Supporting Material for The Mechanism for the Hydrogenation of Ketones Catalyzed by Knölker's Iron-Catalyst

Xi Lu,[a] Yawei Zhang,[b] Peng Yun,[b] Mingtao Zhang*[b] and Tonglei Li[c]

[a] *Department of Chemistry, Nankai University, Tianjin 300071, People's Republic of China;*

[b] *Computational Center for Molecular Science, College of Chemistry, Nankai University, Tianjin 300071, People's Republic of China;* [c] *Department of Industrial and Physical Pharmacy College of Pharmacy Purdue University, West Lafayette, Indiana (USA);*

E-mail: zhan1301@purdue.edu.

Gaussian 09, Revision B.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

Table of Contents

Figure S1. The geometry of 1a optimized at the theory level of B3LYP/LACVP*

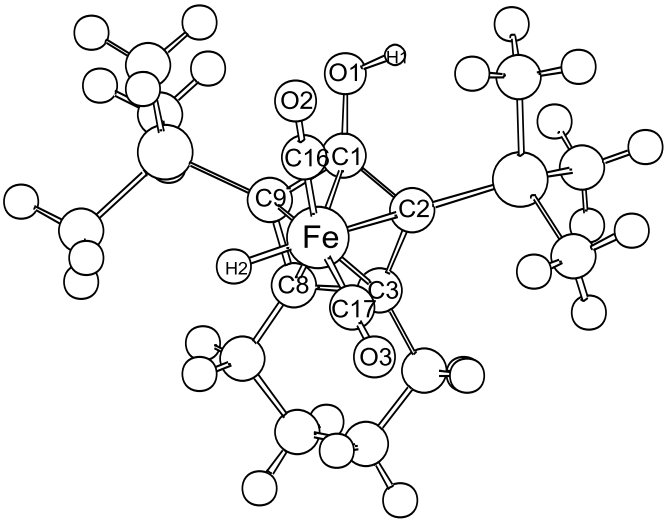


Table S1. Differences of bond lengths between crystal and B3LYP-optimized structure in gas (Å)

Bonds	Bond Lengths (Å)	
	Crystal	B3LYP/LACVP*
Fe-C1	2.135	2.180
Fe-C2	2.149	2.165
Fe-C3	2.099	2.120
Fe-C8	2.098	2.125
Fe-C9	2.109	2.139
Fe-H2	1.384	1.505
Fe-C16	1.752	1.761
Fe-C17	1.741	1.754
C16-O2	1.143	1.155
C17-O3	1.153	1.156
C1-C2	1.437	1.434
C2-C3	1.452	1.455
C3-C8	1.430	1.423
C8-C9	1.445	1.447
C1-C9	1.445	1.436
C1-O1	1.366	1.357
O1-H1	0.750	0.970
C2-Si1	1.888	1.887
C9-Si2	1.887	1.896
SRE[a]	0.0036	
RMSE[b]	0.0598	

a. Square Root Error; b. Root Mean Square Error.

Table S2. Differences of bond angles between crystal and B3LYP-optimized structure in gas (degree, º)

Bond Angles	Degrees of Bond Angles (º)	
	Crystal	B3LYP-optimized
C16-Fe-C17	95.0	95.8
C16-Fe-H2	86.3	84.7
C17-Fe-H2	79.9	83.4
C1-O1-H1	112.2	109.3
C9-C1-C2	112.4	112.1
C1-C2-C3	104.1	104.2
C2-C3-C8	109.7	109.6
C3-C8-C9	109.3	109.0
C8-C9-C1	104.4	104.9
SRE[a]	2.6792	
RMSE[b]	1.6368	
a. Square Root Error; b. Root Mean Square Error		

Table S3. B3LYP-optimized electronic energies for other high-spin states of 1a in gas

Unit	Singlet	Triplet	Quintet	Septet
Hartree	-1592.867843	-1592.814585	-1592.788992	-1592.705847
kcal/mol	0	33.4	49.5	101.7

Table S4. B3LYP-calculated energies and thermochemistry in gas at 298 K and 1 atm (Hartree)

Complexes	E_{SCF}(B3LYP)	H_{corr}(B3LYP)	G_{corr}(B3LYP)
1a	-1592.867843	0.443512	0.352330
1a/1bTS	-1592.861640	0.442317	0.352954
1b	-1592.866688	0.443442	0.352987
1b/1cTS	-1592.862737	0.442393	0.354741
1c	-1592.868087	0.443541	0.352904
1c/1aTS	-1592.859855	0.442490	0.355153
2	-1707.376424	0.476835	0.377231
2/3TS	-1707.321199	0.475760	0.380861

3	-1707.339338	0.478580	0.383551
3/4TS	-1707.330809	0.476844	0.380466
4	-1707.412043	0.481411	0.385139
5	-1591.654314	0.422861	0.332132
6	-1479.482475	0.431543	0.344649
7	-1594.026551	0.465482	0.374729
7/8TS	-1594.025925	0.464440	0.374774
8	-1594.036041	0.467885	0.377305
9	-1707.392291	0.480586	0.384542
9/10TS	-1707.379462	0.479464	0.384620
10	-1707.405471	0.479771	0.383254
10/4TS	-1707.403873	0.476046	0.380801
11	-1707.376350	0.476251	0.374079
11/12TS	-1707.313564	0.474622	0.378463
12	-1707.379280	0.479939	0.385038
12/13TS	-1707.313106	0.476192	0.380913
13	-1707.378286	0.480271	0.382828
1b/14TS	-1707.329941	0.475702	0.380266
14	-1707.367163	0.481422	0.386992
14/10TS	-1707.357769	0.480452	0.385728
1b/15TS	-1707.370457	0.474057	0.379375
1b/16TS	-1977.739167	0.587882	0.480533
15	-1707.386911	0.479839	0.383169
16	-1977.751712	0.594861	0.484745
17	-1977.779509	0.596669	0.486439
CH_2O	-114.500473	0.030635	0.005161
CH_3OH	-115.714407	0.055708	0.028748
$PhCOCH_3$	-384.895995	0.147220	0.105870
$PhCH(OH)CH_3$	-386.087174	0.170885	0.128007
CO	-113.309454	0.008336	-0.014107

Table S5. Single-point energies[a] obtained at the M06/6-311+G* level in toluene (Hartree)

Complexes	E(M06) + ΔG(sol,M06)

1a	-2732.665831
1a/1bTS	-2732.658265
1b	-2732.664422
1b/1cTS	-2732.658581
1c	-2732.665953
1c/1aTS	-2732.655736
2	-2847.146393
2/3TS	-2847.08874
3	-2847.103926
3/4TS	-2847.092869
4	-2847.179603
5	-2731.452745
6	-2619.299426
7	-2733.816645
7/8TS	-2733.817006
8	-2733.824903
9	-2847.160124
9/10TS	-2847.143547
10	-2847.170441
10/4TS	-2847.166597
11	-2847.144564
11/12TS	-2847.083535
12	-2847.149961
12/13TS	-2847.083941
13	-2847.150477
1b/14TS	-2847.101808
14	-2847.13826
14/10TS	-2847.122305
1b/15TS	-2847.138985
1b/16TS	-3117.362709
15	-2847.157678
16	-3117.378975
17	-3117.403912
CH_2O	-114.470524
CH_3OH	-115.680336
$PhCOCH_3$	-384.710495

$PhCH(OH)CH_3$	-385.899832
CO	-113.281197

a. single-point calculations were performed at the B3LYP-optimized structures

Table S6. Solvation single-point energies (Hartree) for hydrogenation of $PhCOCH_3$ obtained at different theory levels in toluene

Methods/Basis Sets	1a	$PhCOCH_3$	1b/16TS
	E(methods) + ΔG(sol, methods)		
B3LYP/LACVP*(Gas)[a]	-1592.515513	-384.790125	-1977.258634
B3LYP/LACVP*(SMD)	-1592.878580	-384.907254	-1977.757274
B3LYP/6-31g**,Lanl2dz(SMD)[b]	-1592.926264	-384.919419	-1977.818073
B3LYP/6-311+g*,Lanl2dz(SMD)	-1593.167832	-385.001051	-1978.139960
B3LYP/6-311+g*(SMD)	-2733.447585	-385.001051	-3118.418172
B3LYP/6-311+g**(SMD)	-2733.491213	-385.013667	-3118.476300
B3LYP/6-311++g**,Lanl2dz(SMD)	-1593.213545	-385.013760	-1978.199186
M06/LACVP*(SMD)	-1592.211110	-384.627952	-1976.819279
M06/LACVP*(PCM)[c]	-1592.164971	-384.611132	-1976.757782
M06/6-31g**,Lanl2dz(SMD)	-1592.256571	-384.639053	-1976.877467
M06/6-31g**(SMD)	-2732.376140	-384.639053	-3117.007704
M06/6-311+g*(SMD)	-2732.665831	-384.710495	-3117.362709

a. B3LYP-optimized energies in gas. b. SMD single-point calculations were performed at the B3LYP-optimized structures. c. PCM single-point calculations were performed at the B3LYP -optimized structures.

Table S7. The bond distances involved hydrogen-transfer of the geometries on the IRC of 1b/15TS. All units are Å.

IRC	H-CH_2O	Fe-H	CpO-H	H-OCH_2
9.85898	1.14542	1.83694	1.7082	0.99206
9.5947	1.14557	1.83723	1.70808	0.99188
9.3543	1.14531	1.83727	1.70706	0.99201
9.09021	1.1455	1.83786	1.70743	0.99194
8.84039	1.14532	1.83813	1.70656	0.99194
8.57143	1.14528	1.83846	1.70662	0.99208
8.32913	1.1451	1.83896	1.70613	0.99223
8.065	1.14494	1.83922	1.70606	0.99166
7.80958	1.14422	1.83953	1.70571	0.99203

7.5454	1.14529	1.83997	1.7052	0.99183
7.29457	1.14472	1.84039	1.70532	0.99227
7.04266	1.14463	1.84084	1.7044	0.99158
6.79641	1.14473	1.84169	1.70419	0.99208
6.54936	1.14417	1.84308	1.70393	0.99216
6.30922	1.14344	1.84492	1.70349	0.99214
6.07332	1.14374	1.84724	1.70221	0.99159
5.83386	1.1422	1.85061	1.70149	0.99247
5.59618	1.1416	1.85411	1.69975	0.99205
5.35619	1.14015	1.8571	1.69648	0.99217
5.09815	1.13974	1.85742	1.69247	0.99294
4.84888	1.14073	1.85488	1.68764	0.99255
4.59234	1.1394	1.84948	1.68223	0.99294
4.34292	1.13682	1.84329	1.67735	0.99338
4.09395	1.13693	1.83739	1.67305	0.9939
3.83209	1.13652	1.83159	1.67191	0.99371
3.60713	1.13637	1.82648	1.67189	0.99409
3.34861	1.13669	1.81934	1.6686	0.99448
3.10888	1.13645	1.80923	1.65654	0.99505
2.88729	1.13827	1.79638	1.63039	0.99659
2.63839	1.1401	1.78377	1.59469	0.99867
2.37417	1.13871	1.77285	1.55377	1.00173
2.1087	1.14066	1.76239	1.51079	1.00481
1.84571	1.1464	1.75286	1.46691	1.00886
1.59949	1.15462	1.74512	1.42435	1.0164
1.44631	1.16829	1.73658	1.38815	1.03435
1.30249	1.19103	1.72015	1.33125	1.08387
1.03823	1.23236	1.68856	1.2137	1.20495
0.78642	1.27779	1.6559	1.11741	1.3183
0.52934	1.32848	1.62644	1.0658	1.39972
0.26508	1.38061	1.60321	1.04149	1.45449
0.00000	1.43583	1.58192	1.02671	1.49588
-0.26382	1.48959	1.56518	1.01714	1.52848
-0.53078	1.5424	1.55033	1.01203	1.55662
-0.79787	1.59248	1.53939	1.00513	1.58021
-1.06445	1.64207	1.52862	0.99935	1.60292
-1.33238	1.68722	1.52319	0.99728	1.62037
-1.59982	1.72935	1.51842	0.99375	1.63826
-1.86764	1.76939	1.5159	0.99173	1.65367
-2.13557	1.80706	1.51545	0.99103	1.66651
-2.40113	1.84527	1.51183	0.9884	1.68222

