-1.249691	3.424177	C	1.253253	-0.429073	-0.064679
H	1.292072	-1.202769	4.461198	Si	3.126609	-0.199010	-0.024747
H	-0.131643	-1.008819	3.397083	C	3.605377	1.402444	-0.932000
H	1.092131	-2.259580	3.030354	H	3.167836	2.231906	-0.351924
C	3.600187	-0.594621	2.704749	C	3.647646	-0.106583	1.805071
H	3.818922	-0.539024	3.778660	H	4.750065	-0.082138	1.833345
H	3.732904	-1.625216	2.360103	C	3.953874	-1.686312	-0.900065
H	4.294571	0.039738	2.146508	H	4.062562	-1.367880	-1.951371
C	1.070459	1.824313	-1.595194	Pd	-1.498490	-0.500638	-0.023805
C	0.110582	0.842397	-1.841715	C	5.354087	-1.976874	-0.355784
Si	-3.636888	-0.482975	-0.134814	H	5.309902	-2.344372	0.678497
C	-3.732853	-2.362704	0.223429	H	5.852620	-2.755740	-0.949924
C	-3.571664	0.462323	1.522558	H	6.006378	-1.094920	-0.358742
C	-5.165957	0.042596	-1.143312	C	3.118130	-2.964751	-0.892776
H	-3.171300	-2.502905	1.165268	H	3.651667	-3.785718	-1.392817
C	-3.070790	-3.247090	-0.836053	H	2.902887	-3.301523	0.132114
C	-5.167433	-2.839247	0.465632	H	2.159140	-2.835094	-1.407917
H	-3.611252	1.533385	1.272594	C	3.172351	-1.337978	2.575494
C	-2.258479	0.201418	2.257621	H	3.557272	-2.276200	2.153214
C	-4.762299	0.139912	2.424005	H	3.487485	-1.297627	3.627780
H	-6.036004	-0.304265	-0.560236	H	2.074650	-1.398167	2.568746
C	-5.290788	1.553596	-1.318633	C	3.117634	1.165234	2.464669
C	-5.201369	-0.644766	-2.508484	H	3.507105	2.076640	1.992763
H	-3.494640	-3.076159	-1.835807	H	2.020222	1.213162	2.409253
H	-1.987691	-3.087844	-0.905946	H	3.391326	1.203036	3.528708
H	-3.231505	-4.310197	-0.602196	C	3.021899	1.451107	-2.342830
H	-5.179281	-3.891698	0.781784	H	3.410171	0.629513	-2.962148
H	-5.693919	-2.260939	1.234627	H	1.927459	1.377294	-2.338749
H	-5.765941	-2.779289	-0.454014	H	3.291838	2.388051	-2.850006
H	-1.382056	0.528492	1.676790	C	5.119862	1.606358	-0.970231
H	-2.233425	0.716562	3.230429	H	5.377220	2.567585	-1.436633
H	-2.129107	-0.874250	2.461211	H	5.575388	1.593757	0.028996
H	-5.726320	0.318435	1.929207	H	5.609123	0.823673	-1.567504
H	-4.743796	-0.910253	2.746960	H	0.918670	-1.484961	-0.055985
H	-4.744542	0.752743	3.336330	P	-3.416848	-1.977437	-0.090873
H	-4.481168	1.945812	-1.949957	C	-3.085581	-3.786127	-0.170219
H	-6.235109	1.813802	-1.817458	H	-2.485333	-4.015219	-1.056569
H	-5.259744	2.097838	-0.365951	H	-2.523496	-4.100623	0.714867
H	-6.079308	-0.327872	-3.088973	H	-4.023040	-4.354112	-0.217827
H	-4.311353	-0.387883	-3.100898	C	-4.587544	-1.904523	1.323217
H	-5.238075	-1.738529	-2.429288	H	-5.447769	-2.565507	1.158714
C	0.283547	-0.245076	-2.871397	H	-4.066835	-2.211905	2.235724
H	1.276806	-0.276559	-3.315755	H	-4.940510	-0.878935	1.470427
H	0.108140	-1.237355	-2.442713	C	-4.527755	-1.765002	-1.537995
H	-0.458850	-0.101201	-3.667796	H	-5.394362	-2.435139	-1.476983
C	2.386672	1.851890	-2.330507	H	-4.871627	-0.727660	-1.598834
H	2.568172	0.942650	-2.903484	H	-3.966208	-1.983076	-2.452118
H	2.424742	2.714867	-3.009495	S	0.349859	2.218180	0.022177
H	3.231212	1.944694	-1.638536				
Zn	2.290355	-1.652464	-0.422180	P _s			
O	1.933513	-3.184158	0.972650	C	5.277193	-1.297220	-0.577791
C	0.809095	-3.404989	0.421766	C	4.544133	-2.357493	-0.052846
O	0.475859	-2.797713	-0.635678	C	3.257439	-2.131537	0.411409
C	-0.154014	-4.352737	1.073878	C	2.705735	-0.851138	0.367110
H	-0.901799	-3.758079	1.616085	C	3.435426	0.244621	-0.128721
H	-0.687224	-4.939686	0.321724	C	4.728143	-0.024341	-0.610460
H	0.356868	-5.005312	1.784721	H	6.280367	-1.461174	-0.963532
C	3.198076	-1.455272	-2.297920	H	4.966766	-3.358691	-0.017756
C	4.308762	-1.240712	-1.715800	H	2.659068	-2.952376	0.802827
O	4.392874	-1.263446	-0.456360	H	5.321273	0.784518	-1.028084
C	5.514707	-0.938331	-2.555410	C	0.557138	0.821513	0.171844
H	5.666198	-1.741729	-3.282286	C	-0.741974	0.962462	-0.175365
H	5.330290	-0.022120	-3.127220	H	-0.996035	1.958573	-0.548437
H	6.406394	-0.816034	-1.938759	C	2.897505	1.612844	-0.118402
S	-1.916410	2.488783	-0.867392	C	1.570540	1.882612	0.029001
				Si	-2.236942	-0.177108	-0.091544
10 _s				C	-3.446068	0.357381	-1.481106
C	-4.141639	2.907698	0.078060	C	-1.804286	-2.012760	-0.351676
C	-3.274338	3.993199	0.090623	C	-3.038415	0.085436	1.619056
C	-1.900178	3.784915	0.072260	H	-3.207582	-0.307040	-2.329667
C	-1.390585	2.485885	0.041071	C	-3.269542	1.795193	-1.966458
C	-2.256326	1.371699	0.026958	C	-4.909584	0.115926	-1.104616
C	-3.628512	1.610467	0.045662	H	-1.194605	-2.319356	0.511441
H	-5.218385	3.062745	0.094132	C	-0.974103	-2.228835	-1.614671
H	-3.665334	5.007859	0.115499	C	-3.056747	-2.889157	-0.377604
H	-1.218517	4.633792	0.081547	H	-4.004124	-0.446349	1.615944

C	-2.172754	-0.498458	2.733350				
C	-3.303884	1.568247	1.878814	2 _{NH}			
H	-3.411574	2.519926	-1.151440	C	-4.163638	-3.733225	0.249110
H	-2.275530	1.970774	-2.394001	C	-2.917445	-3.827557	0.863691
H	-4.008889	2.039803	-2.742246	C	-1.789889	-3.270174	0.272837
H	-5.571118	0.312199	-1.960154	C	-1.909899	-2.612800	-0.951877
H	-5.103434	-0.909859	-0.768619	C	-3.152526	-2.521896	-1.577786
H	-5.228470	0.787949	-0.296091	C	-4.273601	-3.079443	-0.974341
H	-0.024731	-1.680417	-1.583290	H	-5.041339	-4.169821	0.718615
H	-0.739745	-3.293503	-1.755825	H	-2.817458	-4.345083	1.815468
H	-1.517753	-1.901363	-2.512678	H	-0.816488	-3.338501	0.754366
H	-3.669809	-2.778170	0.527007	H	-5.239965	-2.999959	-1.467114
H	-3.693777	-2.653188	-1.241667	C	0.230636	-1.547871	-0.868275
H	-2.790237	-3.952002	-0.462710	C	1.257729	-1.061429	-0.347809
H	-1.185810	-0.012919	2.764007	Si	3.102348	-0.872896	-0.1637342
H	-2.634881	-0.345241	3.718843	C	3.598619	0.497415	1.064905
H	-2.004943	-1.576391	2.610880	H	3.620122	0.001572	2.051605
H	-3.771816	1.725916	2.860816	C	3.695888	-2.558831	0.481421
H	-2.362148	2.136360	1.873993	H	3.399458	-3.279252	-0.299230
H	-3.962732	2.019488	1.124650	C	3.719956	-0.520580	-1.922436
C	1.010476	3.278593	-0.018885	H	4.799307	-0.308323	-1.838626
H	1.745488	4.042429	0.239214	Pd	-0.197552	-0.165284	1.008670
H	0.624461	3.526217	-1.017275	C	3.536927	-1.732403	-2.833654
H	0.173513	3.378063	0.681428	H	2.477587	-2.016788	-2.907639
C	3.913557	2.698816	-0.335570	H	3.879840	-1.509986	-3.853482
H	3.530766	3.696405	-0.121251	H	4.092011	-2.612074	-2.484312
H	4.795575	2.539932	0.295842	C	3.025197	0.706739	-2.515493
H	4.264499	2.711236	-1.376547	H	3.394723	0.914817	-3.529075
S	1.077224	-0.657405	1.009220	H	1.938734	0.556027	-2.589614
				H	3.172926	1.614830	-1.918638
C ₆ H ₅ N (H) C≡CSiPr ₃				C	2.985156	-2.947925	1.776373
C	1.026508	-1.838369	1.178943	H	1.894766	-2.978554	1.653831
C	0.642523	-0.702435	0.472414	H	3.310593	-3.937295	2.126967
C	1.558537	0.298707	0.175790	H	3.206302	-2.233976	2.583257
C	2.884142	0.160371	0.591723	C	5.211715	-2.626277	0.656980
C	3.277747	-0.975371	1.301943	H	5.756467	-2.341761	-0.253235
C	2.349701	-1.966531	1.591138	H	5.544012	-1.957106	1.463369
H	0.301907	-2.615896	1.405819	H	5.535068	-3.639837	0.931617
H	-0.388464	-0.589440	0.144430	C	2.645873	1.687096	1.162439