-2.66824	1.88011	1.51163	0.98739	1.69447
-2.93621	1.91355	1.51256	0.987	1.70561
-3.2036	1.94581	1.51288	0.98638	1.71735
-3.47003	1.9812	1.51039	0.98438	1.73057
-3.73693	2.01272	1.51069	0.98357	1.74088
-4.00487	2.04232	1.5124	0.98403	1.74939
-4.27116	2.0744	1.51109	0.98218	1.76178
-4.53796	2.10368	1.51148	0.98135	1.7717
-4.8049	2.13115	1.51233	0.98282	1.77941
-5.06366	2.15772	1.5125	0.98235	1.7891
-5.32447	2.18197	1.51339	0.9813	1.79835
-5.57879	2.20597	1.51261	0.97978	1.80697
-5.83708	2.22682	1.5129	0.97974	1.81285
-6.09243	2.24734	1.51245	0.98077	1.81759
-6.35311	2.26708	1.5129	0.97958	1.82145
-6.60261	2.28435	1.51356	0.98038	1.82457
-6.85462	2.30532	1.51298	0.98026	1.82817
-7.11838	2.32517	1.51262	0.97989	1.83204
-7.37005	2.34485	1.51255	0.98047	1.83435
-7.63378	2.36591	1.51244	0.98029	1.83737
-7.89669	2.38748	1.51254	0.97963	1.84066

Figure S2. Free energy Δ*G*(gas) profile for the $\eta^5 \rightarrow \eta^2$ ring slippage mechanism at the B3LYP level in gas, ( ) indicated Δ*H*(gas). (kcal/mol)

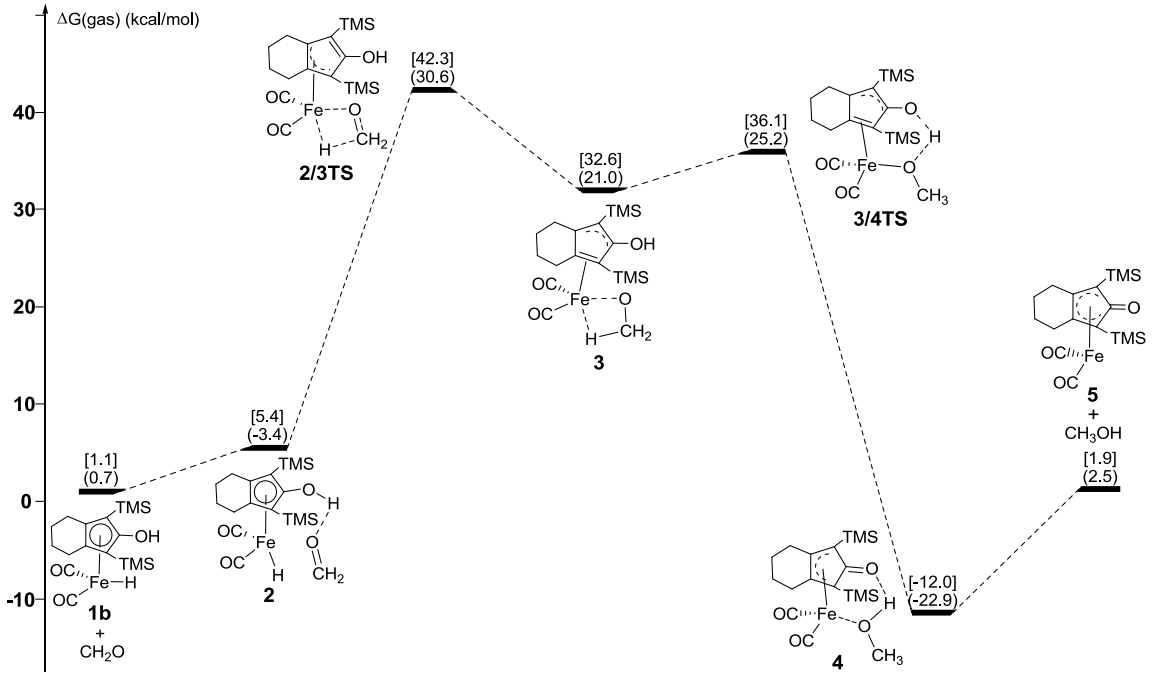


Figure S3. Free energy Δ*G*(gas) profile for the CO leaving mechanism at the B3LYP level in gas, ( ) indicated Δ*H*(gas). (kcal/mol)

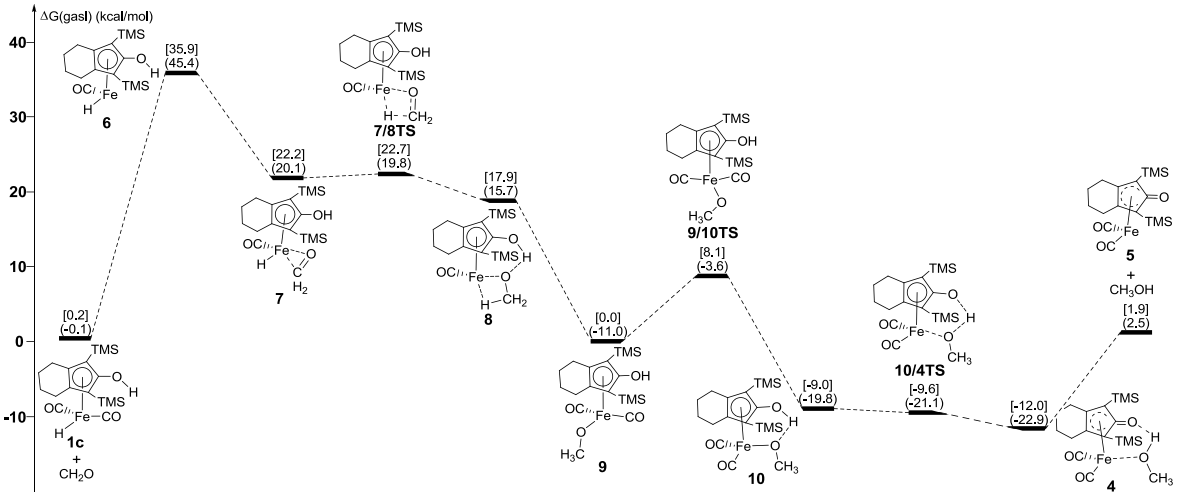


Figure S4. Free energy Δ*G*(gas) profile for the single proton-transfer mechanism at the B3LYP level in gas, ( ) indicated Δ*H*(gas). (kcal/mol)

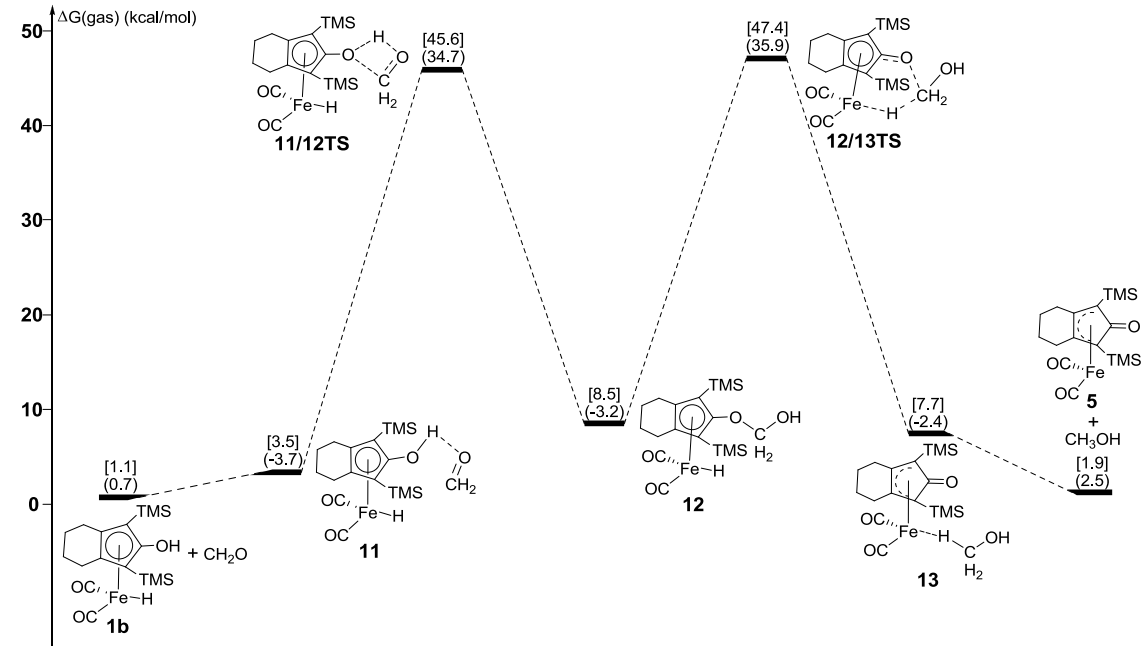


Figure S5. Free energy Δ*G*(gas) profile for the single hydride-transfer mechanism at the B3LYP level in gas, ( ) indicated Δ*H*(gas). (kcal/mol)

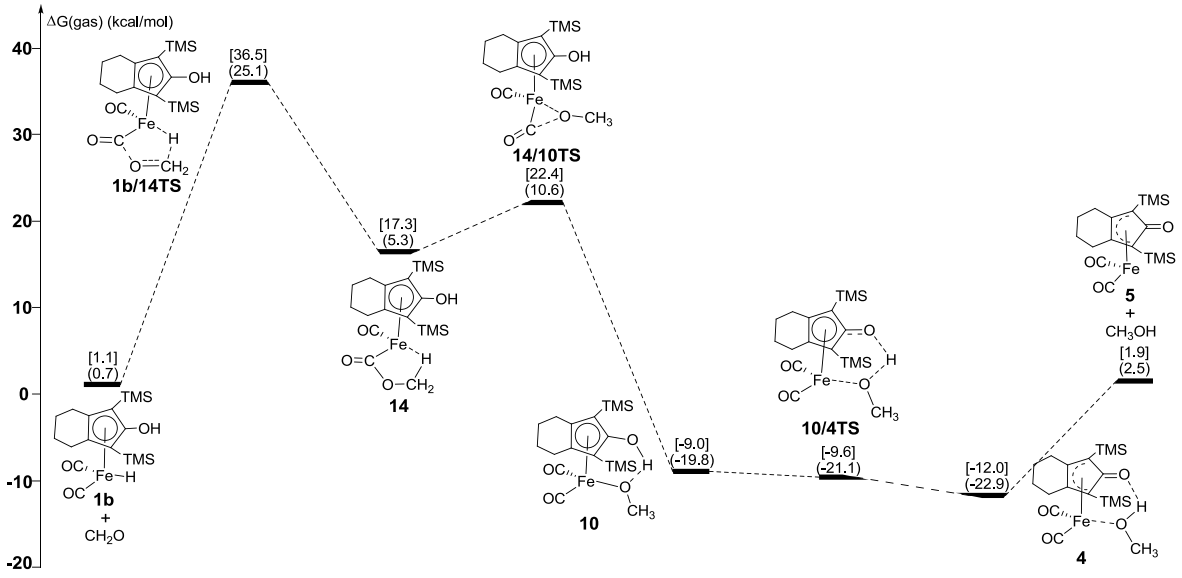


Figure S6. Free energy Δ*G*(gas) profile forhe concerted hydrogen-transfer mechanism

at the B3LYP level in gas, ( ) indicated Δ*H*(gas). (kcal/mol)