H	1.261210	1.189406	-0.375510	H	2.496706	2.170081	0.186637
H	2.666405	-2.847192	2.145412	H	1.648080	1.395268	1.528006
C	3.555351	2.278277	-0.351335	H	3.045440	2.445300	1.852365
C	3.232673	3.289315	-0.959279	C	5.015224	0.998621	0.763479
Si	2.634722	4.782390	-1.839828	H	5.360295	1.681358	1.551795
C	1.543677	4.235490	-3.305408	H	5.753211	0.190634	0.683871
H	0.527596	4.140951	-2.883969	H	5.041577	1.561014	-0.179847
C	1.602093	5.782029	-0.597471	Zn	-0.862535	1.555280	-0.742195
H	2.309767	6.074321	0.195878	O	0.600347	2.894130	-1.369700
C	4.156348	5.769329	-2.400596	C	0.252758	3.701987	-0.452529
H	3.780913	6.632606	-2.976078	O	-0.683243	3.413532	0.346586
C	4.938475	6.293921	-1.197303	C	0.989502	4.999832	-0.293482
H	5.280603	5.464626	-0.561843	H	0.293110	5.798496	-0.026458
H	5.831781	6.849379	-1.515577	H	1.703817	4.896503	0.531660
H	4.340059	6.964624	-0.568054	H	1.538797	5.253684	-1.201874
C	5.064565	4.940251	-3.307141	O	-1.429619	0.488555	-2.575247
H	5.949807	5.514082	-3.615470	C	-2.584559	0.993137	-2.423914
H	5.421191	4.040904	-2.786153	O	-2.839627	1.737541	-1.435993
H	4.553141	4.607281	-4.219123	C	-3.666114	0.719811	-3.428643
C	0.515636	4.916025	0.036071	H	-4.559813	0.354116	-2.913094
H	0.935262	4.024966	0.519751	H	-3.941719	1.658253	-3.919920
H	-0.051461	5.475189	0.793373	H	-3.339870	0.001082	-4.183916
H	-0.210013	4.574447	-0.716676	H	-3.231843	-2.007127	-2.534963
C	1.002791	7.045760	-1.209438	P	-1.796721	0.773740	2.388951
H	1.760603	7.695928	-1.667315	C	-1.326347	2.281601	3.314397
H	0.269775	6.792813	-1.988731	H	-0.402744	2.092708	3.872171
H	0.470722	7.642183	-0.455257	H	-1.141104	3.084918	2.592531
C	1.939249	2.875938	-3.877219	H	-2.118943	2.577545	4.013349
H	2.965399	2.891303	-4.269867	C	-3.431634	1.216114	1.692544
H	1.899923	2.084103	-3.120445	H	-4.122061	1.521442	2.489088
H	1.277993	2.589323	-4.707276	H	-3.323781	2.027142	0.965158
C	1.494644	5.290811	-4.411812	H	-3.836987	0.347048	1.161088
H	0.781882	5.004064	-5.197365	C	-2.274855	-0.394213	3.725606
H	1.197219	6.281633	-4.044650	H	-3.022653	0.052285	4.393596
H	2.474348	5.403565	-4.896270	H	-2.688444	-1.302222	3.272994
H	4.313285	-1.077613	1.625297	H	-1.390427	-0.671603	4.308143
N	3.837465	1.151041	0.305942	N	-0.795289	-2.014202	-1.581649
H	4.780262	1.001131	0.637768	H	-1.049818	-1.364796	-2.335874

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C	4.606987	2.979530	-0.000639
C	3.965185	3.986948	-0.718321
C	2.693246	3.773916	-1.238733
C	2.093000	2.535620	-1.037148
C	2.711977	1.466361	-0.356462
C	3.981814	1.747337	0.171088
H	5.601511	3.153384	0.405249
H	4.452191	4.948314	-0.866022
H	2.170980	4.568899	-1.770129
H	4.515045	0.948181	0.691258
C	0.067600	1.354601	-0.883123
C	-0.999259	0.640472	-0.613403
Si	-2.603325	1.300785	0.094537
C	-2.219865	3.063893	0.717643
H	-1.771925	3.572616	-0.154837
C	-3.846625	1.398167	-1.341386
H	-4.775713	1.825051	-0.926157
C	-3.243127	0.218114	1.525553
H	-2.688497	0.575424	2.411622
Pd	1.015520	0.262828	0.567692
C	-4.736270	0.454086	1.767038
H	-5.335627	0.075815	0.926974
H	-5.076598	-0.076223	2.667095
H	-4.988645	1.514349	1.895327
C	-2.962594	-1.275086	1.383090
C	-3.339496	-1.828712	2.255721
H	-3.443391	-1.703125	0.492031
H	-1.888487	-1.485290	1.310403
C	-4.163896	0.021017	-1.920669
H	-4.607828	-0.652378	-1.176748
H	-4.871408	0.097513	-2.758312
H	-3.260253	-0.475084	-2.301145
C	-3.336201	2.333464	-2.435985
C	-3.145708	3.349721	-2.065798
H	-2.399501	1.949724	-2.868161
H	-4.057099	2.413311	-3.261354
C	-1.191847	3.091131	1.847907
H	-1.579143	2.587659	2.745579
H	-0.248806	2.594579	1.576934
H	-0.952147	4.123798	2.138478
C	-3.472764	3.836795	1.125066
H	-3.233153	4.880125	1.373874
H	-4.238527	3.852469	0.338564
H	-3.928277	3.396174	2.023039
Zn	-0.431941	-1.385282	-0.893939
O	-0.487361	-3.275351	0.092823
C	-1.473187	-3.564927	-0.651150
O	-1.895554	-2.738482	-1.514422
C	-2.187223	-4.870237	-0.470960
H	-2.602582	-5.215695	-1.420103
H	-1.523964	-5.622025	-0.038714
H	-3.021634	-4.709421	0.222278
O	1.156569	-1.654773	-2.146420
C	2.408376	-1.677176	-2.106429
O	3.163756	-0.858875	-1.484803
C	3.115443	-2.784301	-2.837200
H	4.162943	-2.538051	-3.019112
H	3.068057	-3.685435	-2.214245
H	2.596267	-3.006761	-3.772466
H	2.718095	0.092779	-0.922009
P	1.659446	-1.316659	2.193925
C	0.442993	-2.227705	3.226769
H	-0.223284	-1.520652	3.733123
H	-0.155574	-2.860208	2.561270
H	0.944258	-2.857487	3.973172
C	2.594791	-2.709648	1.448425
H	2.992774	-3.385048	2.216625
H	1.909553	-3.264954	0.797056
H	3.416398	-2.310740	0.842198
C	2.844603	-0.696405	3.454918
H	3.217900	-1.510210	4.089793
H	3.686695	-0.215343	2.945404
H	2.355837	0.055383	4.083017
N	0.760969	2.307519	-1.482271
H	0.362930	2.846242	-2.245722

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C	4.513315	3.237357	-0.088166
C	3.841342	4.196120	-0.838189
C	2.508682	3.997960	-1.190611
C	1.886629	2.821153	-0.790047
C	2.525926	1.816312	-0.033151
C	3.852820	2.073444	0.314922
H	5.557020	3.392305	0.179536
H	4.350961	5.105278	-1.149860
H	1.967987	4.752963	-1.761052
C	4.404241	1.337420	0.903308
H	0.004247	1.434989	-0.617372
C	-1.046380	0.650617	-0.448426
Si	-2.744731	1.187132	0.128743
C	-2.566788	2.987962	0.734872
H	-2.137274	3.534650	-0.123106
C	-3.913725	1.140815	-1.371444
H	-4.910726	1.446823	-1.012219
C	-3.384092	0.091149	1.555177
H	-2.983851	0.567959	2.466743
Pd	1.142374	0.306234	0.595171
C	-4.912101	0.117048	1.641431
H	-5.364771	-0.397206	0.782610
H	-5.263028	-0.399846	2.545423
H	-5.323031	1.133904	1.664392
C	-2.888401	-1.351930	1.537965
H	-3.291666	-1.915741	2.391742
H	-3.202822	-1.879348	0.625002
H	-1.793203	-1.410654	1.605754
C	-4.021709	-0.261559	-1.964647
H	-4.381932	-1.001595	-1.238645
H	-4.708349	-0.280239	-2.822773
H	-3.046263	-0.618743	-2.322772
C	-3.462168	2.135927	-2.438465
H	-3.448426	3.170090	-2.069204
H	-2.449624	1.890298	-2.793503
H	-4.123174	2.107932	-3.316034
C	-1.595298	3.124090	1.906036
H	-1.975941	2.603545	2.796498
H	-0.602751	2.710627	1.683979
H	-1.461294	4.178262	2.186935
C	-3.906593	3.637051	1.080205
H	-3.780124	4.700740	1.326665
H	-4.633996	3.574017	0.260116
H	-4.359013	3.162520	1.962953
Zn	-0.499171	-1.350089	-0.688899
O	-0.303296	-3.283704	0.194175
C	-1.282124	-3.648552	-0.525363
O	-1.825691	-2.836525	-1.331703
C	-1.844273	-5.030325	-0.380532
H	-1.086860	-5.724961	-0.011896
H	-2.658765	-4.990842	0.352567
H	-2.263690	-5.376258	-1.327689
O	1.017310	-1.675480	-2.159294
C	2.218269	-1.557876	-2.395505
O	3.030379	-0.720370	-1.801610
C	2.907977	-2.418102	-3.404409
H	3.449410	-3.206452	-2.868744
H	2.175867	-2.880183	-4.067341
H	3.643240	-1.840129	-3.969036
H	2.576616	-0.152955	-1.108663
P	2.037060	-1.396826	1.989146
C	0.976454	-2.355031	3.144949
H	0.445095	-1.671249	3.815022
H	0.243589	-2.915123	2.553346
H	1.574534	-3.055256	3.742624
C	2.864660	-2.757923	1.070936
H	3.354556	-3.457086	1.760647
H	2.105481	-3.296565	0.490529
H	3.612849	-2.336228	0.389954
C	3.383014	-0.831238	3.106305
H	3.788923	-1.661882	3.697888
H	4.185478	-0.387068	2.507358