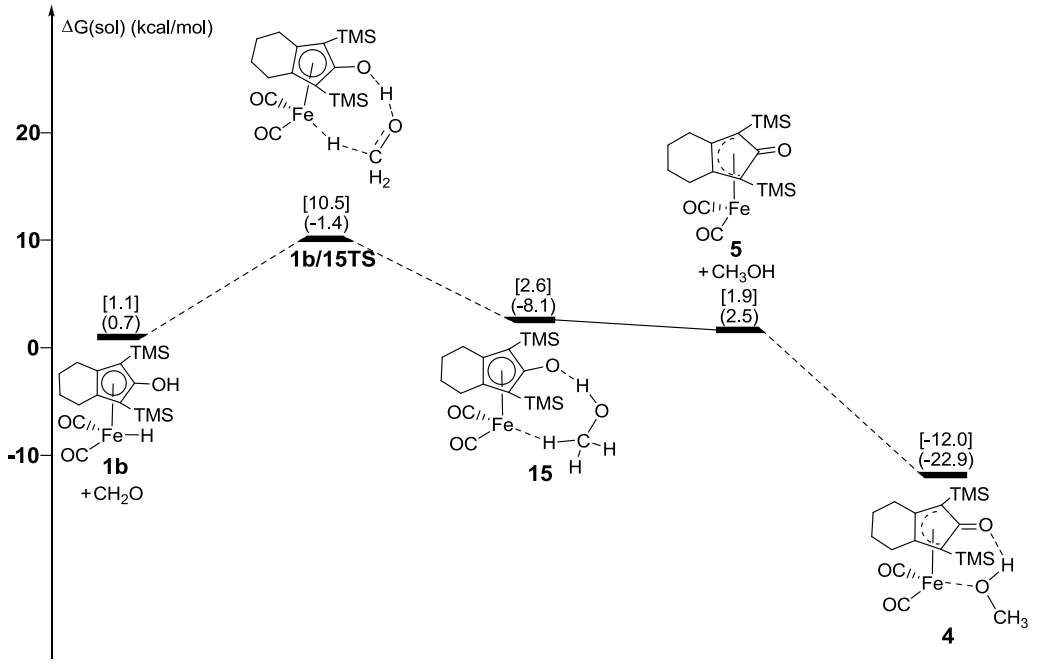
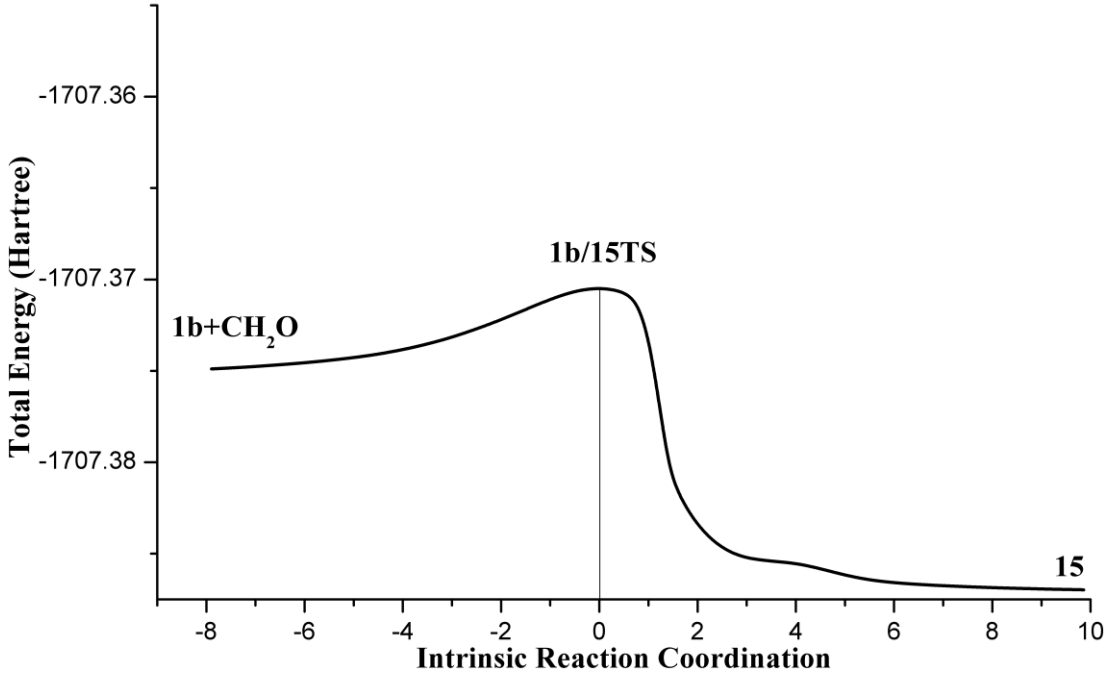


Figure S7. The Intrinsic Rection Coordination for the transition state 1b/15TS



Cartesian Coordinates of B3LYP-Optimized Structures in Gas

1a

Fe	0.011862	0.134299	1.148747
C	0.186603	-1.008419	-0.700054
O	0.384900	-2.342879	-0.848068
H	-0.465820	-2.803406	-0.779524
C	-1.071629	-0.320872	-0.669618
C	-0.709066	1.086240	-0.603530
C	-1.623162	2.281894	-0.709098
H	-2.526853	2.146591	-0.105339
H	-1.960248	2.364098	-1.753984
C	-0.903586	3.581682	-0.312557
H	-1.531046	4.441119	-0.576932
H	-0.767589	3.608972	0.776702
C	0.461701	3.682687	-1.006350
H	0.928768	4.651989	-0.796095
H	0.310313	3.636502	-2.094592
C	1.412523	2.550626	-0.572140
H	2.259013	2.500616	-1.267966
H	1.835577	2.775041	0.412629
C	0.707589	1.210985	-0.546127
C	1.296256	-0.110877	-0.543573
Si	-2.804052	-1.045609	-0.850607
C	-3.504890	-0.575924	-2.547450
H	-3.597835	0.510813	-2.658774
H	-4.502199	-1.008658	-2.695550
H	-2.859798	-0.936810	-3.357516
C	-3.971621	-0.454299	0.514690
H	-4.096634	0.633830	0.524152
H	-3.605275	-0.753326	1.503137
H	-4.966341	-0.896794	0.375598
C	-2.738946	-2.947222	-0.746892
H	-2.298567	-3.313412	0.190189
H	-2.222866	-3.417876	-1.594584
H	-3.766837	-3.330349	-0.770958
Si	3.128094	-0.599551	-0.515151
C	3.730401	-0.698251	-2.312384
H	4.790615	-0.977522	-2.357623
H	3.618083	0.261564	-2.831458

H	3.164462	-1.448920	-2.876858
C	4.147831	0.689185	0.425759
H	5.176562	0.325927	0.544776
H	3.735698	0.860450	1.426760
H	4.198608	1.654658	-0.088394
C	3.365582	-2.277450	0.320728
H	4.428746	-2.549668	0.312579
H	2.805635	-3.065580	-0.190601
H	3.035042	-2.256022	1.365225
C	0.271581	-1.256556	2.196993
O	0.473657	-2.161056	2.886789
C	-1.060606	0.984410	2.245061
O	-1.737532	1.583625	2.966302
H	1.088237	0.782092	1.977251

1a/1bTS

Fe	0.047597	0.289185	1.141699
C	-0.037396	-1.213914	-0.380507
O	-0.086624	-2.571578	-0.251995
H	-0.946387	-2.827969	0.114691
C	-1.154434	-0.320271	-0.542664
C	-0.574182	0.977980	-0.779949
C	-1.270006	2.267542	-1.140515
H	-2.126461	2.448068	-0.484119
H	-1.672488	2.179520	-2.162366
C	-0.304568	3.464335	-1.093137
H	-0.785479	4.338361	-1.548125
H	-0.092747	3.726770	-0.047977
C	1.009191	3.140548	-1.817419
H	1.648891	4.029185	-1.871213
H	0.783487	2.851540	-2.854031
C	1.777012	1.999948	-1.122054
H	2.574830	1.637682	-1.781587
H	2.276632	2.387023	-0.226629
C	0.855795	0.847177	-0.776419
C	1.210954	-0.514816	-0.484538
Si	-2.984486	-0.807756	-0.655791
C	-3.409446	-0.986846	-2.492625
H	-3.279044	-0.039606	-3.029367
H	-4.451663	-1.302530	-2.626123

H	-2.769288	-1.732907	-2.978207
C	-4.127046	0.464339	0.151590
H	-4.119498	1.426765	-0.370161
H	-3.861928	0.642729	1.199139
H	-5.158488	0.089913	0.130000
C	-3.282369	-2.479056	0.203074
H	-2.913896	-2.498573	1.236484
H	-2.861284	-3.331772	-0.345439
H	-4.363566	-2.658040	0.255947
Si	2.939317	-1.283589	-0.337173
C	3.524589	-1.719480	-2.089509
H	4.525145	-2.169365	-2.067907
H	3.573716	-0.835063	-2.736506
H	2.846581	-2.439590	-2.563052
C	4.145541	-0.049039	0.443591
H	5.115902	-0.536147	0.603788
H	3.781106	0.292457	1.419228
H	4.322837	0.834090	-0.179443
C	2.904896	-2.843124	0.725747
H	3.919203	-3.251025	0.822568
H	2.261873	-3.614729	0.293532
H	2.531335	-2.621454	1.731594
C	-1.169488	-0.065548	2.341049
O	-1.962846	-0.341535	3.139256
C	0.697656	1.679828	1.990165
O	1.167493	2.583637	2.538266
H	0.911128	-0.527130	2.063098

1b

Fe	0.011628	0.480358	1.073896
C	0.013660	-1.254125	-0.206949
O	0.101225	-2.570743	0.129380
H	-0.689435	-2.825631	0.630274
C	-1.187448	-0.495530	-0.400170
C	-0.728075	0.802396	-0.886537
C	-1.562677	1.964374	-1.364838
H	-2.415667	2.135574	-0.701415
H	-1.983334	1.712860	-2.351301
C	-0.720308	3.244351	-1.489827
H	-1.301952	4.016912	-2.006561

H	-0.493103	3.631432	-0.487055
C	0.587395	2.966635	-2.242153
H	1.138840	3.898214	-2.415293
H	0.345184	2.555758	-3.232822
C	1.486843	1.971560	-1.484339
H	2.258764	1.590369	-2.163235
H	2.022341	2.490050	-0.680006
C	0.688585	0.808333	-0.934580
C	1.185001	-0.474490	-0.452760
Si	-2.943297	-1.193229	-0.322658
C	-3.347808	-1.953617	-2.010456
H	-3.328969	-1.197241	-2.804388
H	-4.346033	-2.409056	-2.010296
H	-2.624862	-2.732706	-2.280043
C	-4.238474	0.120326	0.096404
H	-4.342652	0.868394	-0.696692
H	-4.015677	0.645113	1.031268
H	-5.214970	-0.366626	0.214263
C	-3.042181	-2.556690	1.001518
H	-2.586025	-2.248918	1.950482
H	-2.594574	-3.508640	0.684807
H	-4.096385	-2.777688	1.210582
Si	2.947923	-1.169499	-0.319335
C	3.211749	-2.334771	-1.790844
H	4.214214	-2.780012	-1.765771
H	3.105458	-1.808708	-2.747391
H	2.481366	-3.151819	-1.775754
C	4.237218	0.218540	-0.377044
H	5.232864	-0.213749	-0.214101
H	4.073857	0.964300	0.408949
H	4.262634	0.739668	-1.340014
C	3.155830	-2.116678	1.301716
H	4.147746	-2.583909	1.347815
H	2.400111	-2.901766	1.396227
H	3.057243	-1.449500	2.165429
C	-1.243095	1.323974	1.961349
O	-2.083845	1.849446	2.557029
C	1.335835	1.240260	1.935358
O	2.224175	1.713025	2.504681
H	0.001189	-0.486700	2.234863

1b/1cTS

Fe	-0.052990	0.252579	1.153681
C	0.027313	-1.200927	-0.412036
O	0.196135	-2.552601	-0.316461
H	-0.578261	-2.936199	0.122831
C	-1.218750	-0.487160	-0.488439
C	-0.849634	0.885652	-0.718522
C	-1.753869	2.057082	-1.023159
H	-2.601359	2.096893	-0.331828
H	-2.180141	1.903632	-2.026610
C	-0.992559	3.395149	-1.009539
H	-1.625419	4.174706	-1.449994
H	-0.794040	3.698784	0.026395
C	0.332916	3.287685	-1.775378
H	0.818071	4.268728	-1.840632
H	0.126011	2.968825	-2.807216
C	1.293793	2.283175	-1.112377
H	2.130814	2.078335	-1.790762
H	1.732503	2.732487	-0.213100
C	0.583233	0.989415	-0.773325
C	1.148490	-0.312895	-0.564326
Si	-2.960252	-1.222433	-0.404126
C	-3.620973	-1.377809	-2.173316
H	-3.693034	-0.399164	-2.662795
H	-4.622159	-1.826373	-2.184083
H	-2.966236	-2.006904	-2.788146
C	-4.134415	-0.166558	0.635865
H	-4.349003	0.805111	0.178636
H	-3.719730	0.012641	1.633847
H	-5.092676	-0.687851	0.756254
C	-2.906319	-2.957272	0.373447
H	-2.408837	-2.960924	1.351985
H	-2.436840	-3.710024	-0.273209
H	-3.933908	-3.301504	0.545016
Si	2.982871	-0.812511	-0.654789
C	3.416233	-0.970750	-2.495027
H	4.466716	-1.261055	-2.622076
H	3.265139	-0.029000	-3.036223
H	2.798988	-1.735750	-2.980881
C	4.073163	0.512439	0.146909

H	5.123677	0.197660	0.103477
H	3.816099	0.653539	1.202780
H	4.000898	1.484926	-0.350742
C	3.298548	-2.462010	0.207887
H	4.361019	-2.723336	0.120356
H	2.706855	-3.267456	-0.235531
H	3.054365	-2.415148	1.274617
C	-0.564370	1.670113	2.052473
O	-0.932866	2.591544	2.647184
C	1.122110	-0.261849	2.343898
O	1.878335	-0.624846	3.140980
H	-1.000726	-0.507073	2.042894

1c

Fe	0.003758	0.132038	1.140246
C	-0.138496	-0.987292	-0.722201
O	-0.161227	-2.333309	-0.897498
H	-1.062005	-2.662920	-0.754819
C	-1.277419	-0.120930	-0.543879
C	-0.716152	1.216260	-0.518788
C	-1.450750	2.532852	-0.500959
H	-2.282695	2.504061	0.208553
H	-1.889510	2.701977	-1.497081
C	-0.504079	3.697500	-0.169697
H	-1.021431	4.649915	-0.335629
H	-0.236613	3.657993	0.894723
C	0.766719	3.624451	-1.026589
H	1.394632	4.507964	-0.862564
H	0.479163	3.635872	-2.087772
C	1.587125	2.353310	-0.732465
H	2.315623	2.195355	-1.536957
H	2.174709	2.496172	0.181478
C	0.700973	1.129489	-0.620535
C	1.093949	-0.267489	-0.690146
Si	-3.109660	-0.586917	-0.533148
C	-3.877789	-0.077546	-2.189034
H	-3.808973	1.005445	-2.346077
H	-4.939702	-0.349926	-2.232806
H	-3.372614	-0.565432	-3.031324
C	-4.045380	0.223154	0.894142

H	-4.078884	1.314235	0.807334
H	-3.576727	-0.018002	1.854007
H	-5.081740	-0.137281	0.916353
C	-3.302875	-2.472771	-0.342436
H	-2.798483	-2.868465	0.548673
H	-2.975857	-3.042230	-1.223456
H	-4.368888	-2.701538	-0.219418
Si	2.810463	-1.052594	-0.831820
C	3.169543	-1.390865	-2.663354
H	4.156342	-1.852526	-2.794073
H	3.154002	-0.467351	-3.254953
H	2.423613	-2.071672	-3.090083
C	4.138873	0.106893	-0.136966
H	5.104700	-0.414405	-0.132942
H	3.922706	0.402776	0.895992
H	4.264486	1.019333	-0.729545
C	2.871055	-2.671456	0.142233
H	3.874484	-3.112229	0.086694
H	2.153673	-3.401505	-0.243615
H	2.637905	-2.500401	1.199627
C	1.149310	0.902826	2.219787
O	1.888596	1.450344	2.920564
C	-0.301463	-1.262664	2.168471
O	-0.555891	-2.173946	2.832543
H	-1.021578	0.835898	1.992457

1c/1aTS

Fe	-0.003168	0.121751	1.226439
C	0.007961	-0.941417	-0.654034
O	0.071908	-2.283762	-0.912992
H	-0.728416	-2.710952	-0.571134
C	-1.178754	-0.139150	-0.563635
C	-0.711276	1.223397	-0.433373
C	-1.524301	2.494045	-0.393912
H	-2.372597	2.392946	0.289096
H	-1.946551	2.673446	-1.395631
C	-0.663902	3.703991	0.006255
H	-1.229202	4.627006	-0.170166
H	-0.448725	3.656604	1.081574
C	0.653238	3.727568	-0.779978

H	1.214620	4.644260	-0.563832
H	0.426419	3.744744	-1.856110
C	1.533370	2.503341	-0.462233
H	2.333393	2.429168	-1.208917
H	2.027209	2.642723	0.505907
C	0.720262	1.225770	-0.464066
C	1.189436	-0.133129	-0.573782
Si	-2.947797	-0.767696	-0.836790
C	-3.264826	-0.742224	-2.702934
H	-3.187274	0.274072	-3.107100
H	-4.268091	-1.118251	-2.938855
H	-2.538769	-1.366499	-3.236931
C	-4.242046	0.282698	0.054830
H	-4.306930	1.299010	-0.346884
H	-4.044171	0.351567	1.129937
H	-5.228642	-0.181599	-0.070079
C	-3.119300	-2.555247	-0.206220
H	-2.750335	-2.674249	0.819564
H	-2.630192	-3.299263	-0.849182
H	-4.182809	-2.825022	-0.192206
Si	2.967251	-0.781059	-0.788953
C	3.309171	-0.813031	-2.653468
H	4.325929	-1.171156	-2.857736
H	3.211241	0.182745	-3.102240
H	2.609852	-1.481380	-3.169394
C	4.214192	0.354560	0.072941
H	5.219275	-0.075357	-0.025200
H	4.001031	0.445441	1.143969
H	4.245743	1.362502	-0.352775
C	3.150716	-2.519706	-0.074221
H	4.170795	-2.886230	-0.246610
H	2.449494	-3.219025	-0.537138
H	2.974207	-2.529254	1.006962
C	1.265340	-0.414724	2.307952
O	2.112666	-0.721784	3.033674
C	-1.292810	-0.371491	2.294567
O	-2.163576	-0.662738	3.001078
H	0.016685	1.363816	2.071869

2

Fe	-0.129826	0.306290	1.097504
Si	-2.880677	-1.110099	-0.835638
Si	2.965789	-0.267820	-0.917988
O	0.110304	-2.168947	-0.916708
O	1.788573	1.442053	2.968903
O	-2.434722	0.560414	2.850871
C	0.034929	-0.827323	-0.743431
C	-1.238395	-0.172701	-0.677431
C	-0.939056	1.250473	-0.640486
C	-1.906748	2.413431	-0.703525
H	-2.480030	2.492949	0.227713
H	-2.643157	2.228077	-1.494676
C	-1.182243	3.743297	-0.987578
H	-0.939238	3.803191	-2.058194
H	-1.857275	4.579888	-0.772213
C	0.117197	3.874695	-0.182143
H	-0.102281	3.793768	0.891235
H	0.567606	4.861381	-0.343267
C	1.117990	2.781172	-0.589286
H	1.493725	3.001340	-1.599129
H	1.991541	2.795208	0.071991
C	0.469166	1.418453	-0.601677
C	1.118866	0.111175	-0.655649
C	-2.919406	-2.576010	0.358756
H	-2.876710	-2.238780	1.400588
H	-2.069607	-3.240553	0.175769
H	-3.842457	-3.155230	0.230117
C	-3.010753	-1.733169	-2.619842
H	-2.160084	-2.379832	-2.862835
H	-3.015717	-0.902961	-3.336628
H	-3.930478	-2.311322	-2.773670
C	-4.359586	0.010667	-0.448162
H	-5.278057	-0.589912	-0.472307
H	-4.482687	0.820716	-1.175065
H	-4.289601	0.458060	0.549868
C	3.759673	1.134424	-1.920439
H	4.779517	0.841427	-2.200641
H	3.831659	2.073310	-1.362206
H	3.209685	1.334493	-2.847791
C	3.137009	-1.850113	-1.950463
H	2.458447	-1.852887	-2.810787

H	2.953472	-2.760470	-1.371427
H	4.162933	-1.913934	-2.335024
C	3.908681	-0.479566	0.707615
H	4.967831	-0.685509	0.506660
H	3.508123	-1.321271	1.282873
H	3.855122	0.413998	1.338930
C	1.019688	1.000486	2.226745
C	-1.510070	0.478108	2.160161
H	0.888669	-2.550499	-0.456560
H	0.107119	-0.990084	1.836954
C	1.035102	-3.661385	1.793826
H	-0.030536	-3.387514	1.731126
H	1.384774	-4.098848	2.746907
O	1.799511	-3.494464	0.863859

2/3TS

H	-0.736945	-0.014251	2.561278
C	0.149096	-1.307498	-0.352797
C	-1.106027	-0.581778	-0.499092
C	-0.700917	0.711018	-1.013294
C	0.727547	0.762702	-1.005793
C	1.274120	-0.525632	-0.656822
C	0.667174	1.910938	1.908388
O	1.365155	2.703951	2.357642
C	0.200968	-0.848674	2.831883
O	1.323098	-0.569586	2.222344
H	0.141656	-0.680054	3.929403
H	-0.316565	-1.787288	2.553754
C	-1.870577	1.574755	1.325324
O	-2.843432	2.164424	1.518339
O	0.133911	-2.574954	0.110347
H	1.027059	-2.806563	0.416948
Fe	-0.387009	0.684393	1.097733
C	1.496884	1.968012	-1.505833
C	-1.527053	1.758424	-1.724660
C	-0.762746	3.084048	-1.870982
C	0.642996	2.847436	-2.438364
H	1.857218	2.568577	-0.661211
H	2.396233	1.630307	-2.033382
H	-1.763440	1.377052	-2.730851

H	-2.490513	1.926210	-1.235277
H	-1.326730	3.760058	-2.524675
H	-0.687575	3.579136	-0.892414
H	0.552242	2.355898	-3.417536
H	1.155508	3.801025	-2.612313
Si	-2.774949	-1.477823	-0.537228
Si	3.098230	-0.980182	-0.486707
C	-2.707039	-2.792090	-1.901731
H	-1.891930	-3.500765	-1.718324
H	-3.644130	-3.360797	-1.950130
H	-2.541769	-2.339040	-2.886939
C	-3.110714	-2.314904	1.126935
H	-3.172505	-1.578839	1.937502
H	-4.061440	-2.862160	1.100716
H	-2.317502	-3.027103	1.377008
C	-4.206791	-0.291433	-0.911420
H	-4.306927	0.504595	-0.165451
H	-4.114689	0.176858	-1.897619
H	-5.145693	-0.860072	-0.907215
C	4.032550	0.290200	0.553035
H	3.596796	0.329095	1.556347
H	5.090024	0.010055	0.641482
H	3.995585	1.296487	0.120146
C	3.298642	-2.687974	0.326008
H	2.870675	-3.510964	-0.261816
H	4.368960	-2.908109	0.425715
H	2.880617	-2.696741	1.340287
C	3.867060	-1.090580	-2.221588
H	3.816451	-0.139326	-2.764779
H	4.925921	-1.372502	-2.157329
H	3.358818	-1.845392	-2.833842

3

H	-1.272380	-0.385331	-2.792910
C	0.463242	1.320380	0.019591
C	-0.815692	0.769202	0.345571
C	-0.482093	-0.544432	0.907735
C	0.990343	-0.630955	0.949904
C	1.582108	0.512137	0.435248
C	-0.477343	-2.550951	-1.424109

O	-0.078824	-3.621051	-1.579266
C	-0.188664	0.057864	-2.994584
O	0.683701	-0.323641	-2.024591
H	0.014549	-0.351402	-4.000576
H	-0.377303	1.144304	-3.052485
C	-2.657934	-1.280357	-0.779852
O	-3.767067	-1.595244	-0.712112
O	0.553426	2.486051	-0.625457
H	1.484811	2.675430	-0.831507
Fe	-0.949818	-0.868299	-1.074947
C	1.664525	-1.871553	1.470019
C	-1.232539	-1.267779	2.017208
C	-0.601587	-2.632046	2.340214
C	0.893418	-2.487666	2.655173
H	1.713138	-2.609171	0.655882
H	2.701244	-1.661385	1.754650
H	-1.195930	-0.649577	2.929752
H	-2.292706	-1.387585	1.777581
H	-1.122189	-3.084052	3.193538
H	-0.733664	-3.315267	1.489657
H	1.013719	-1.845335	3.539284
H	1.332449	-3.459942	2.909181
Si	-2.295287	1.927511	0.589896
Si	3.408771	0.747901	0.035018
C	-1.730988	3.439710	1.592225
H	-0.930742	3.986941	1.082923
H	-2.565622	4.135210	1.747449
H	-1.358893	3.144303	2.581147
C	-2.960398	2.525918	-1.081604
H	-3.386485	1.701057	-1.665269
H	-3.748341	3.277206	-0.943457
H	-2.162729	2.982759	-1.678348
C	-3.711772	1.125312	1.562990
H	-4.163221	0.265993	1.059050
H	-3.393725	0.806148	2.561626
H	-4.501565	1.876095	1.697064
C	4.050988	-0.708365	-0.983594
H	3.380495	-0.878071	-1.833274
H	5.062194	-0.515138	-1.363059
H	4.088591	-1.634646	-0.399401
C	3.675880	2.333705	-0.992328

H	3.399861	3.259468	-0.467935
H	4.747339	2.424274	-1.210862
H	3.169741	2.303600	-1.966355
C	4.407589	0.949875	1.634905
H	4.309755	0.078684	2.293206
H	5.475062	1.078483	1.415309
H	4.074654	1.828040	2.201102

3/4TS

H	-1.317675	0.011435	2.877938
C	0.340990	-1.282951	-0.200535
C	-0.899267	-0.657989	-0.531547
C	-0.496294	0.683773	-0.941918
C	0.979630	0.711615	-0.972505
C	1.504287	-0.495893	-0.538807
C	-0.041013	2.222518	1.707979
O	0.512320	3.191000	1.992961
C	-0.299687	-0.448479	3.164376
O	0.625834	-0.324697	2.145999
H	-0.023253	0.074461	4.095905
H	-0.573688	-1.492859	3.394492
C	-2.418168	1.373077	0.966977
O	-3.491698	1.795731	0.986070
O	0.399403	-2.422545	0.513208
H	0.812426	-2.100777	1.356767
Fe	-0.781832	0.704582	1.141314
C	-1.238532	1.612695	-1.886192
C	-0.522690	2.962853	-2.050099
C	0.943655	2.759335	-2.454512
C	1.716544	1.957837	-1.389437
H	-1.042714	3.563729	-2.805942
H	-1.287314	1.128244	-2.875066
H	-2.276877	1.764278	-1.577541
H	0.979780	2.222319	-3.413094
H	1.439224	3.724231	-2.614889
H	2.719724	1.704427	-1.748145
H	1.863503	2.594700	-0.505345
H	-0.571059	3.528088	-1.108555
Si	-2.467760	-1.693292	-0.773454
Si	3.318728	-0.898483	-0.187364