H	2.999318	-0.058977	3.780687
N	0.538721	2.544595	-1.130041
H	0.032885	3.113391	-1.801350

TS_{34NH}

C	-5.192344	2.430308	-0.065172
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C	-4.623759	3.665923	0.218962	C	-3.148534	3.868510	0.273611
C	-3.240956	3.788670	0.337229	C	-2.414424	2.696179	0.148290
C	-2.457257	2.651325	0.178354	C	-2.985697	1.448739	-0.148095
C	-2.992846	1.378541	-0.113771	C	-4.362825	1.443635	-0.382700
C	-4.377212	1.306899	-0.240377	H	-6.209796	2.561485	-0.399454
H	-6.273453	2.336164	-0.150732	H	-5.122660	4.716948	0.175711
H	-5.253954	4.543126	0.349345	H	-2.660312	4.812688	0.514331
H	-2.785881	4.756461	0.547124	H	-4.867233	0.514214	-0.646820
H	-4.847653	0.350963	-0.471938	C	-0.408618	1.489770	0.139897
C	-0.407963	1.518285	0.100709	C	0.750794	0.832223	0.180193
C	0.748768	0.878498	0.063737	Si	2.424079	1.345978	-0.518583
Si	2.465601	1.406361	-0.492848	C	2.471201	0.850635	-2.359576
C	2.713148	0.765398	-2.272664	H	1.677785	1.460639	-2.824768
H	1.961049	1.312174	-2.866461	C	2.573918	3.245101	-0.390484
C	2.546400	3.313981	-0.516819	H	3.622663	3.471463	-0.646010
H	3.585353	3.561200	-0.794206	C	3.868834	0.542887	0.437852
C	3.796954	0.700795	0.680553	H	4.055859	-0.425024	-0.053554
H	4.014990	-0.311951	0.305476	Pd	-1.534810	-0.073656	-0.357218
Pd	-1.499834	-0.075336	-0.412739	C	5.149151	1.377191	0.342736
C	5.097911	1.506413	0.650700	H	5.050135	2.327832	0.885169
H	4.961598	2.511384	1.073837	H	5.994275	0.840726	0.795846
H	5.873876	1.013274	1.252611	H	5.431016	1.617996	-0.689877
H	5.502624	1.632372	-0.361191	C	3.554954	0.247465	1.904107
C	3.310131	0.550927	2.121290	H	4.442618	-0.150039	2.416230
H	4.095740	0.117300	2.755667	H	3.242883	1.149689	2.450755
H	3.031158	1.519445	2.560721	H	2.767864	-0.508447	2.011886
C	2.436133	-0.107692	2.196256	C	2.348788	3.733592	1.041307
C	2.293823	3.922989	0.862351	H	3.116649	3.352160	1.726721
H	3.065783	3.635713	1.586697	H	2.373107	4.831043	1.101711
H	2.277474	5.021320	0.817781	H	1.384350	3.401219	1.455253
C	1.337119	3.597685	1.296799	C	1.691374	3.981781	-1.396822
C	1.631072	3.925400	-1.577365	H	1.985081	3.761346	-2.430293
H	1.913292	3.616810	-2.591091	H	0.631571	3.708535	-1.307120
H	0.581162	3.634839	-1.436770	H	1.762199	5.070887	-1.263431
H	1.673782	5.023709	-1.548054	C	2.137142	-0.616636	-2.620464
C	2.433144	-0.726917	-2.440571	H	2.843921	-1.290906	-2.114513
H	3.101260	-1.336767	-1.815215	H	1.121282	-0.871319	-2.283723
H	1.394768	-0.983865	-2.183560	H	2.183185	-0.843594	-3.694987
C	2.588857	-1.039191	-3.483030	C	3.808325	1.207661	-3.007714
H	4.101596	1.095721	-2.818785	H	3.791550	1.012316	-4.089080
H	4.189853	0.808627	-3.875990	H	4.080428	2.262898	-2.870957
H	4.348267	2.163447	-2.749686	H	4.620586	0.598885	-2.585946
H	4.877059	0.540105	-2.272451	Zn	0.698238	-1.311778	0.350875
Zn	0.740695	-1.247633	0.371368	O	0.188281	0.519479	3.062327
O	-0.816357	0.298045	3.014721	C	-0.022565	-0.759802	3.256266
C	-0.435214	-0.941481	3.233602	O	0.185552	-1.632759	2.411188
O	0.072994	-1.669618	2.384595	C	-0.557417	-1.072347	4.612604
C	-0.682646	-1.383352	4.636204	H	-1.582825	-0.693386	4.679877
H	-0.316414	-2.399472	4.781218	H	-0.552796	-2.149141	4.782018
H	-0.185879	-0.697339	5.328729	H	0.029103	-0.555360	5.376748
H	-1.755031	-1.332952	4.848282	O	0.688408	-3.323402	-0.335093
O	0.800658	-3.288829	-0.241487	C	1.941575	-3.357148	-0.140550
C	2.023261	-3.306398	0.092249	O	2.544719	-2.342395	0.316997
O	2.574046	-2.266656	0.562820	C	2.721103	-4.585363	-0.499912
C	2.842050	-4.545285	-0.108803	H	3.580794	-4.701275	0.163462
H	3.447696	-4.416532	-1.013270	H	2.085991	-5.472881	-0.472695
H	3.530369	-4.683258	0.728512	H	3.100556	-4.465577	-1.521447
H	2.204995	-5.422460	-0.234655	H	0.472749	0.687164	2.117946
H	-0.682824	0.535307	2.068859	P	-2.526087	-2.176244	-0.875665
P	-2.385613	-2.141678	-1.163660	C	-2.435138	-3.461698	0.433127
C	-2.537830	-3.496188	0.064155	H	-1.389184	-3.760893	0.564876
H	-1.538754	-3.747904	0.432682	H	-2.808841	-3.047657	1.375512
H	-3.153291	-3.158943	0.904704	H	-3.033602	-4.339855	0.158767
H	-2.994771	-4.386708	-0.385802	C	-4.333798	-2.126209	-1.199363
C	-4.097894	-2.061713	-1.826519	H	-4.719920	-3.127702	-1.428067
H	-4.400560	-3.024720	-2.256964	H	-4.846627	-1.734128	-0.314439
H	-4.785601	-1.802312	-1.014238	H	-4.539056	-1.456757	-2.041374
H	-4.164154	-1.280770	-2.591063	C	-1.919503	-3.093597	-2.345640
C	-1.494774	-2.979711	-2.534589	H	-2.509508	-4.004163	-2.511464
H	-2.039653	-3.869478	-2.875573	H	-1.986409	-2.454106	-3.231812
H	-1.375580	-2.284983	-3.372651	H	-0.871917	-3.364886	-2.176970
H	-0.503705	-3.275439	-2.171669	N	-1.014719	2.668970	0.341502
N	-1.052974	2.685317	0.309985	H	-0.506122	3.490735	0.652511
H	-0.565100	3.526975	0.597664				
				TS _{45NH}			
4 _{NH}				C	-3.708005	4.096604	-0.690098
C	-5.132448	2.605095	-0.248844	C	-2.636766	4.974045	-0.802776
C	-4.527140	3.811929	0.076926	C	-1.332407	4.530078	-0.587511

C	-1.131490	3.197501	-0.251640	C	2.093642	1.978789	-0.426141
C	-2.198785	2.292723	-0.123736	C	3.323224	2.611598	-0.277812
C	-3.484905	2.754880	-0.357345	H	4.385092	4.443127	0.131169
H	-4.722729	4.451661	-0.857882	H	2.315838	5.780679	0.442270
H	-2.811311	6.015299	-1.064104	H	0.090947	4.701154	0.172787
H	-0.490121	5.213460	-0.686099	H	4.249559	2.053409	-0.406624
H	-4.333188	2.074248	-0.274609	C	-0.224924	0.796823	-0.817526
C	0.139383	1.312698	0.282147	C	-1.338777	-0.048311	-0.773381
C	1.118799	0.383809	0.487813	Si	-3.171375	0.314639	-0.496451
Si	2.932452	0.614601	0.021239	C	-3.423158	1.760948	0.730816
C	2.982009	1.315819	-1.758091	C	-3.067229	2.677467	0.225276
H	2.558276	2.333873	-1.701048	C	-3.946976	0.791635	-2.172227
C	3.812119	1.820610	1.214085	H	-5.034993	0.880563	-2.016392
H	4.872730	1.808035	0.910724	C	-3.971101	-1.272958	0.207997
C	3.839753	-1.071426	0.055134	H	-3.871140	-1.184247	1.304193
H	3.657957	-1.519713	-0.936979	Pd	1.706825	0.055183	-0.902315
Pd	-1.637204	0.387797	0.353725	C	-5.460112	-1.379100	-0.130869
C	5.353467	-0.908222	0.223702	H	-5.613915	-1.515794	-1.210663
H	5.605658	-0.539424	1.227612	H	-5.911574	-2.248133	0.367387
H	5.861713	-1.874946	0.103844	H	-6.036675	-0.495795	0.169070
H	5.797684	-0.213573	-0.499240	C	-3.265443	-2.568076	-0.202422
C	3.325019	-2.063046	1.100261	H	-3.795405	-3.439079	0.207074
H	3.943182	-2.971686	1.102777	H	-3.239343	-2.692726	-1.295229
H	3.343511	-1.648907	2.117575	H	-2.232308	-2.633045	0.161856
H	2.297994	-2.400219	0.913039	C	-3.700849	-0.285520	-3.228065
C	3.718871	1.341586	2.661840	H	-4.096697	-1.265264	-2.930753
H	4.166658	0.350452	2.804182	H	-4.170382	-0.018471	-4.185116
H	4.230663	2.033952	3.345338	H	-2.625782	-0.408364	-3.420771
H	2.671414	1.275041	2.987892	C	-3.418693	2.137403	-2.665363
C	3.312497	3.258931	1.112714	H	-3.675189	2.963616	-1.989259
H	3.338982	3.648700	0.084900	H	-2.323673	2.116572	-2.771216
H	2.283616	3.340685	1.494050	H	-3.828785	2.388255	-3.653642
H	3.920866	3.936698	1.727605	C	-2.649165	1.596273	2.038058
C	2.105327	0.507888	-2.715430	H	-2.921394	0.659914	2.544073
H	2.419491	-0.545889	-2.758075	H	-1.559626	1.579876	1.891804
H	1.046728	0.527565	-2.421768	H	-2.870537	2.421092	2.730659
H	2.166841	0.905678	-3.738243	C	-4.907176	1.979668	1.031341
C	4.401246	1.434610	-2.310492	H	-5.055781	2.870276	1.657414
H	4.404655	1.917400	-3.297875	H	-5.510142	2.111389	0.123406
H	5.063104	2.019314	-1.657525	H	-5.321047	1.127470	1.587280
H	4.854360	0.441954	-2.440133	Zn	-0.291395	-0.994726	0.904737
Zn	0.410799	-1.435004	-0.283854	O	1.177578	-1.980736	-1.625523
O	0.571392	-0.819438	2.766841	C	0.762502	-2.910852	-0.894459
C	-0.140338	-1.854822	2.544595	O	0.378769	-2.784474	0.314162
O	-0.293383	-2.397092	1.417838	C	0.703538	-4.302172	-1.465811
C	-0.889667	-2.423868	3.710949	H	1.247199	-4.988152	-0.807821
H	-1.911744	-2.023541	3.673858	H	-0.338659	-4.639105	-1.482160
H	-0.951908	-3.511824	3.630633	H	1.118724	-4.334578	-2.474525
H	-0.438017	-2.123423	4.658113	O	0.574221	-0.194347	2.625208
O	-0.785034	-2.182509	-1.878491	C	-0.403248	-0.660961	3.290166
C	0.242135	-2.810492	-2.275096	O	-1.319151	-1.317899	2.711697
O	1.325135	-2.748858	-1.615173	C	-0.505937	-0.381827	4.758143
C	0.204348	-3.597047	-3.549126	H	0.473764	-0.157724	5.184078
H	0.783345	-4.517534	-3.443424	H	-1.149285	0.496371	4.891756
H	-0.822628	-3.816317	-3.846224	H	-0.975982	-1.220361	5.276781
H	0.677996	-2.999720	-4.336438	H	-1.169309	-0.964736	-1.354287
H	0.876221	-0.262145	1.749335	P	3.837309	-0.814631	-0.233932
P	-3.502776	-1.145547	0.124922	C	3.896929	-2.645750	-0.136442
C	-3.227439	-2.952369	0.305051	H	3.074490	-2.994609	0.498201
H	-2.441139	-3.255806	-0.395621	H	3.774136	-3.076519	-1.135339
H	-2.880373	-3.184235	1.317127	H	4.850298	-2.977962	0.292237
H	-4.150717	-3.505610	0.090622	C	5.420283	-0.455040	-1.093712
C	-5.012920	-0.892537	1.140914	H	6.264007	-0.885563	-0.540486
H	-5.818819	-1.568486	0.828900	H	5.389870	-0.891317	-2.097110
H	-4.778511	-1.077725	2.194586	H	5.575101	0.623036	-1.196983
H	-5.355396	0.143522	1.049771	C	4.166356	-0.344902	1.505136
C	-4.145458	-1.047087	-1.589174	H	5.053993	-0.855791	1.898242
H	-5.011341	-1.705567	-1.733739	H	4.298474	0.738562	1.579801
H	-4.423930	-0.013783	-1.821929	H	3.285300	-0.607570	2.102855
H	-3.336426	-1.346626	-2.264552	N	-0.269198	2.100158	-0.465596
N	0.128515	2.626902	-0.023043	H	-1.149163	2.569454	-0.269629
H	0.984133	3.169096	-0.102838				
5 _{NH}				6 _{NH}			
C	3.409136	3.973757	0.027567	C	-3.471082	3.078211	-2.384086
C	2.252840	4.723122	0.196801	C	-2.333394	3.646440	-2.941599
C	1.005431	4.122818	0.046863	C	-1.070899	3.205439	-2.550993
C	0.941309	2.770810	-0.269188	C	-0.974637	2.193785	-1.602905
				C	-2.107266	1.581768	-1.035376

C	-3.352207	2.050143	-1.442468	N	0.249723	1.743602	-1.099106
H	-4.457692	3.430753	-2.676952	H	1.122038	2.067050	-1.509585
H	-2.421859	4.441695	-3.678003				
H	-0.171142	3.653067	-2.971565	TS _{67NH}			
H	-4.262401	1.629207	-1.016232	C	-1.769791	4.058140	-1.765174
C	0.227655	0.856603	-0.080341	C	-0.709499	3.797999	-2.641511
C	1.369100	0.180048	0.366827	C	0.138911	2.735122	-2.408829
Si	3.189659	0.445541	-0.041740	C	-0.026208	1.878229	-1.296459
C	3.448055	0.815852	-1.900533	C	-1.089361	2.147156	-0.399475
H	3.082773	1.844563	-2.073778	C	-1.939942	3.236114	-0.664652
C	3.831796	1.927530	0.977120	H	-2.440067	4.896653	-1.937339
H	4.927739	1.954128	0.857446	H	-0.547388	4.431919	-3.510306
C	4.130958	-1.150095	0.440083	H	0.963762	2.533786	-3.093592
H	4.166217	-1.758828	-0.479349	H	-2.731998	3.457554	0.052108
Pd	-1.686452	0.245217	0.411917	C	0.862756	-0.269681	-0.332137
C	5.573169	-0.864121	0.864531	C	2.017655	-0.804178	0.136055
H	5.607848	-0.302169	1.808032	Si	3.797496	-0.235095	-0.038208
H	6.124258	-1.800315	1.029524	C	4.314551	-0.473153	-1.865776
H	6.129018	-0.282754	0.118822	H	3.721269	0.257695	-2.447537
C	3.431796	-1.988206	1.513032	C	4.122314	1.588005	0.453910
H	4.061733	-2.839020	1.807858	H	5.220760	1.644230	0.544229
H	3.232662	-1.405818	2.426153	C	4.868889	-1.374135	1.069975
C	2.476376	-2.409494	1.175467	H	5.058953	-2.265941	0.446769
C	3.507665	1.755495	2.461582	Pd	-1.793426	0.681752	0.877109
H	3.864834	0.800471	2.870442	C	6.222922	-0.764623	1.435967
H	3.957077	2.558703	3.062141	H	6.100140	0.091689	2.113894
C	2.421002	1.804702	2.621152	H	6.854921	-1.495671	1.959808
C	3.262174	3.256242	0.484548	H	6.785743	-0.409775	0.564212
H	3.541095	3.479188	-0.553852	C	4.163972	-1.845742	2.342511
H	2.163371	3.257492	0.553939	H	4.821837	-2.497592	2.935090
C	3.616484	4.093367	1.102273	H	3.888442	-0.999573	2.988755
C	2.682087	-0.118049	-2.837965	H	3.246933	-2.408323	2.135832
H	2.932640	-1.174176	-2.667297	C	3.514104	1.918247	1.815548
H	1.593099	-0.025379	-2.720226	H	3.868304	1.247899	2.609537
C	2.913703	0.110180	-3.888385	H	3.748860	2.948600	2.123573
C	4.936784	0.821425	-2.253008	H	2.419602	1.825003	1.771771
H	5.094057	1.112246	-3.300908	C	3.700691	2.644034	-0.566226
H	5.514438	1.517080	-1.629495	H	4.040999	2.416611	-1.585964
H	5.375143	-0.178592	-2.130897	H	2.607359	2.750523	-0.592175
Zn	0.418839	-1.622554	-0.397723	H	4.107150	3.630709	-0.301856
O	-1.171107	-1.010353	2.168674	C	3.940636	-1.868338	-2.364162
C	-0.621438	-2.137041	2.183292	H	4.502792	-2.643132	-1.822746
O	-0.136003	-2.737309	1.172215	H	2.873728	-2.084461	-2.224968
C	-0.504378	-2.851442	3.503664	H	4.178810	-1.989781	-3.430415
H	-0.886140	-3.872582	3.405910	C	5.790187	-0.182065	-2.129506
H	0.556212	-2.933476	3.768704	H	6.026046	-0.242348	-3.201660
H	-1.038481	-2.316961	4.292149	H	6.095752	0.813085	-1.779258
O	-0.538642	-2.114468	-2.192906	H	6.428891	-0.920208	-1.623844
C	0.481209	-2.807674	-2.495680	Zn	-0.688912	-1.611679	-0.275941
O	1.454347	-2.907497	-1.689368	O	-2.504544	-0.750892	2.355925
C	0.573129	-3.468829	-3.836784	C	-2.201615	-1.972123	2.263989
H	-0.401508	-3.514648	-4.325517	O	-1.503675	-2.498872	1.354131
H	1.255250	-2.877455	-4.459430	C	-2.747216	-2.901953	3.317291
H	1.005901	-4.467377	-3.737449	H	-3.514489	-3.535594	2.858048
H	1.219847	-0.227145	1.376151	H	-1.955294	-3.567616	3.671310
P	-3.774969	-0.924469	0.304578	H	-3.186304	-2.350054	4.150160
C	-3.699842	-2.567081	1.114423	O	-1.926805	-2.237345	-1.880346
H	-2.829128	-3.107362	0.725411	C	-1.147913	-3.235704	-2.052198
H	-3.578783	-2.444560	2.195404	O	-0.143078	-3.407497	-1.318216
H	-4.609199	-3.144278	0.908423	C	-1.471463	-4.210929	-3.147458
C	-5.377272	-0.275032	0.925139	H	-2.400687	-4.733744	-2.898007
H	-6.190611	-0.979755	0.711064	H	-1.646310	-3.673560	-4.084120
H	-5.311193	-0.120387	2.006647	H	-0.668621	-4.939371	-3.272428
H	-5.610894	0.687393	0.459018	H	1.912465	-1.787657	0.611704
C	-4.150152	-1.395146	-1.425240	P	-3.726717	0.274503	-0.462961
H	-5.016945	-2.065793	-1.475684	C	-4.535857	-1.349662	-0.240346
H	-4.341304	-0.500070	-2.025035	H	-3.858198	-2.127830	-0.606506
C	-3.266641	-1.892279	-1.842604	H	-4.733429	-1.502250	0.826054
C	-0.308322	2.132513	3.157161	H	-5.479015	-1.389884	-0.798259
C	-0.629028	2.981507	2.355457	C	-5.080126	1.440449	-0.042068