C	-2.030328	-3.154875	-1.898564
H	-2.902982	-3.798467	-2.067078
H	-1.675557	-2.812191	-2.878296
H	-1.240633	-3.770379	-1.453313
C	-3.097999	-2.364754	0.882010
H	-2.306220	-2.924116	1.392036
H	-3.429862	-1.560618	1.549726
H	-3.947309	-3.042967	0.730598
C	-3.849082	-0.701129	-1.612811
H	-4.209330	0.141239	-1.013328
H	-3.537655	-0.313686	-2.589446
H	-4.705074	-1.366653	-1.784386
C	4.049222	0.434066	0.943575
H	3.421540	0.537844	1.836394
H	5.063035	0.164047	1.265144
H	4.107787	1.414700	0.457338
C	4.271507	-0.964668	-1.828928
H	3.880214	-1.756165	-2.479334
H	4.217560	-0.022559	-2.387236
H	5.332730	-1.177979	-1.647840
C	3.511798	-2.580146	0.662958
H	2.998577	-3.383570	0.125087
H	4.578020	-2.835435	0.715119
H	3.132858	-2.566836	1.691559

4

Fe	-0.008492	0.220190	1.026263
Si	-2.939192	-0.981955	-0.815901
Si	2.925091	-0.801863	-0.980844
O	0.068425	-2.307504	-0.810566
O	2.264427	1.248196	2.565725
O	-2.108529	1.363258	2.728228
C	0.016055	-1.041816	-0.850954
C	-1.206242	-0.223702	-0.698585
C	-0.787812	1.151841	-0.734824
C	-1.651176	2.391647	-0.854780
H	-2.188888	2.581670	0.081132
H	-2.424627	2.208563	-1.610055
C	-0.831343	3.634806	-1.248362
H	-0.610559	3.601262	-2.324792

H	-1.432999	4.535646	-1.080491
C	0.491772	3.713699	-0.476845
H	0.290292	3.724490	0.603510
H	1.017839	4.646272	-0.712343
C	1.390827	2.516007	-0.820798
H	1.750980	2.624086	-1.855636
H	2.284320	2.508306	-0.189488
C	0.643394	1.209034	-0.721142
C	1.169736	-0.137085	-0.732824
C	-3.050277	-2.581404	0.183373
H	-2.827987	-2.407537	1.242141
H	-2.335672	-3.318827	-0.193420
H	-4.060638	-3.003843	0.112650
C	-3.264644	-1.351188	-2.647402
H	-2.513354	-2.046104	-3.039894
H	-3.229120	-0.440539	-3.258011
H	-4.251997	-1.808270	-2.789752
C	-4.269648	0.212966	-0.178222
H	-5.243797	-0.292448	-0.198979
H	-4.361427	1.118330	-0.788055
H	-4.086285	0.522314	0.857071
C	2.983492	-1.547437	-2.719924
H	3.960776	-2.000205	-2.928791
H	2.794646	-0.790560	-3.490991
H	2.218097	-2.325210	-2.816179
C	3.344029	-2.139840	0.290043
H	2.571714	-2.915256	0.298431
H	3.437153	-1.722494	1.299930
H	4.300829	-2.616140	0.041769
C	4.228434	0.569621	-0.834242
H	5.224788	0.137721	-0.994095
H	4.231919	1.033733	0.159269
H	4.094016	1.362758	-1.578136
C	1.353287	0.827167	1.994833
C	-1.277824	0.893328	2.080378
C	0.557327	-2.255424	2.866209
H	0.279040	-1.663464	3.740457
H	1.642447	-2.210899	2.724342
H	0.248876	-3.294148	3.026054
O	-0.146321	-1.714657	1.746348
H	-0.022502	-2.268350	0.920489

5

Fe	6.284889	6.683393	2.492152
Si	6.587793	3.113750	2.855298
Si	9.464365	8.217173	3.233097
O	8.281594	5.429459	4.353981
O	5.682448	9.546220	2.314741
O	3.546752	5.764850	1.982902
C	8.088054	5.628234	3.137739
C	7.226066	4.797166	2.255663
C	7.183665	5.457118	0.993514
C	6.580742	4.965618	-0.304785
H	5.486297	4.978153	-0.237682
H	6.857567	3.914932	-0.447432
C	7.038706	5.796693	-1.518175
H	8.059737	5.501831	-1.799414
H	6.399175	5.565745	-2.377812
C	7.022789	7.300452	-1.217629
H	6.011144	7.608665	-0.919975
H	7.277082	7.873078	-2.117019
C	8.018497	7.639816	-0.097552
H	9.043609	7.518725	-0.481290
H	7.929100	8.688244	0.200372
C	7.865202	6.729557	1.093264
C	8.385062	6.890079	2.413430
C	5.692793	3.329494	4.505749
H	4.770765	3.913244	4.395844
H	6.341004	3.844667	5.221002
H	5.417619	2.353478	4.925022
C	8.092872	1.986792	3.073536
H	8.795784	2.424132	3.791184
H	8.626722	1.835484	2.127447
H	7.794893	1.000108	3.449468
C	5.391073	2.337412	1.604509
H	4.989308	1.406163	2.024199
H	5.874023	2.081811	0.654656
H	4.536915	2.988732	1.386019
C	11.165918	7.439560	3.522031
H	11.838694	8.140850	4.031232
H	11.642786	7.145625	2.579018

H	11.072746	6.544554	4.146882
C	8.699672	8.733450	4.882532
H	8.522776	7.851552	5.505982
H	7.744420	9.254112	4.744390
H	9.370685	9.411909	5.424276
C	9.655516	9.748226	2.130462
H	10.302000	10.475401	2.638483
H	8.698748	10.247711	1.937345
H	10.121244	9.517896	1.165563
C	5.893493	8.416327	2.423101
C	4.609752	6.142852	2.228518

6

Fe	0.015855	0.088211	1.086610
C	-0.138918	-0.927002	-0.799205
O	-0.154106	-2.285096	-0.895164
H	-1.063142	-2.604240	-0.779285
C	-1.276749	-0.083211	-0.582576
C	-0.707213	1.248411	-0.460476
C	-1.432507	2.560428	-0.321765
H	-2.243003	2.475195	0.407521
H	-1.900155	2.806605	-1.288953
C	-0.475578	3.696987	0.074563
H	-0.993541	4.659219	-0.015431
H	-0.192341	3.583783	1.129551
C	0.782751	3.683399	-0.802872
H	1.417034	4.550252	-0.582935
H	0.481970	3.773281	-1.856770
C	1.600099	2.391324	-0.613251
H	2.323656	2.294256	-1.430991
H	2.193050	2.458516	0.306301
C	0.715031	1.163969	-0.592198
C	1.102485	-0.219282	-0.759912
Si	-3.098222	-0.571593	-0.614706
C	-3.773900	-0.299770	-2.365398
H	-3.701555	0.754740	-2.658154
H	-4.829453	-0.590816	-2.435977
H	-3.215669	-0.884961	-3.106198
C	-4.134507	0.401335	0.630074
H	-4.278426	1.443679	0.326092

H	-3.663606	0.398230	1.618766
H	-5.129571	-0.052516	0.720592
C	-3.278651	-2.423936	-0.193195
H	-2.767347	-2.698495	0.738045
H	-2.949067	-3.101586	-0.993956
H	-4.342719	-2.645817	-0.043271
Si	2.800840	-1.032086	-0.924780
C	3.038420	-1.589555	-2.721366
H	4.007038	-2.086144	-2.859607
H	2.996957	-0.740611	-3.414566
H	2.254401	-2.297382	-3.014836
C	4.183840	0.172907	-0.447254
H	5.142729	-0.361063	-0.451815
H	4.040027	0.578108	0.561107
H	4.277748	1.016004	-1.140117
C	2.911991	-2.533097	0.223127
H	3.884303	-3.030204	0.114648
H	2.128356	-3.263943	0.001427
H	2.807372	-2.233002	1.273014
C	1.095578	0.810575	2.268973
O	1.796383	1.353582	3.014963
H	-1.121094	0.361473	2.081839

7

Fe	0.077412	0.172357	1.155919
C	-0.174061	-1.017931	-0.592081
O	-0.239046	-2.380384	-0.501525
H	-0.152460	-2.569530	0.463296
C	-1.308278	-0.149972	-0.477351
C	-0.754793	1.185803	-0.522932
C	-1.493652	2.500193	-0.550978
H	-2.300175	2.507502	0.187120
H	-1.970253	2.605400	-1.538301
C	-0.546629	3.689262	-0.326207
H	-1.080394	4.625611	-0.527514
H	-0.237672	3.717695	0.727702
C	0.691058	3.576199	-1.225744
H	1.317732	4.471279	-1.136984
H	0.363599	3.524920	-2.274050

C	1.531795	2.329038	-0.891039
H	2.230772	2.128617	-1.711487
H	2.153647	2.527515	-0.010487
C	0.664174	1.105405	-0.676652
C	1.060038	-0.287117	-0.680407
Si	-3.129544	-0.673426	-0.511273
C	-3.726464	-0.514059	-2.304360
H	-3.632555	0.513442	-2.676120
H	-4.781356	-0.802958	-2.392218
H	-3.146438	-1.162955	-2.971207
C	-4.196764	0.436259	0.597183
H	-4.314854	1.446392	0.190146
H	-3.780739	0.529373	1.607137
H	-5.201177	0.003768	0.689934
C	-3.341396	-2.469858	0.040273
H	-3.034801	-2.633147	1.080063
H	-2.752642	-3.145413	-0.586521
H	-4.398087	-2.756299	-0.037879
Si	2.767412	-1.094501	-0.855987
C	2.974278	-1.630194	-2.662258
H	3.945978	-2.114496	-2.821239
H	2.912175	-0.776596	-3.348273
H	2.193627	-2.345037	-2.947479
C	4.143390	0.130962	-0.406563
H	5.110160	-0.386584	-0.452707
H	4.032499	0.522650	0.611101
H	4.198049	0.983409	-1.092037
C	2.915898	-2.593397	0.285121
H	3.948519	-2.964797	0.289627
H	2.264502	-3.410595	-0.040157
H	2.641783	-2.334557	1.313915
C	1.355692	0.925946	2.113873
O	2.178690	1.466900	2.714861
H	-0.829162	1.049743	1.982916
C	-0.860192	-0.892560	2.634540
H	-1.898777	-1.115290	2.371274
H	-0.704686	-0.477017	3.635836
O	0.104827	-1.566041	2.083641

7/8TS

H	-0.913658	0.870688	2.077209
C	-1.298314	-0.141914	-0.494585
C	-0.740079	1.193460	-0.541598
C	0.677395	1.104178	-0.685789
C	1.068743	-0.293210	-0.678570
C	-0.168842	-1.016442	-0.597765
C	1.360936	0.930392	2.089419
O	2.201665	1.470039	2.668190
O	-0.238988	-2.378857	-0.491781
H	-0.248583	-2.554558	0.478411
C	-0.937353	-0.775688	2.672844
O	-0.020743	-1.525298	2.122921
H	-0.754458	-0.398872	3.686581
H	-1.991518	-0.960903	2.439626
Fe	0.075843	0.172848	1.139228
Si	-3.117288	-0.671501	-0.527239
Si	2.768346	-1.120265	-0.829048
C	-3.698344	-0.585161	-2.329941
H	-4.751197	-0.881749	-2.416618
H	-3.604169	0.428044	-2.739144
H	-3.109081	-1.256496	-2.965596
C	-3.328370	-2.444094	0.099345
H	-2.993828	-2.568434	1.135864
H	-4.388239	-2.726398	0.059957
H	-2.761117	-3.147843	-0.516446
C	-4.200889	0.479320	0.522931
H	-4.311710	1.473126	0.075672
H	-5.206880	0.050423	0.615074
H	-3.804165	0.611374	1.536480
C	2.962941	-1.737334	-2.610440
H	3.929607	-2.237035	-2.751541
H	2.174781	-2.456937	-2.860616
H	2.905601	-0.914240	-3.333169
C	4.157190	0.112669	-0.443406
H	4.057526	0.551799	0.555826
H	5.119292	-0.414702	-0.472889
H	4.213351	0.931830	-1.168326
C	2.906233	-2.567987	0.377505
H	3.933531	-2.953488	0.395267
H	2.638995	-2.259231	1.394324

H	2.240926	-3.388709	0.092051
C	1.554051	2.320615	-0.902109
C	-1.471635	2.512012	-0.566998
C	-0.515787	3.693248	-0.337128
C	0.722135	3.574038	-1.235520
H	2.180105	2.514251	-0.023579
H	2.249021	2.113689	-1.724343
H	-1.950321	2.625296	-1.552495
H	-2.276892	2.523578	0.172783
H	-1.041943	4.634721	-0.534586
H	-0.207087	3.713902	0.717108
H	0.395340	3.526975	-2.284220
H	1.354496	4.464882	-1.144386

8

Fe	0.083235	0.101299	1.112761
C	-0.168192	-0.991771	-0.666514
O	-0.238078	-2.351836	-0.569809
H	-0.253666	-2.518736	0.409683
C	-1.287403	-0.115074	-0.532669
C	-0.729601	1.226044	-0.515722
C	-1.460417	2.545485	-0.486019
H	-2.264302	2.529815	0.256790
H	-1.945635	2.704176	-1.461979
C	-0.500972	3.714049	-0.207242
H	-1.023090	4.664525	-0.368820
H	-0.194250	3.693190	0.847744
C	0.740068	3.626159	-1.104668
H	1.374200	4.511013	-0.975684
H	0.417645	3.621317	-2.155676
C	1.566872	2.358068	-0.816997
H	2.267381	2.182042	-1.641814
H	2.187026	2.512396	0.073335
C	0.684625	1.137988	-0.657708
C	1.075614	-0.261768	-0.691826
Si	-3.113963	-0.629145	-0.567233
C	-3.741064	-0.311007	-2.328004
H	-3.645852	0.744508	-2.609875
H	-4.799299	-0.585022	-2.422615
H	-3.176346	-0.902104	-3.058520

C	-4.156701	0.389418	0.649077
H	-4.219297	1.447314	0.372628
H	-3.769667	0.332769	1.673334
H	-5.181377	-0.003506	0.664960
C	-3.322767	-2.459398	-0.147302
H	-2.969409	-2.695959	0.863108
H	-2.765845	-3.092495	-0.843541
H	-4.384409	-2.733013	-0.199322
Si	2.776002	-1.087591	-0.843991
C	3.001067	-1.623136	-2.648654
H	3.968318	-2.120346	-2.794554
H	2.960255	-0.767905	-3.334286
H	2.215165	-2.327285	-2.945732
C	4.160246	0.123680	-0.379987
H	5.122297	-0.402871	-0.423949
H	4.048339	0.511046	0.639135
H	4.226976	0.978861	-1.061239
C	2.883662	-2.587199	0.299407
H	3.915397	-2.958065	0.347622
H	2.244813	-3.401936	-0.055113
H	2.561509	-2.330671	1.314828
C	1.333917	0.867437	2.116188
O	2.179137	1.401579	2.695094
H	-1.161974	0.176957	2.390931
C	-1.016598	-0.955795	2.737099
H	-2.029240	-1.364925	2.599457
H	-0.795488	-0.831832	3.809741
O	-0.033180	-1.583720	2.025215

9

Fe	0.052144	0.405581	0.902557
C	-0.048301	-1.293280	-0.535037
O	0.060554	-2.616482	-0.265419
H	-0.807959	-2.970802	-0.017931
C	-1.254383	-0.517265	-0.590595
C	-0.808385	0.802495	-1.026899
C	-1.657902	1.982375	-1.428903
H	-2.523595	2.094453	-0.766771
H	-2.064304	1.788136	-2.433844
C	-0.833549	3.280435	-1.462334

H	-1.429599	4.079141	-1.919835
H	-0.605882	3.596271	-0.436031
C	0.476599	3.078407	-2.236626
H	1.023047	4.026060	-2.309631
H	0.237699	2.773986	-3.266306
C	1.379734	2.019077	-1.577235
H	2.181764	1.735846	-2.267726
H	1.860376	2.423019	-0.675715
C	0.604232	0.798875	-1.163582
C	1.117200	-0.495926	-0.778626
Si	-3.037706	-1.122309	-0.431500
C	-3.851783	-1.082702	-2.141134
H	-3.892147	-0.063989	-2.543986
H	-4.880878	-1.460645	-2.097583
H	-3.299021	-1.700024	-2.859368
C	-4.048311	-0.087867	0.786768
H	-4.095360	0.970896	0.510629
H	-3.634961	-0.148311	1.799811
H	-5.079250	-0.462408	0.824376
C	-3.070464	-2.918801	0.201626
H	-2.572801	-3.044118	1.172693
H	-2.657042	-3.645562	-0.510792
H	-4.116472	-3.211738	0.355901
Si	2.901992	-1.142771	-0.720249
C	3.161964	-2.221830	-2.259646
H	4.177012	-2.638040	-2.282601
H	3.018192	-1.647194	-3.182902
H	2.456203	-3.060706	-2.274979
C	4.142095	0.281521	-0.690721
H	5.140754	-0.106098	-0.452182
H	3.855682	1.000350	0.084132
H	4.214830	0.812635	-1.645829
C	3.157687	-2.187790	0.834249
H	4.151165	-2.653767	0.817755
H	2.410771	-2.983046	0.917403
H	3.096971	-1.566038	1.734496
C	0.224851	-0.742327	2.252841
O	0.273739	-1.533198	3.089382
C	-1.042990	1.533941	1.728263
O	-1.728737	2.302682	2.242172
C	1.894356	1.772045	2.695784

H	2.743425	2.474525	2.716596
H	2.224924	0.851841	3.217000
H	1.095208	2.222495	3.317056
O	1.526897	1.555815	1.369489

9/10TS

H	2.033120	-0.151458	3.584123
C	-1.275078	-0.182295	-0.668316
C	-0.775202	1.163307	-0.599363
C	0.658634	1.131850	-0.777850
C	1.085414	-0.223609	-0.902579
C	-0.105638	-1.012174	-0.839971
O	1.466766	-1.057355	1.774017
C	0.395670	1.421388	2.129407
O	0.620335	2.335617	2.795152
H	-0.843161	-2.771526	-0.627926
O	-0.084382	-2.356638	-1.065177
C	1.736267	-1.122302	3.140551
H	0.893012	-1.504779	3.747880
H	2.578557	-1.815742	3.295812
C	-1.103829	-0.748610	2.115500
O	-1.858325	-1.294086	2.797338
C	1.481387	2.396811	-0.912741
C	-1.561714	2.453870	-0.584901
C	-0.653356	3.685374	-0.411098
C	0.592399	3.592581	-1.303141
H	2.011600	2.624158	0.019730
H	2.256776	2.247059	-1.672805
H	-2.091955	2.544323	-1.545763
H	-2.332737	2.440602	0.191980
H	-1.225429	4.590145	-0.648282
H	-0.343701	3.776469	0.637643
H	0.278484	3.488297	-2.351772
H	1.177476	4.517481	-1.240236
Si	-3.085759	-0.737073	-0.816678
Si	2.865931	-0.877414	-1.093450
C	-3.601709	-0.437285	-2.613492
H	-2.958390	-0.991321	-3.307075
H	-4.636004	-0.760273	-2.785536
H	-3.538119	0.624573	-2.879444

C	-4.232809	0.209415	0.352321
H	-3.920352	0.118310	1.398175
H	-4.295314	1.274603	0.107471
H	-5.247191	-0.202260	0.274765
C	-3.253725	-2.590005	-0.431704
H	-4.319370	-2.850356	-0.407929
H	-2.797678	-3.230206	-1.197098
H	-2.846180	-2.859526	0.550666
C	3.304832	-0.667893	-2.932232
H	4.326232	-1.020237	-3.125338
H	2.628850	-1.249080	-3.571101
H	3.251289	0.378564	-3.257286
C	4.050211	0.155357	-0.040885
H	4.121157	1.198954	-0.366340
H	3.713528	0.132821	1.000197
H	5.059904	-0.272351	-0.084946
C	2.993212	-2.694800	-0.616082
H	2.429940	-3.337960	-1.298646
H	4.043059	-3.015147	-0.625979
H	2.591408	-2.825388	0.392609
Fe	0.058224	0.049918	1.057811

10

Fe	-0.001236	0.126827	1.007931
C	-0.009069	-0.929705	-0.862365
O	-0.053260	-2.277262	-0.807028
H	-0.036039	-2.442246	0.205810
C	-1.175188	-0.096553	-0.792010
C	-0.664511	1.262430	-0.711790
C	-1.436615	2.558720	-0.726953
H	-2.323356	2.498080	-0.088827
H	-1.809219	2.724944	-1.749212
C	-0.554702	3.747770	-0.314118
H	-1.092190	4.684515	-0.502130
H	-0.360030	3.704371	0.766807
C	0.774978	3.730394	-1.078357
H	1.361870	4.628938	-0.855270
H	0.563666	3.753322	-2.156963
C	1.609719	2.478620	-0.747661
H	2.397444	2.354103	-1.499999

H	2.129379	2.619702	0.207558
C	0.759094	1.225514	-0.714488
C	1.200476	-0.155803	-0.762732
Si	-2.926931	-0.804199	-1.001758
C	-2.975004	-1.638069	-2.699649
H	-2.784645	-0.921215	-3.507625
H	-3.953073	-2.098854	-2.885957
H	-2.212452	-2.422217	-2.757985
C	-4.230909	0.571067	-0.943180
H	-4.070913	1.337388	-1.709871
H	-4.270856	1.069300	0.032528
H	-5.220609	0.131594	-1.122190
C	-3.319497	-2.063019	0.351800
H	-3.351054	-1.592861	1.341164
H	-2.565917	-2.855326	0.381291
H	-4.297471	-2.526217	0.169364
Si	2.943390	-0.903033	-0.893292
C	3.297917	-1.185090	-2.734028
H	4.287765	-1.636912	-2.876024
H	3.276257	-0.248196	-3.304142
H	2.556437	-1.861681	-3.174618
C	4.247065	0.282712	-0.190797
H	5.230108	-0.203002	-0.239553
H	4.060767	0.532804	0.859570
H	4.320555	1.219872	-0.752967
C	3.035069	-2.534482	0.051375
H	4.079732	-2.845820	0.176690
H	2.500248	-3.328216	-0.479235
H	2.576594	-2.434785	1.040856
C	-1.350288	0.681343	2.018994
O	-2.248210	1.073165	2.626329
C	1.283742	0.662928	2.111930
O	2.128007	1.021120	2.808494
C	-0.323902	-2.133590	2.905413
H	-0.166966	-3.218952	2.994654
H	-1.387773	-1.933691	3.125100
H	0.276228	-1.650881	3.695777
O	0.058087	-1.720180	1.624902

10/4TS

H	0.012283	-1.921487	3.634831
C	-1.175037	-0.078681	-0.767265
C	-0.653709	1.272562	-0.682598
C	0.772106	1.223606	-0.693780
C	1.199915	-0.157702	-0.743005
C	-0.017875	-0.939911	-0.856681
O	0.102090	-1.762070	1.574587
C	1.295233	0.683151	2.121997
O	2.140015	1.053296	2.812185
H	-0.024656	-2.308075	0.418027
O	-0.070530	-2.256472	-0.741559
C	-0.463028	-2.331424	2.732722
H	-1.548343	-2.161881	2.804734
H	-0.285326	-3.415342	2.724465
C	-1.340231	0.675972	2.044866
O	-2.239054	1.053383	2.660635
C	1.630905	2.471178	-0.731157
C	-1.413180	2.576140	-0.695940
C	-0.520471	3.757405	-0.284596
C	0.804800	3.730107	-1.055980
H	2.157719	2.607181	0.220661
H	2.412861	2.340093	-1.488209
H	-1.784674	2.745502	-1.718113
H	-2.300379	2.522490	-0.057701
H	-1.051421	4.698707	-0.468441
H	-0.320618	3.710115	0.795178
H	0.587718	3.756093	-2.133395
H	1.400490	4.623437	-0.835285
Si	-2.929857	-0.762430	-1.013225
Si	2.937044	-0.914376	-0.886243
C	-2.945295	-1.598963	-2.710233
H	-2.188655	-2.390196	-2.745032
H	-3.922731	-2.050613	-2.920606
H	-2.726587	-0.886543	-3.514950
C	-4.220903	0.626430	-0.986453
H	-4.279799	1.125759	-0.012205
H	-4.033720	1.390817	-1.748920
H	-5.210484	0.197498	-1.190037
C	-3.377946	-2.020209	0.324549
H	-4.346996	-2.484574	0.102060
H	-2.624898	-2.811954	0.377341

H	-3.453143	-1.551394	1.312454
C	3.262585	-1.214843	-2.729740
H	4.249477	-1.669184	-2.883799
H	2.512890	-1.895099	-3.150311
H	3.231822	-0.283812	-3.308960
C	4.257983	0.269616	-0.211428
H	4.337726	1.197604	-0.787831
H	4.080913	0.537348	0.836354
H	5.235837	-0.226656	-0.258626
C	3.050995	-2.542548	0.061326
H	2.429422	-3.311242	-0.406983
H	4.089482	-2.896862	0.080737
H	2.704318	-2.424409	1.093227
Fe	0.008369	0.138291	1.021365