C	-1.013367	4.006744	1.397412	H	-5.983901	1.206191	-0.618315
H	-0.187875	4.242155	0.712502	H	-5.303257	1.369334	1.027507
H	-1.304673	4.937200	1.898342	H	-4.772855	2.466129	-0.270590
H	-1.856811	3.674877	0.776941	C	-3.569785	0.457449	-2.272791
C	0.086543	1.109015	4.111930	H	-4.552132	0.376588	-2.754294
H	0.667680	0.314944	3.621448	H	-3.129179	1.434262	-2.503103
H	-0.787983	0.623879	4.560500	H	-2.913542	-0.338849	-2.640034
H	0.699877	1.527957	4.919032	C	-0.198433	1.295771	2.118576

C	-0.209351	2.392800	1.494175	C	5.236395	-1.118997	-0.630708
C	0.154817	3.817602	1.427945	H	6.170584	-0.682454	-1.006271
H	0.689910	4.055188	0.500252	H	5.375503	-1.424803	0.412697
H	0.802574	4.047322	2.283474	H	4.993758	-2.009950	-1.220312
H	-0.728372	4.463229	1.478320	C	3.921349	0.662613	-2.448645
C	0.320650	0.383586	3.145903	H	4.937358	0.997970	-2.691911
H	0.859620	-0.439852	2.654768	H	3.637164	-0.147742	-3.126205
H	-0.496765	-0.040630	3.737425	H	3.217818	1.496061	-2.550647
H	1.021823	0.902482	3.811887	C	0.728493	-2.239485	1.507469
N	0.907311	0.884785	-1.123323	C	0.255271	-3.021448	0.539726
H	1.749757	1.013386	-1.675811	C	-0.616323	-4.235536	0.608888
				H	-1.526255	-4.104943	0.005354
7 _{NH}				H	-0.920791	-4.453546	1.638370
C	2.058615	-2.544904	-2.811692	H	-0.096726	-5.117686	0.209760
C	1.369122	-1.431039	-3.313044	C	0.555944	-2.204721	2.975125
C	0.364419	-0.823384	-2.586748	H	0.048865	-1.277021	3.275763
C	-0.039388	-1.356296	-1.347140	H	1.522449	-2.220891	3.490588
C	0.699045	-2.449029	-0.785590	H	-0.051405	-3.051883	3.326468
C	1.736258	-3.032830	-1.558906	N	-1.149063	-0.854249	-0.707830
H	2.849874	-3.009154	-3.395575	H	-1.453568	-1.468907	0.043404
H	1.626771	-1.036340	-4.294169				
H	-0.185720	0.027828	-2.982514	TS _{78NH}			
C	2.265553	-3.887487	-1.137926	C	-2.504126	3.639398	-1.856260
C	-1.193034	0.521900	-0.296586	C	-1.820313	3.059205	-2.931932
C	-2.376265	1.041040	0.085734	C	-0.739644	2.225566	-2.709864
Si	-4.090039	0.280856	-0.067754	C	-0.284865	1.959232	-1.407145
C	-4.489822	0.086456	-1.925146	C	-0.919670	2.602926	-0.300909
H	-3.876952	-0.766801	-2.261552	C	-2.047990	3.415854	-0.570482
C	-4.239258	-1.426816	0.806779	H	-3.366145	4.278238	-2.031900
H	-5.280992	-1.459301	1.166314	H	-2.155706	3.238941	-3.951191
C	-5.319170	1.498931	0.756415	H	-0.243817	1.734543	-3.546568
H	-5.484759	2.291469	0.005179	H	-2.529241	3.902014	0.278261
Pd	1.983050	-1.036240	0.476068	C	0.717386	0.093187	-0.172594
C	-6.673046	0.871043	1.089312	C	1.859092	-0.418560	0.332635
H	-6.574714	0.152151	1.915458	Si	3.645931	0.004360	-0.097180
H	-7.391817	1.633840	1.420110	C	3.901176	-0.111557	-1.985748
H	-7.123542	0.336316	0.245053	H	3.380670	0.753359	-2.434216
C	-4.755594	2.157298	2.016784	C	4.081872	1.760202	0.512256
H	-5.485316	2.850909	2.458628	H	5.180258	1.792878	0.602382
H	-4.527057	1.404923	2.786161	C	4.781756	-1.300144	0.733331
H	-3.836138	2.722271	1.831494	H	4.995034	-2.035195	-0.062171
C	-3.341613	-1.530564	2.041466	Pd	-1.778328	0.626863	0.689832
H	-3.508017	-0.703171	2.743787	C	6.117761	-0.716093	1.193633
H	-3.518030	-2.470417	2.585799	H	5.975841	-0.006674	2.021169
H	-2.269187	-1.506115	1.789602	H	6.784753	-1.507337	1.563757
C	-4.057816	-2.632969	-0.113354	H	6.652034	-0.183731	0.396397
H	-4.837314	-2.685937	-0.883266	C	4.122046	-2.057408	1.885429
H	-3.096976	-2.610708	-0.646466	H	4.835149	-2.748648	2.356500
H	-4.099109	-3.573087	0.457253	H	3.769557	-1.374272	2.672816
C	-4.054436	1.314269	-2.722045	H	3.262887	-2.652286	1.553893
H	-4.585437	2.218346	-2.388717	C	3.475087	1.995821	1.895156
H	-2.981061	1.508533	-2.612627	H	3.769930	1.226501	2.622988
H	-4.273630	1.192302	-3.792716	H	3.771776	2.973066	2.304549
C	-5.958517	-0.229505	-2.197915	H	2.378367	1.979614	1.830951
H	-6.132852	-0.436570	-3.263468	C	3.655428	2.868377	-0.448743
H	-6.320578	-1.098134	-1.630737	H	4.156807	2.796680	-1.422409
H	-6.597385	0.624594	-1.931333	H	2.572407	2.837884	-0.635735
Zn	0.509008	1.558230	0.166206	H	3.891034	3.860001	-0.034158
O	2.762485	-0.175211	2.259762	C	3.303904	-1.395809	-2.560486
C	2.271027	0.935971	2.624743	H	3.762153	-2.284299	-2.102649
O	1.408604	1.608243	2.010510	H	2.224661	-1.481590	-2.376235
C	2.816806	1.517136	3.904098	H	3.474230	-1.467388	-3.644296
H	3.525296	2.312155	3.643251	C	5.379447	0.005452	-2.357814
H	2.009315	1.979054	4.477479	H	5.519684	0.001688	-3.447987
H	3.334679	0.762950	4.499356	H	5.839613	0.923918	-1.969504
O	1.855167	2.622851	-1.088627	H	5.953953	-0.843362	-1.961033
C	1.221284	3.694906	-0.805101	Zn	-0.548116	-1.615401	0.024193
O	0.243399	3.681408	-0.016817	O	-2.509796	-0.592859	2.437352
C	1.683692	4.980132	-1.430733	C	-1.952058	-1.704383	2.619071
H	2.698775	5.203638	-1.085705	O	-1.164545	-2.293508	1.816195
H	1.732558	4.864652	-2.517765	C	-2.207125	-2.406613	3.929412
H	1.018870	5.805198	-1.170509	H	-2.301314	-3.484150	3.772945
H	-2.321277	2.064385	0.471126	H	-1.338303	-2.246065	4.578701
P	3.848853	0.086282	-0.712505	H	-3.092925	-2.005719	4.425745
C	4.565155	1.516957	0.182974	O	-1.390596	-2.646112	-1.630417
H	3.882988	2.366730	0.071290	C	-0.400660	-3.447288	-1.588467
H	4.672874	1.259459	1.241965	O	0.494504	-3.321037	-0.711064
H	5.547401	1.775891	-0.231257	C	-0.291647	-4.551005	-2.599865

H	-1.116620	-4.524360	-3.313688	H	-6.110001	-0.510251	-0.944484
H	0.663681	-4.461629	-3.126794	H	-1.433116	0.718908	2.493302
H	-0.279837	-5.514383	-2.081036	H	-2.535628	1.551195	3.599046
H	1.731181	-1.226582	1.062780	H	-2.959565	-0.033872	2.930387
P	-3.591479	-0.262492	-0.681861	H	-5.221730	2.506506	1.229438
C	-4.271859	-1.896485	-0.208625	H	-5.191526	1.110830	2.323746
H	-3.542400	-2.671310	-0.467760	H	-4.585614	2.674139	2.872145
H	-4.447280	-1.910309	0.871961	H	-2.335740	2.840366	-1.947040
H	-5.214307	-2.092806	-0.734819	H	-3.841426	3.662769	-2.364674
C	-5.032824	0.843779	-0.408799	H	-3.298745	3.621204	-0.681662
H	-5.925498	0.475548	-0.930134	H	-4.748838	1.658673	-3.505660
H	-5.237352	0.904002	0.665884	H	-3.289301	0.724301	-3.164921
H	-4.787974	1.848636	-0.771618	H	-4.872498	0.091857	-2.691709
C	-3.514654	-0.371852	-2.507036	C	0.106312	0.461264	-3.213339
H	-4.484231	-0.677160	-2.920373	H	0.896652	0.552229	-3.960976
H	-3.235176	0.605753	-2.914831	H	-0.183540	-0.596668	-3.186304
H	-2.750701	-1.110213	-2.773010	H	-0.760027	1.032122	-3.580926
C	-0.473453	1.660554	1.819577	C	2.800261	1.827217	-2.743610
C	-0.265808	2.729292	1.062554	H	2.773633	1.001479	-3.457898
C	0.443271	4.006652	1.393899	H	2.620756	2.764562	-3.292034
H	1.253147	4.200665	0.675402	H	3.822337	1.863097	-2.351781
H	0.878093	3.976784	2.398986	Zn	-0.692031	-1.500368	0.245961
-0.241889	4.863963	1.342825		O	1.707512	-2.650007	-1.228360
C	-0.024234	1.209222	3.150145	C	0.710033	-3.389191	-1.315558
H	0.573058	0.290221	3.048342	O	-0.454742	-3.121828	-0.858598
H	-0.875295	0.977645	3.800355	C	0.835815	-4.723276	-2.009186
H	0.603332	1.966946	3.642006	H	1.861120	-4.901001	-2.337860
N	0.740948	1.065124	-1.204515	H	0.512215	-5.519956	-1.332475