11

Fe	0.033194	0.239424	1.075631
C	-0.017763	-0.694283	-0.848555
O	-0.044866	-2.016971	-1.190800
C	-1.167221	0.148988	-0.694919
C	-0.627449	1.490466	-0.511096
C	-1.376885	2.794469	-0.387430
H	-2.249637	2.686906	0.262837
H	-1.765058	3.071296	-1.379880
C	-0.464290	3.920109	0.124848
H	-0.985390	4.881188	0.041031
H	-0.251743	3.762467	1.191298
C	0.851650	3.955199	-0.662058
H	1.459039	4.817858	-0.363733
H	0.621927	4.087062	-1.729221
C	1.669124	2.662899	-0.472762
H	2.435697	2.600947	-1.253942
H	2.212487	2.701399	0.478969
C	0.791531	1.430459	-0.539260
C	1.201732	0.045972	-0.712623
Si	-2.944350	-0.452190	-0.978939
C	-3.088120	-0.912948	-2.810126
H	-2.918182	-0.043773	-3.457158
H	-4.084447	-1.310411	-3.040724
H	-2.348246	-1.676494	-3.074648

C	-4.213111	0.896333	-0.573216
H	-4.092057	1.792833	-1.190851
H	-4.175321	1.199777	0.479496
H	-5.220370	0.503230	-0.762282
C	-3.343500	-1.956841	0.095982
H	-4.380321	-2.272044	-0.078064
H	-3.240963	-1.720073	1.161376
H	-2.696218	-2.811190	-0.123622
Si	2.911089	-0.746896	-0.931919
C	3.107618	-1.189134	-2.762744
H	4.076173	-1.668456	-2.952447
H	3.045609	-0.299815	-3.401686
H	2.319205	-1.882478	-3.076099
C	4.295726	0.441178	-0.414948
H	5.259063	-0.079831	-0.488462
H	4.185457	0.776274	0.622879
H	4.357362	1.329628	-1.052629
C	3.058804	-2.307129	0.127736
H	4.024311	-2.798148	-0.048177
H	2.265364	-3.021837	-0.110022
H	2.994818	-2.065182	1.194955
C	-1.255183	0.613033	2.204827
O	-2.130178	0.828168	2.930027
C	1.349307	0.501198	2.203159
O	2.236004	0.647688	2.931505
H	-0.024071	-1.152040	1.655319
C	-0.260089	-4.076954	1.906005
H	0.098754	-3.188034	2.452568
H	-0.373274	-5.013964	2.483159
O	-0.525481	-4.038213	0.722417
H	-0.302495	-2.588375	-0.436734

11/12TS

Fe	-0.044025	-0.498916	1.113044
C	0.041184	0.943630	-0.599569
O	0.131247	2.246206	-0.586329
C	1.161276	0.009693	-0.586545
C	0.577151	-1.314792	-0.731911
C	1.274902	-2.636739	-0.940251
H	2.154005	-2.723980	-0.295276

H	1.647881	-2.679441	-1.975362
C	0.322743	-3.819964	-0.705886
H	0.809212	-4.749884	-1.023876
H	0.114858	-3.917756	0.368369
C	-0.991196	-3.616653	-1.469839
H	-1.631749	-4.502388	-1.384191
H	-0.761613	-3.497217	-2.538473
C	-1.760434	-2.377554	-0.972976
H	-2.512853	-2.098952	-1.720712
H	-2.318793	-2.624392	-0.062432
C	-0.838965	-1.198435	-0.735167
C	-1.202710	0.197185	-0.577990
Si	2.967822	0.556840	-0.723527
C	3.113806	1.671076	-2.252109
H	2.926099	1.095809	-3.167174
H	4.116954	2.107459	-2.334809
H	2.384132	2.487714	-2.229511
C	4.155725	-0.903825	-0.947320
H	3.909823	-1.521953	-1.817324
H	4.192156	-1.555393	-0.066956
H	5.168890	-0.510062	-1.101038
C	3.560469	1.486968	0.821024
H	4.617553	1.759015	0.706289
H	3.473442	0.852790	1.710384
H	3.010951	2.411649	1.023369
Si	-2.912372	1.000057	-0.660555
C	-3.196981	1.583726	-2.442055
H	-4.170093	2.079397	-2.549160
H	-3.172335	0.744667	-3.148073
H	-2.420222	2.295408	-2.744978
C	-4.288209	-0.211216	-0.171855
H	-5.244395	0.327302	-0.146203
H	-4.126614	-0.638932	0.823996
H	-4.400905	-1.039211	-0.879341
C	-3.049177	2.489713	0.503985
H	-4.089160	2.836351	0.551163
H	-2.435041	3.324534	0.152125
H	-2.741399	2.225481	1.522937
C	1.231450	-1.175766	2.106768
O	2.099274	-1.590626	2.750281
C	-1.361226	-1.034496	2.139767

O	-2.245916	-1.363751	2.809261
H	0.036497	0.703608	2.044890
C	0.089177	3.469682	1.303635
H	0.118027	2.411476	1.571106
H	-0.637635	4.136266	1.769394
O	1.020418	4.052685	0.644218
H	1.276555	3.306395	-0.010803

12

Fe	-0.155696	-0.561683	1.119814
C	0.087080	0.953423	-0.387987
O	0.240429	2.309227	-0.304475
C	1.138881	-0.019087	-0.516028
C	0.449710	-1.277825	-0.784417
C	1.047591	-2.631888	-1.081843
H	1.895259	-2.842042	-0.423048
H	1.449092	-2.624284	-2.106240
C	-0.004294	-3.746683	-0.969309
H	0.416607	-4.685460	-1.348358
H	-0.253848	-3.910719	0.087919
C	-1.272243	-3.376115	-1.747766
H	-1.982453	-4.211169	-1.752226
H	-1.001076	-3.188557	-2.796593
C	-1.956174	-2.124953	-1.165483
H	-2.667714	-1.726089	-1.898700
H	-2.550949	-2.400073	-0.286509
C	-0.950603	-1.048301	-0.812650
C	-1.207951	0.349859	-0.517982
Si	2.995901	0.371166	-0.639282
C	3.190639	1.710668	-1.969074
H	2.917379	1.308266	-2.952359
H	4.230013	2.056519	-2.032822
H	2.546961	2.578841	-1.792378
C	4.012709	-1.131803	-1.180055
H	3.658615	-1.570984	-2.118596
H	4.037455	-1.922264	-0.422194
H	5.048028	-0.805168	-1.342248
C	3.740497	0.951400	1.008298
H	4.819748	1.107889	0.883908
H	3.604816	0.188458	1.783194

H	3.320308	1.883128	1.401069
Si	-2.847230	1.309667	-0.549499
C	-3.056805	2.008801	-2.298412
H	-3.985464	2.587169	-2.381834
H	-3.093459	1.212447	-3.051707
H	-2.223935	2.673413	-2.555513
C	-4.313583	0.177494	-0.147549
H	-5.228390	0.783162	-0.113400
H	-4.207289	-0.307169	0.829325
H	-4.470540	-0.604909	-0.897217
C	-2.843728	2.724197	0.704413
H	-3.850123	3.154364	0.782253
H	-2.160761	3.524660	0.403911
H	-2.550806	2.379275	1.702678
C	1.029785	-1.420188	2.083718
O	1.839070	-1.960160	2.708720
C	-1.533999	-1.057601	2.081658
O	-2.450970	-1.358422	2.717640
H	-0.029358	0.516669	2.165910
C	0.751987	2.943831	0.885564
H	1.094439	2.160665	1.568659
H	-0.064792	3.509855	1.337614
O	1.730301	3.875562	0.563837
H	2.521303	3.405184	0.256900

12/13TS

Fe	0.013096	0.335254	1.147645
C	-0.029202	-0.947552	-0.797634
O	-0.106220	-2.215104	-0.957091
C	-1.169064	-0.034787	-0.639561
C	-0.620979	1.303634	-0.610168
C	-1.350058	2.623152	-0.690781
H	-2.233458	2.624370	-0.045370
H	-1.721561	2.752131	-1.719684
C	-0.429095	3.803096	-0.342233
H	-0.938507	4.746296	-0.573146
H	-0.227016	3.803765	0.737801
C	0.892693	3.704296	-1.113465
H	1.508327	4.595627	-0.944150
H	0.672281	3.674661	-2.190304

C	1.691115	2.447712	-0.719739
H	2.470232	2.264634	-1.469716
H	2.218461	2.625363	0.224804
C	0.804583	1.222242	-0.616280
C	1.201310	-0.165039	-0.613139
Si	-2.948331	-0.594723	-0.953766
C	-3.098521	-0.993745	-2.799316
H	-2.902024	-0.109593	-3.417740
H	-4.101833	-1.360159	-3.050548
H	-2.373059	-1.765717	-3.079693
C	-4.217746	0.733424	-0.484144
H	-4.135343	1.631641	-1.105328
H	-4.129610	1.038589	0.565177
H	-5.229291	0.331258	-0.625148
C	-3.410712	-2.160329	0.024100
H	-4.454047	-2.424714	-0.189114
H	-3.334802	-2.009591	1.109327
H	-2.787272	-3.010229	-0.273955
Si	2.937744	-0.884292	-0.841550
C	3.241753	-1.045415	-2.706990
H	4.233749	-1.467372	-2.912164
H	3.182466	-0.074380	-3.213669
H	2.494443	-1.704842	-3.163413
C	4.273188	0.226160	-0.078393
H	5.244926	-0.279344	-0.149497
H	4.084619	0.426531	0.982338
H	4.370124	1.190228	-0.588602
C	3.109980	-2.599216	-0.055110
H	4.099706	-3.011909	-0.288320
H	2.356066	-3.290436	-0.443882
H	3.029678	-2.562919	1.038955
C	-1.283947	0.924963	2.169987
O	-2.162078	1.297039	2.826077
C	1.306698	0.842668	2.219042
O	2.171518	1.166863	2.915726
H	-0.027735	-0.932112	2.052482
C	-0.231435	-2.800727	1.246994
H	-1.087347	-2.231999	0.952447
H	0.793436	-2.548664	1.063336
O	-0.403119	-3.915993	1.916856
H	-1.352074	-4.101185	2.040894

13

Fe	0.002048	0.193652	1.036768
C	0.014929	-0.912275	-1.038988
O	-0.067643	-2.117383	-1.332632
C	-1.118705	0.016758	-0.782657
C	-0.549821	1.325662	-0.622722
C	-1.243793	2.664558	-0.627014
H	-2.163040	2.633156	-0.035138
H	-1.555020	2.876188	-1.661877
C	-0.320597	3.794252	-0.143815
H	-0.804720	4.761610	-0.321216
H	-0.167368	3.709229	0.940905
C	1.031831	3.730955	-0.864229
H	1.655832	4.591114	-0.595505
H	0.858966	3.795458	-1.948046
C	1.790939	2.429738	-0.543720
H	2.599814	2.287880	-1.269576
H	2.280006	2.516984	0.433271
C	0.886396	1.214587	-0.581597
C	1.253870	-0.166479	-0.674872
Si	-2.893628	-0.545539	-1.117294
C	-3.014315	-1.013535	-2.946445
H	-2.830125	-0.149196	-3.596166
H	-4.008462	-1.408096	-3.190882
H	-2.271072	-1.781055	-3.187000
C	-4.169953	0.800232	-0.721502
H	-4.054201	1.687261	-1.354281
H	-4.129424	1.122097	0.325719
H	-5.177526	0.403225	-0.900592
C	-3.294053	-2.060816	-0.050341
H	-4.252717	-2.507390	-0.339885
H	-3.371495	-1.775822	1.007107
H	-2.514248	-2.819783	-0.179566
Si	2.960063	-0.977617	-0.829803
C	3.287131	-1.242979	-2.676968
H	4.248966	-1.744684	-2.841235
H	3.308264	-0.294733	-3.227971
H	2.500252	-1.868021	-3.113810
C	4.328940	0.108926	-0.089844

H	5.273922	-0.449262	-0.101485
H	4.126241	0.382475	0.952020
H	4.492659	1.033319	-0.654403
C	2.985949	-2.646652	0.057227
H	3.941449	-3.155396	-0.122542
H	2.180596	-3.289501	-0.310481
H	2.874016	-2.534999	1.142548
C	-1.338892	0.792160	2.044464
O	-2.225753	1.217628	2.647798
C	1.266616	0.656585	2.194060
O	2.107512	1.000798	2.905862
H	-0.145558	-1.439485	1.778438
C	-0.185504	-2.575477	1.874337
H	-0.133951	-2.965180	0.852236
H	0.705267	-2.843576	2.445660
O	-1.306851	-2.976908	2.597560
H	-2.068093	-2.974879	1.996183