H	1.241478	0.789790	-2.044031	H	0.161513	-4.746499	-2.871508
				O	-1.649059	-2.220897	2.031745
8 _{NH}				C	-0.625995	-1.847230	2.666348
C	3.077325	4.253314	0.828341	O	0.335445	-1.260870	2.068471
C	2.026197	4.283832	1.746980	C	-0.538995	-2.050451	4.150725
C	0.919195	3.476029	1.546476	H	-0.798181	-1.109469	4.650615
C	0.869261	2.635995	0.434362	H	-1.236590	-2.823133	4.478991
C	1.916246	2.576125	-0.500074	H	0.483833	-2.304022	4.440811
C	3.017511	3.417480	-0.277149	N	-0.230522	1.819445	0.242371
H	3.945853	4.890770	0.974306	H	-0.910976	1.783129	0.989622
H	2.070897	4.938668	2.613277				
H	0.082322	3.482240	2.245754	9 _{NH}			
H	3.844541	3.415677	-0.982688	C	1.137854	5.100797	0.299619
C	-0.436836	0.982287	-0.806027	C	-0.149167	5.139479	0.836239
C	-1.593216	0.138855	-0.769230	C	-1.055382	4.131320	0.548537
H	-1.737075	-0.372281	-1.728598	C	-0.682779	3.070395	-0.283026
Pd	2.003328	-0.367116	-0.898662	C	0.617936	3.006429	-0.829574
P	3.706111	-0.652172	0.731390	C	1.509070	4.045649	-0.521151
C	5.485181	-0.270563	0.450228	H	1.848626	5.892818	0.519398
H	5.580854	0.775206	0.136580	H	-0.447697	5.961085	1.482997
H	6.076238	-0.422774	1.362844	H	-2.064763	4.151162	0.959559
H	5.884704	-0.905807	-0.346544	H	2.512351	4.025522	-0.938815
C	3.351515	0.382644	2.205922	C	-1.274902	0.865668	-1.199995
H	4.071755	0.198457	3.014101	C	-2.155550	-0.169482	-1.186898
H	3.384063	1.442317	1.922927	H	-1.837944	-1.046587	-1.745618
H	2.338488	0.139258	2.547737	Pd	1.292470	0.636455	0.212566
C	3.778934	-2.330881	1.467817	P	2.042350	0.094061	2.323170
H	4.505968	-2.389330	2.288106	C	1.945865	1.673043	3.261432
H	2.777701	-2.567600	1.843994	H	0.912338	2.038395	3.243501
H	4.030035	-3.059757	0.691312	H	2.269898	1.540546	4.301965
C	1.806691	1.643204	-1.624771	H	2.576166	2.424794	2.774171
C	0.555084	0.960779	-1.861822	C	1.098014	-1.052804	3.393700
Si	-3.295636	0.607994	-0.101958	H	1.470507	-0.999561	4.424754
C	-4.300716	-0.987980	0.179184	H	0.036521	-0.784685	3.377915
C	-3.227223	1.618122	1.534718	H	1.218867	-2.071399	3.008604
C	-4.127817	1.719676	-1.415441	C	3.769194	-0.435438	2.612417
H	-4.056055	-1.296846	1.210197	H	4.002259	-0.402779	3.684125
C	-3.914623	-2.146989	-0.741634	H	3.915042	-1.452169	2.234320
C	-5.810854	-0.756129	0.084131	H	4.449795	0.218201	2.059116
H	-2.709573	2.566615	1.299490	C	0.968918	1.856294	-1.679801
C	-2.494526	0.932137	2.691077	C	0.053172	0.817936	-1.852918
C	-4.632650	2.001017	2.004966	Si	-3.690543	-0.420708	-0.166052
H	-5.139735	1.955136	-1.045762	C	-3.888497	-2.297031	0.155703
C	-3.364499	3.029160	-1.603678	C	-3.515550	0.459396	1.534348
C	-4.271877	1.007398	-2.759830	C	-5.225760	0.270638	-1.063339
H	-4.067105	-1.895548	-1.800988	H	-3.344760	-2.479301	1.100387
H	-2.873894	-2.473134	-0.631291	C	-3.242186	-3.175584	-0.916055
H	-4.537706	-3.026532	-0.529180	C	-5.342607	-2.720432	0.373723
H	-6.360943	-1.664540	0.365519	H	-3.537891	1.551672	1.369124
H	-6.169295	0.055979	0.726661	C	-2.188755	0.119125	2.211748

C	-4.685609	0.140761	2.465083	H	3.725749	-2.320499	2.093718
H	-6.113079	-0.013590	-0.474003	H	3.656885	-1.372454	3.588354
C	-5.180120	1.794057	-1.158814	H	2.221150	-1.512168	2.561677
C	-5.356219	-0.335249	-2.460164	C	3.169675	1.089681	2.491842
H	-3.672641	-2.985266	-1.910224	H	3.515313	2.026831	2.035489
H	-2.158705	-3.015673	-0.985931	H	2.069730	1.094926	2.475157
H	-3.410012	-4.240399	-0.696010	H	3.473970	1.111495	3.548035
H	-5.401362	-3.780873	0.656365	C	2.879306	1.514290	-2.285322
H	-5.848167	-2.144244	1.158634	H	3.265532	0.722474	-2.942757
H	-5.932340	-2.604716	-0.545641	H	1.788859	1.405047	-2.251108
H	-1.314812	0.411682	1.609841	H	3.110938	2.472558	-2.771877
H	-2.106151	0.607492	3.195325	C	5.020536	1.681511	-0.989549
H	-2.108699	-0.965428	2.384239	H	5.231369	2.668999	-1.423647
H	-5.657865	0.390196	2.019343	H	5.518110	1.638807	-0.011615
H	-4.704566	-0.926323	2.725932	H	5.504433	0.939895	-1.640411
H	-4.605776	0.696540	3.410032	H	0.971325	-1.592361	0.010082
H	-4.298673	2.122763	-1.730089	P	-3.712845	-1.668423	-0.092691
H	-6.060447	2.191799	-1.683173	C	-3.725216	-3.505902	-0.213781
H	-5.147593	2.277216	-0.172148	H	-3.177371	-3.821688	-1.107481
H	-6.243098	0.049480	-2.983632	H	-3.231980	-3.940510	0.661515
H	-4.479794	-0.086128	-3.074688	H	-4.751484	-3.889781	-0.271330
H	-5.436395	-1.429655	-2.437755	C	-4.850087	-1.408060	1.325942
C	0.236838	-0.288543	-2.850166	H	-5.812880	-1.907307	1.159765
H	1.237401	-0.325131	-3.279336	H	-4.388718	-1.807268	2.234807
H	0.050035	-1.267625	-2.397353	H	-5.017638	-0.337249	1.480370
H	-0.493311	-0.163458	-3.661790	C	-4.768650	-1.223669	-1.528234
C	2.264593	1.929887	-2.440304	H	-5.746725	-1.717725	-1.472448
H	2.551045	0.968091	-2.869857	H	-4.909062	-0.138846	-1.568691
H	2.197679	2.673413	-3.247037	H	-4.262895	-1.527679	-2.450384
H	3.087794	2.234769	-1.783873	N	0.257342	1.712656	0.024431
Zn	2.215933	-1.655936	-0.385732	H	1.118533	2.245368	0.053553
O	1.786134	-3.144773	1.034708				
C	0.657702	-3.326818	0.478025	P _{NH}			
O	0.360790	-2.726621	-0.593427	C	5.188983	-1.535326	0.091644
C	-0.352308	-4.219716	1.136063	C	4.209712	-2.526246	0.168733
H	-1.081594	-3.582603	1.654092	C	2.868772	-2.183110	0.144292
H	-0.900060	-4.798167	0.387593	C	2.494198	-0.838609	0.044038
H	0.120839	-4.878423	1.866902	C	3.464014	0.178142	-0.034848
O	3.144377	-1.439656	-2.251849	C	4.812494	-0.204813	-0.009874
C	4.262395	-1.305425	-1.659436	H	6.242202	-1.802452	0.110287
O	4.344949	-1.401699	-0.403833	H	4.494686	-3.572771	0.248190
C	5.478344	-0.993060	-2.481101	H	2.094074	-2.947506	0.200691
H	5.533819	-1.668738	-3.338889	H	5.584959	0.557438	-0.071668
H	5.379864	0.023961	-2.878068	C	0.666725	0.802345	-0.089296
H	6.387570	-1.059848	-1.881678	C	-0.679000	1.027450	-0.129696
N	-1.580950	2.077430	-0.582864	H	-0.963386	2.075751	-0.187592
H	-2.499867	2.153553	-0.169658	C	3.015599	1.561518	-0.138473
				C	1.683950	1.859965	-0.167990
10 _{NH}				C	4.100375	2.594007	-0.211188
C	-3.571345	3.339420	0.111703	H	3.728806	3.616461	-0.268779
C	-2.481992	4.201649	0.108854	H	4.752849	2.532265	0.669238
C	-1.180908	3.705614	0.076597	H	4.738139	2.425393	-1.088608
C	-0.979573	2.327048	0.049909	C	1.146522	3.252664	-0.284408
C	-2.075457	1.439379	0.051011	H	0.503042	3.344646	-1.169053
C	-3.360706	1.955464	0.080072	H	0.522083	3.500993	0.583650
H	-4.584897	3.733136	0.139806	H	1.922891	4.013514	-0.361356
H	-2.641523	5.277643	0.131628	Si	-2.138566	-0.119173	-0.014484
H	-0.328859	4.383852	0.072912	C	-3.591168	0.640102	-1.008341
H	-4.221991	1.287277	0.082424	C	-1.770008	-1.848786	-0.758762
C	0.240001	0.336019	0.010268	C	-2.616099	-0.338237	1.821725
C	1.268501	-0.534010	-0.025479	H	-3.510965	0.180761	-2.009048
Si	3.114185	-0.227133	-0.026749	C	-3.494177	2.153373	-1.198599
C	3.516098	1.426921	-0.899694	C	-4.964655	0.276323	-0.442041
H	3.094339	2.230075	-0.268532	H	-1.024246	-2.346786	-0.110481
C	3.719281	-0.146289	1.781864	C	-1.198468	-1.760867	-2.173183
H	4.820224	-0.081982	1.769795	C	-3.005611	-2.750416	-0.747402
C	3.995498	-1.644024	-0.964903	H	-3.564759	-0.898268	1.866791
H	4.042206	-1.299451	-2.012866	C	-1.551000	-1.133137	2.575206
Pd	-1.584962	-0.518518	-0.003571	C	-2.822350	1.018180	2.494835
C	5.428619	-1.875619	-0.483629	H	-3.504707	2.685782	-0.236372
H	5.445347	-2.270091	0.541850	H	-2.578583	2.445510	-1.725961
H	5.941697	-2.613366	-1.116797	H	-4.347123	2.530548	-1.780596
H	6.034158	-0.960907	-0.488579	H	-5.767871	0.635437	-1.101040
C	3.219164	-2.960053	-0.950298	H	-5.105522	-0.803768	-0.313995
H	3.764317	-3.746889	-1.490958	H	-5.126998	0.742435	0.539246
H	3.063351	-3.324929	0.075679	H	-0.266053	-1.185466	-2.220102
H	2.232330	-2.858933	-1.416469	H	-0.998567	-2.759823	-2.586220
C	3.315106	-1.407178	2.544067	H	-1.912079	-1.273336	-2.851827

C	-3.542465	-0.926518	-3.654352	H	4.387400	-2.125268	-4.972564
H	-2.671242	-1.433897	-3.219591	H	4.391825	-0.394645	-4.639287
H	-3.940010	-1.565573	-4.455255	H	2.747815	6.225682	-1.374051
H	-3.183507	-0.003425	-4.132592	H	3.548614	5.137775	-0.240145
C	-5.841633	0.008939	-3.244534	H	4.944494	-0.495107	4.246385
H	-6.634583	0.219849	-2.514738	H	5.375430	-1.006590	2.614226
H	-5.582128	0.958731	-3.733688	S	-1.713047	-3.269756	0.305301
H	-6.271394	-0.640873	-4.019484				
C	-2.150998	2.716836	-1.153758	TS_{45S-PCy3}			
H	-2.266514	2.822271	-0.066356	C	1.906292	4.834912	0.171869
H	-1.262664	2.083566	-1.311985	C	0.823828	5.546071	0.673146
H	-1.930730	3.712854	-1.566714	C	-0.412752	4.922324	0.791507
C	-4.555568	3.114858	-1.744108	C	-0.552273	3.581642	0.430086
H	-4.292298	4.061072	-2.236361	C	0.540919	2.826842	-0.027783
H	-5.470797	2.740941	-2.221560	C	1.757980	3.491116	-0.177011
H	-4.802034	3.353523	-0.700974	H	2.872274	5.319499	0.045175
Zn	-0.732838	0.200860	2.069091	H	0.932589	6.590729	0.955293
O	-1.318082	2.253661	2.066065	H	-1.275434	5.479922	1.152220
C	-0.309420	2.501495	2.788858	H	2.617693	2.964463	-0.583211
O	0.489523	1.576198	3.129759	C	-1.702035	1.276562	-0.222452
C	-0.061016	3.903975	3.262048	C	-2.591891	0.284269	-0.484409
H	1.012066	4.091285	3.355520	Si	-4.437515	0.182906	-0.099425
H	-0.525387	4.625384	2.585158	C	-4.667278	0.472748	1.774106
H	-0.509305	4.026113	4.254010	H	-4.458477	1.544110	1.932572
O	-2.161099	-0.847932	3.167688	C	-5.489423	1.415851	-1.111818
C	-1.307389	-1.756426	3.401190	H	-6.497362	0.967697	-1.125605
O	-0.130492	-1.674525	2.940565	C	-5.004348	-1.603539	-0.526430
C	-1.702219	-2.962064	4.201728	H	-4.742856	-2.211172	0.358367
H	-0.854824	-3.324511	4.788693	Pd	0.298722	0.857595	-0.464900
H	-2.554852	-2.742571	4.847179	C	-6.518392	-1.702513	-0.729195
H	-1.992765	-3.756155	3.503185	H	-6.820831	-1.205040	-1.661561
H	0.630673	-3.712755	1.882167	H	-6.833907	-2.751856	-0.812241
P	1.881193	0.582539	-0.522096	H	-7.096222	-1.248604	0.084818
C	2.700049	-0.537600	-1.770965	C	-4.310615	-2.238787	-1.731620
C	1.983316	2.345301	-1.128382	H	-4.702545	-3.249169	-1.914244
C	2.795368	0.475180	1.091132	H	-4.469447	-1.655991	-2.649695
C	2.045707	-0.330369	-3.143408	H	-3.226300	-2.350753	-1.604869
C	4.227799	-0.561191	-1.872261	C	-4.990861	1.503634	-2.553777
H	2.384421	-1.535951	-1.414877	H	-4.965132	0.524368	-3.050691
C	1.497347	3.285259	-0.014793	H	-5.632214	2.161232	-3.157667
C	3.307327	2.815848	-1.737851	H	-3.972147	1.915194	-2.591049
H	1.223472	2.380528	-1.931122	C	-5.621440	2.811710	-0.507786
C	2.806597	-0.983858	1.559507	H	-5.991964	2.791914	0.525084
C	4.173379	1.120156	1.261602	H	-4.659236	3.339027	-0.502715
H	2.111367	1.013543	1.768872	H	-6.320999	3.422506	-1.096268
C	2.529095	-1.362520	-4.156247	C	-3.658580	-0.321736	2.602205
H	2.286505	0.676210	-3.524264	H	-3.762814	-1.405239	2.434260
H	0.949080	-0.375063	-3.041729	H	-2.620855	-0.040777	2.374273
C	4.678755	-1.611074	-2.885775	H	-3.808070	-0.155263	3.678485
H	4.613793	0.424381	-2.176373	C	-6.089690	0.189372	2.254051
H	4.668381	-0.780980	-0.891377	H	-6.214882	0.467085	3.310284
C	1.446845	4.734510	-0.486559	H	-6.847881	0.737458	1.678433
H	2.178752	3.214979	0.850047	H	-6.326410	-0.881270	2.177189
H	0.506361	2.966189	0.344354	Zn	-1.577944	-1.413712	0.067353
C	3.224193	4.273027	-2.186280	O	-1.738982	-0.389044	-2.907457
H	4.123691	2.708135	-1.008711	C	-0.612247	-0.959596	-2.707450
H	3.572269	2.180253	-2.593188	O	-0.268227	-1.471497	-1.605770
C	3.257668	-1.080213	3.010540	C	0.357977	-0.971206	-3.844035
H	3.485131	-1.578001	0.922071	H	0.829500	-1.953982	-3.931764
H	1.806220	-1.424598	1.451546	H	-0.123946	-0.684620	-4.779890
C	4.617744	1.007204	2.720181	H	1.145512	-0.241359	-3.609347
H	4.916800	0.636180	0.610045	O	-0.544598	-2.193875	1.737763
H	4.147564	2.180146	0.975648	C	-1.218733	-3.259023	1.587639
C	4.049776	-1.368990	-4.252246	O	-2.061394	-3.353158	0.643382
H	2.077322	-1.166792	-5.137265	C	-0.997425	-4.424687	2.501514
H	2.179736	-2.358607	-3.841226	H	-0.579394	-4.097897	3.455977
H	5.774083	-1.618787	-2.957905	H	-1.929357	-4.974272	2.651143
H	4.380390	-2.608173	-2.521050	H	-0.282439	-5.107475	2.025366
C	2.792747	5.180715	-1.042036	H	-2.199057	-0.149599	-1.901773
H	1.130967	5.384057	0.340663	S	-2.139906	2.823705	0.490645
H	0.680481	4.833512	-1.272559	P	2.611203	-0.101787	-0.087573
H	4.190817	4.592943	-2.596419	C	2.454299	-1.911300	0.374167
H	2.492881	4.356898	-3.006801	C	3.893348	-0.071866	-1.444669
C	4.628403	-0.441123	3.196612	C	3.196452	0.829778	1.421512
H	3.263246	-2.131224	3.331535	C	2.441387	-2.818858	-0.863314
H	2.517063	-0.565868	3.641813	C	3.384520	-2.511684	1.434059
H	5.607189	1.466026	2.846972	H	1.439571	-1.946371	0.803344
H	3.915950	1.584518	3.344162	C	4.041014	1.309416	-2.088135

C	5.271476	-0.688070	-1.187136	C	5.265661	0.997211	3.320791
H	3.395062	-0.710118	-2.200918	H	6.198666	0.643288	2.862503
C	2.162132	0.642516	2.544202	H	5.183064	2.074199	3.115963
C	4.631612	0.681239	1.933282	H	5.371528	0.889076	4.409162
H	3.092502	1.878035	1.097866	C	2.845763	2.185674	-0.996728
C	1.933904	-4.207521	-0.489282	H	3.256218	1.577281	-1.814706
H	3.461933	-2.907592	-1.272612	H	1.804659	1.858368	-0.847367
H	1.805084	-2.393461	-1.646813	H	2.825176	3.232355	-1.335470
C	2.885126	-3.902902	1.821116	C	5.030341	2.732218	0.099264
H	4.415682	-2.579608	1.049939	H	4.898488	3.801115	-0.117204
H	3.425144	-1.884229	2.331250	H	5.677153	2.654414	0.982516
C	4.850530	1.225064	-3.379528	H	5.580693	2.301518	-0.748316
H	4.550523	1.989907	-1.383564	Zn	0.312848	-0.838411	-2.169226
H	3.050538	1.742266	-2.290674	O	2.162555	-0.542146	-3.146905
C	6.057847	-0.794361	-2.491205	C	1.641864	0.433681	-3.761336
H	5.836083	-0.057034	-0.486119	O	0.425704	0.744540	-3.578424
H	5.182145	-1.673974	-0.714011	C	2.468208	1.248749	-4.713590
C	2.439566	1.599261	3.697124	H	2.062462	1.151600	-5.725414
H	2.181226	-0.393323	2.918069	H	2.396933	2.305600	-4.436592
H	1.147783	0.804876	2.148560	H	3.511393	0.925788	-4.701646
C	4.877621	1.622581	3.112404	O	0.283921	-3.026524	-2.062823
H	4.837961	-0.354535	2.239019	C	-0.904013	-2.971977	-2.500995
H	5.343950	0.918507	1.133485	O	-1.450290	-1.857881	-2.748090
C	2.787476	-4.825739	0.612164	C	-1.686452	-4.236262	-2.710993
H	1.916517	-4.857843	-1.373622	H	-2.314342	-4.409275	-1.827344
H	0.888047	-4.116045	-0.149869	H	-2.351421	-4.132523	-3.571879
H	3.538857	-4.339716	2.587415	H	-1.019813	-5.092052	-2.839677
H	1.888974	-3.790663	2.280268	H	-0.571001	-4.926301	0.011012
C	6.208405	0.571886	-3.150437	P	-1.656026	1.021983	0.201620
H	4.970082	2.224488	-3.816798	C	-2.030470	0.945610	2.033972
H	4.281867	0.629899	-4.113326	C	-1.611055	2.810961	-0.323114
H	7.041870	-1.243148	-2.303989	C	-3.030120	0.144676	-0.695797
H	5.527791	-1.477297	-3.176026	C	-0.987905	1.764128	2.806265
C	3.857472	1.417730	4.224713	C	-3.438331	1.218353	2.571018
H	1.703655	1.446413	4.496576	H	-1.813336	-0.117725	2.246062
H	2.306850	2.634712	3.340572	C	-1.481465	2.893064	-1.849132
H	5.899547	1.486753	3.490021	C	-2.692411	3.759281	0.201373
H	4.811674	2.663519	2.755678	H	-0.645264	3.149725	0.097686
H	2.390953	-5.806859	0.906888	C	-3.203137	-1.251948	-0.081177
H	3.800634	-5.007538	0.217105	C	-4.372209	0.865560	-0.855761
H	6.758013	0.486734	-4.096486	H	-2.613073	-0.008544	-1.706587
H	6.813514	1.219585	-2.495361	C	-1.047838	1.449677	4.296116
H	4.054770	2.106087	5.056558	H	-1.172120	2.840559	2.653869
H	3.962982	0.397301	4.629572	H	0.022569	1.563073	2.412212
2_{NH}-PCy₃				C	-3.493194	0.903550	4.065379
C	-2.362910	-3.852055	2.700798	H	-3.719524	2.269339	2.404758
C	-1.496266	-2.855284	3.141492	C	-4.181476	0.607283	2.042584
C	-0.311284	-2.587917	2.463221	H	-1.234848	4.327714	-2.302162
C	0.013852	-3.332569	1.328481	H	-2.411365	2.531998	-2.318344
C	-0.841053	-4.346248	0.892704	H	-0.681028	2.234007	-2.211657
C	-2.024685	-4.598272	1.574871	C	-2.440849	5.187758	-0.278812
H	-3.288961	-4.049563	3.234422	H	-3.684309	3.429431	-0.140673
H	-1.742617	-2.272695	4.028171	H	-2.721116	3.742134	1.298457
H	0.358174	-1.799417	2.804344	C	-4.211909	-2.082287	-0.864718
H	-2.688231	-5.384478	1.220072	H	-3.545828	-1.165469	0.963899
C	1.774029	-1.888812	0.590468	H	-2.229675	-1.765251	-0.045169
C	2.432022	-0.827492	0.563964	C	-5.367827	0.000187	-1.625840
Si	3.906056	0.259819	0.908044	H	-4.796073	1.118396	0.127471
C	3.673465	2.043998	0.279011	H	-4.229215	1.815930	-1.386038
H	3.134654	2.566414	1.090334	C	-2.448468	1.691200	4.847929
C	4.039342	0.246296	2.806886	H	-0.306035	2.047882	4.842177
H	4.146026	-0.820755	3.066011	H	-0.768520	0.392457	4.445860
C	5.391498	-0.603947	0.103829	H	-4.499079	1.102912	4.456945
H	6.265514	0.052678	0.250716	H	-3.312991	-0.176477	4.201964
Pd	0.470881	0.063766	0.207449	C	-2.330189	5.257753	-1.796683
C	5.676001	-1.940906	0.784986	H	-1.164100	4.364443	-3.396277
H	4.806072	-2.610075	0.722789	H	-0.260106	4.666200	-1.913394
H	6.514380	-2.458713	0.298885	H	-3.236951	5.850180	0.085549
H	5.930563	-1.824451	1.846036	H	-1.501636	5.554558	0.167030
C	5.168485	-0.801382	-1.396009	C	-5.549800	-1.361633	-0.968375
H	6.013973	-1.335762	-1.851147	H	-4.330559	-3.064563	-0.385030
H	4.260763	-1.387481	-1.590156	H	-3.808727	-2.255240	-1.875362
H	5.047795	0.146057	-1.937477	H	-6.327942	0.525925	-1.710362
C	2.768643	0.767539	3.472695	H	-4.995766	-0.144272	-2.652480
H	1.876990	0.218389	3.139562	H	-2.493395	1.436198	5.914508
H	2.824022	0.683110	4.567324	H	-2.680850	2.766297	4.774315
H	2.604632	1.831118	3.242307	H	-2.145632	6.290137	-2.120617
				H	-3.292223	4.956139	-2.243016

H	-6.274510	-1.965179	-1.529927	C	-1.107509	-3.996113	3.052148
H	-5.970994	-1.224131	0.041964	H	-0.472944	-3.603922	3.850521
N	1.183405	-3.086206	0.574487	H	-2.056310	-4.359580	3.450842
H	1.125011	-3.480835	-0.370100	H	-0.579768	-4.839990	2.591334
TS_{45NH-PCy3}				H	-2.173260	-0.157760	-1.787343
C	1.526462	5.089434	0.344424	P	2.570536	-0.106384	-0.121869
C	0.288391	5.689864	0.527222	C	2.477916	-1.922526	0.271139
C	-0.877151	4.933291	0.424024	C	3.724964	0.092298	-1.574861
C	-0.770072	3.577387	0.140380	C	3.283805	0.753317	1.371966
C	0.468662	2.937939	-0.033241	C	2.112962	-2.717295	-0.986613
C	1.612384	3.719010	0.068058	C	3.598889	-2.627436	1.040061
H	2.436395	5.682602	0.407659	H	1.591888	-1.954270	0.924420
H	0.221821	6.753078	0.746015	C	3.945364	1.578092	-1.875671
H	-1.854406	5.394514	0.560736	C	5.048596	-0.678335	-1.559829
H	2.596835	3.283780	-0.093160	H	3.118351	-0.313481	-2.406546
C	-1.622043	1.444660	-0.306697	C	2.408239	0.415462	2.587706
C	-2.456688	0.379156	-0.512028	C	4.776442	0.638958	1.692642
Si	-4.287885	0.393551	-0.025191	H	3.089777	1.815138	1.150321
C	-4.374354	1.075451	1.763041	C	1.654564	-4.120644	-0.609734
H	-4.072108	2.135423	1.703410	H	2.987140	-2.785560	-0.856274
C	-5.327402	1.495797	-1.195752	H	1.315448	-2.208879	-1.543387
C	-6.370553	1.337309	-0.872864	C	3.141808	-4.037276	1.416085
C	-5.023502	-1.373389	-0.062434	H	4.518343	-2.682549	0.435937
H	-4.727321	-1.831108	0.896701	H	3.855740	-2.076627	1.953493
Pd	0.316939	0.911235	-0.370223	C	4.740024	1.778828	-3.161661
C	-6.554106	-1.351575	-0.121506	H	4.497873	2.042450	-1.040072
H	-6.909369	-0.984283	-1.094319	C	2.975656	2.091615	-1.940468
H	-6.957789	-2.366235	0.000385	H	5.824935	-0.458141	-2.856117
H	-7.011262	-0.722814	0.651300	H	5.666547	-0.353974	-0.709699
C	-4.501173	-2.283355	-1.174584	H	4.864703	-1.750234	-1.416550
H	-4.995488	-3.263692	-1.126483	C	2.785162	1.281506	3.783302
H	-4.696699	-1.868395	-2.172607	H	2.525331	-0.646700	2.857406
H	-3.425884	-2.482835	-1.110070	H	1.346702	0.552096	2.329659
C	-5.200525	1.041312	-2.649568	C	5.128107	1.491233	2.911407
H	-5.550923	0.013155	-2.800126	H	5.056757	-0.407358	1.884623
H	-5.785873	1.686984	-3.319864	H	5.376521	0.970008	0.834158
H	-4.154976	1.080905	-2.986368	C	2.730854	-4.845511	0.190035
C	-5.040665	2.991943	-1.102186	H	1.383526	-4.687755	-1.510300
H	-5.075053	3.372573	-0.070741	H	0.736394	-4.032037	-0.007114
H	-4.057960	3.228575	-1.535786	H	3.933412	-4.555518	1.973262
H	-5.774460	3.571933	-1.678931	H	2.278674	-3.949512	2.097299
C	-3.378854	0.372924	2.687731	C	6.062192	1.023573	-3.116793
H	-3.564074	-0.710817	2.731712	H	4.907175	2.849345	-3.335896
H	-2.338525	0.520077	2.365683	H	4.142923	1.413341	-4.012603
H	-3.458860	0.754482	3.715471	H	6.776004	-1.004998	-2.819852
C	-5.777170	1.033546	2.366337	H	5.251443	-0.884635	-3.695442
H	-5.799935	1.526390	3.348587	C	4.265224	1.135762	4.115707
H	-6.526511	1.528197	1.733677	H	2.164107	1.019035	4.649167
H	-6.106506	-0.002664	2.524298	H	2.563742	2.335025	3.544695
Zn	-1.578627	-1.375667	0.169835	H	6.194139	1.380797	3.149417
O	-1.857499	-0.656821	-2.851337	H	4.972279	2.553207	2.660556
C	-1.181226	-1.724878	-2.691142	H	2.385771	-5.844283	0.488408
O	-1.000265	-2.305498	-1.587009	H	3.614821	-4.999730	-0.451143
C	-0.516082	-2.289770	-3.910266	H	6.621691	1.167063	-4.049956
H	0.455272	-1.790963	-4.023512	H	6.688377	1.437083	-2.308823
H	-0.339034	-3.361111	-3.790528	H	4.533765	1.760724	4.977106
H	-1.103386	-2.083100	-4.807523	H	4.467212	0.092257	4.409942
O	-0.386650	-2.152316	1.711704	N	-1.875028	2.734864	-0.005707
C	-1.331223	-2.955065	1.998709	H	-2.822421	3.093572	0.064826
O	-2.426950	-2.899967	1.371460				