1b/14TS

Fe	-0.017911	0.366479	0.945463
C	-0.120413	-1.207764	-0.552724
O	-0.008969	-2.541515	-0.336472
H	-0.834466	-2.880454	0.044562
C	-1.337017	-0.442073	-0.542380
C	-0.920228	0.901164	-0.921983
C	-1.790943	2.098294	-1.211538
H	-2.592701	2.193206	-0.472675
H	-2.284586	1.938542	-2.183122
C	-0.966834	3.395030	-1.274619
H	-1.590014	4.203921	-1.673445
H	-0.671012	3.691935	-0.259157
C	0.285570	3.205375	-2.139933
H	0.820366	4.154977	-2.256571
H	-0.023078	2.892202	-3.147669
C	1.239072	2.151736	-1.545778
H	1.970535	1.852757	-2.305106
H	1.818503	2.591178	-0.726111
C	0.490837	0.925644	-1.071746
C	1.030372	-0.399413	-0.789372
Si	-3.081746	-1.157538	-0.394806

C	-3.628851	-1.759744	-2.105438
H	-3.690535	-0.930956	-2.820877
H	-4.618166	-2.231922	-2.059649
H	-2.926718	-2.495901	-2.514913
C	-4.336816	0.092460	0.265274
H	-4.517335	0.913003	-0.437211
H	-4.033104	0.527479	1.223157
H	-5.296550	-0.416174	0.422311
C	-3.061705	-2.645376	0.795107
H	-2.524541	-2.429897	1.726741
H	-2.650234	-3.566068	0.357550
H	-4.095027	-2.890209	1.070933
Si	2.802742	-1.085830	-0.959481
C	2.890522	-1.906116	-2.669178
H	3.885685	-2.333791	-2.844637
H	2.689330	-1.191708	-3.476941
H	2.160024	-2.719491	-2.752432
C	4.081046	0.307769	-0.866090
H	5.084492	-0.136648	-0.882198
H	3.994386	0.879549	0.063865
H	4.022462	1.007785	-1.706267
C	3.173836	-2.337421	0.397877
H	4.193054	-2.726790	0.277773
H	2.480130	-3.183267	0.370892
H	3.101280	-1.850838	1.378160
C	-1.190848	1.228089	1.941003
O	-1.983218	1.787111	2.568470
C	1.475401	1.240227	1.716832
O	2.248551	2.082873	1.862685
H	0.172443	-0.790619	2.088117
C	1.014823	-1.022083	3.064773
H	1.044880	-2.124289	2.943011
H	0.322947	-0.734766	3.883034
O	2.117676	-0.364572	2.918609

14

Fe	-0.033518	-0.514981	0.830875
C	0.165288	1.365964	-0.254892
O	0.039069	2.592997	0.318770
H	0.911737	2.902763	0.607827

C	1.369811	0.617072	-0.409034
C	0.926205	-0.626466	-1.027847
C	1.783298	-1.746706	-1.560820
H	2.591575	-1.994678	-0.864187
H	2.268674	-1.392455	-2.483635
C	0.947725	-2.996493	-1.885732
H	1.570027	-3.716863	-2.429910
H	0.634643	-3.484442	-0.953526
C	-0.290713	-2.623824	-2.710861
H	-0.836827	-3.526786	-3.007240
H	0.035481	-2.133512	-3.640027
C	-1.237655	-1.691046	-1.932681
H	-1.970774	-1.253367	-2.619157
H	-1.807078	-2.258829	-1.187333
C	-0.487254	-0.583470	-1.235811
C	-1.002480	0.650860	-0.688947
Si	3.148155	1.169759	-0.104920
C	4.010783	1.419205	-1.773067
H	4.071966	0.484135	-2.342058
H	5.034768	1.787658	-1.633192
H	3.474878	2.148155	-2.392627
C	4.127838	-0.059700	0.945752
H	4.203114	-1.048133	0.480171
H	3.674146	-0.196104	1.933597
H	5.150033	0.311342	1.094112
C	3.171255	2.839618	0.815238
H	2.674805	2.804562	1.794471
H	2.752390	3.670120	0.230723
H	4.215870	3.110316	1.013870
Si	-2.756394	1.385401	-0.698784
C	-2.760816	2.795509	-1.967018
H	-3.743886	3.280567	-2.012918
H	-2.523223	2.430504	-2.973707
H	-2.021107	3.560714	-1.704862
C	-4.049775	0.089019	-1.166933
H	-5.050583	0.513178	-1.013733
H	-3.964665	-0.805414	-0.540756
H	-3.984498	-0.219401	-2.216165
C	-3.189002	2.068398	1.011436
H	-4.150105	2.596627	0.972591
H	-2.431614	2.773207	1.369812

H	-3.286109	1.255449	1.739647
C	0.998798	-1.735553	1.572741
O	1.703130	-2.553605	1.989095
C	-1.618019	-1.436092	1.456157
O	-2.343554	-2.285818	0.996011
H	-0.543499	0.620522	2.389486
C	-1.041799	0.033356	3.202457
H	-1.577601	0.787095	3.786180
H	-0.281790	-0.441414	3.831744
O	-1.979253	-0.906843	2.706009

14/10TS

Fe	0.041526	-0.669892	-0.685652
C	-0.158699	1.390461	-0.017903
O	-0.024891	2.462871	-0.841880
H	-0.891264	2.693401	-1.212609
C	-1.363162	0.695274	0.286267
C	-0.920859	-0.403804	1.140630
C	-1.777272	-1.397279	1.885050
H	-2.584538	-1.779752	1.251212
H	-2.264527	-0.870160	2.720403
C	-0.938907	-2.558234	2.446490
H	-1.560175	-3.164189	3.116630
H	-0.621269	-3.213019	1.624226
C	0.296211	-2.030580	3.188581
H	0.843047	-2.857879	3.655646
H	-0.034530	-1.371369	4.004584
C	1.243836	-1.261285	2.249530
H	1.973784	-0.698884	2.842443
H	1.819355	-1.959631	1.630634
C	0.493036	-0.310105	1.350448
C	1.008202	0.784149	0.567283
Si	-3.139910	1.196634	-0.105112
C	-3.954594	1.818514	1.487776
H	-3.990816	1.035305	2.253957
H	-4.984945	2.147181	1.303268
H	-3.402538	2.666945	1.909485
C	-4.160429	-0.217754	-0.836308
H	-4.248407	-1.069770	-0.153947
H	-3.726484	-0.589350	-1.771016

H	-5.177157	0.133380	-1.054410
C	-3.161547	2.623942	-1.368085
H	-2.681777	2.368729	-2.322683
H	-2.723653	3.555495	-0.984815
H	-4.206334	2.859150	-1.606593
Si	2.758162	1.525832	0.447359
C	2.756519	3.102109	1.504091
H	3.739183	3.589885	1.479488
H	2.520890	2.884020	2.552960
H	2.016635	3.823061	1.137321
C	4.065705	0.326630	1.101005
H	5.061449	0.737062	0.888849
H	3.994546	-0.650706	0.612892
H	4.000230	0.175058	2.184123
C	3.157662	1.957197	-1.347867
H	4.172046	2.369670	-1.420728
H	2.457983	2.699462	-1.744736
H	3.105892	1.065313	-1.981565
C	-1.030807	-1.968376	-1.193503
O	-1.768285	-2.827654	-1.437924
C	1.599405	-1.626527	-1.147576
O	2.434510	-2.302379	-0.605243
H	0.170165	-0.631062	-3.558844
C	0.996475	-1.355330	-3.547060
H	1.574096	-1.229163	-4.466322
H	0.586201	-2.371446	-3.527353
O	1.911548	-1.140100	-2.467465

1b/15TS

Fe	0.000003	0.285951	1.038288
C	0.001632	-0.882001	-0.789528
O	0.005161	-2.213808	-0.931827
H	-0.026939	-2.721222	-0.039843
C	-1.185504	-0.070218	-0.711381
C	-0.706987	1.299676	-0.684010
C	-1.509331	2.576401	-0.727823
H	-2.392976	2.509929	-0.086571
H	-1.886492	2.709051	-1.753381
C	-0.654062	3.795141	-0.346923
H	-1.216292	4.713945	-0.550244

H	-0.449819	3.778805	0.732736
C	0.668694	3.794035	-1.122744
H	1.235258	4.711102	-0.924043
H	0.447183	3.789644	-2.199522
C	1.539047	2.571155	-0.775158
H	2.319294	2.449466	-1.534445
H	2.066927	2.747766	0.169594
C	0.721025	1.298318	-0.699894
C	1.191659	-0.072896	-0.712533
Si	-2.928236	-0.816338	-0.889593
C	-2.988660	-1.661559	-2.580974
H	-2.834680	-0.942447	-3.394827
H	-3.959722	-2.145552	-2.743344
H	-2.208555	-2.426281	-2.655023
C	-4.260642	0.530460	-0.819899
H	-4.142491	1.285512	-1.605041
H	-4.285884	1.045290	0.147654
H	-5.243666	0.063336	-0.962415
C	-3.259791	-2.058844	0.494828
H	-3.401593	-1.546616	1.454491
H	-2.438522	-2.773682	0.610813
H	-4.176612	-2.624494	0.285684
Si	2.932673	-0.833487	-0.849574
C	3.044912	-1.658750	-2.548020
H	4.018951	-2.144393	-2.685835
H	2.917524	-0.931255	-3.358951
H	2.265512	-2.420767	-2.653307
C	4.275420	0.496937	-0.700790
H	5.257974	0.007695	-0.697719
H	4.195611	1.068713	0.231094
H	4.270348	1.206291	-1.535864
C	3.201878	-2.097792	0.528763
H	4.113953	-2.677431	0.337627
H	2.365608	-2.799078	0.613872
H	3.327096	-1.598981	1.497698
C	-1.310965	0.827104	2.089936
O	-2.188828	1.177946	2.751644
C	1.312762	0.812406	2.095475
O	2.191265	1.160476	2.757961
H	-0.011270	-1.098337	1.803861
C	-0.041058	-2.447178	2.295148

H	-0.966383	-2.277721	2.874138
H	0.882315	-2.312691	2.886385
O	-0.050600	-3.286756	1.344814

1b/16TS

Fe	-0.21181100	-0.20142700	-0.72937300
C	-0.98992900	0.21508400	1.27807800
O	-0.56676000	-0.35989200	2.38174100
H	0.51629800	-0.63660700	2.32101900
C	-0.44095900	1.41652700	0.67056600
C	-1.23423700	1.64407100	-0.51803500
C	-1.19285100	2.82434700	-1.45589100
H	-0.16327300	3.14729700	-1.64364600
H	-1.69073300	3.66805000	-0.95586600
C	-1.92499200	2.52778900	-2.77414300
H	-2.01284600	3.45060100	-3.35925200
H	-1.33627900	1.82327800	-3.37739400
C	-3.31464700	1.94020700	-2.49496400
H	-3.87567000	1.81262400	-3.42792500
H	-3.88176200	2.65687200	-1.88401000
C	-3.23876700	0.58978500	-1.75563400
H	-4.21640300	0.36704000	-1.31180100
H	-3.04443600	-0.21820800	-2.47072900
C	-2.18882800	0.59411000	-0.66381600
C	-2.02668600	-0.34146700	0.43069000
Si	0.77483800	2.64170000	1.48239200
C	1.21728600	2.11145500	3.23708600
H	0.32440100	1.91902700	3.84080700
H	1.79174100	2.91133400	3.72217300
H	1.82246300	1.20109700	3.23692100
C	-0.11818700	4.31703200	1.58520300
H	-1.08808900	4.22656300	2.08933900
H	-0.29004000	4.76883800	0.60207300
H	0.48868400	5.02294400	2.16636000
C	2.35055200	2.85641000	0.45747800
H	2.14765800	3.19428100	-0.56529000
H	2.91715700	1.92109900	0.39532300
H	2.99796900	3.60777700	0.92786300
Si	-3.21101200	-1.73865100	0.94716800
C	-4.54818600	-0.90444700	2.00274700

H	-5.29247600	-1.63512300	2.34343100
H	-5.08018200	-0.12324600	1.44617100
H	-4.10665800	-0.43845000	2.89145700
C	-4.02149700	-2.56639500	-0.55475600
H	-4.61157200	-3.42424400	-0.20724700
H	-3.28072700	-2.94841100	-1.26614900
H	-4.70211500	-1.90406000	-1.09970600
C	-2.36478300	-3.08196000	1.96718900
H	-3.12395600	-3.72729900	2.42735800
H	-1.75164700	-2.64567300	2.76004300
H	-1.72618500	-3.72097700	1.34723400
C	1.01124900	0.49732000	-1.80686400
O	1.76481800	0.98419800	-2.52940300
C	-0.56843600	-1.57700500	-1.78034800
O	-0.82104200	-2.47316300	-2.46303400
H	0.96912900	-1.05619200	0.02541900
C	1.85066600	-1.58527100	0.89137700
O	1.74968400	-0.94572200	2.02422500
C	1.36323800	-3.04164300	0.91338000
H	1.28679400	-3.48445500	-0.08329200
H	2.08350500	-3.62426700	1.50041400
H	0.39285000	-3.09189600	1.40863900
C	3.15712700	-1.37006200	0.13936400
C	3.37830300	-1.90536600	-1.13782200
C	4.18978800	-0.65907100	0.76330700
C	4.60366400	-1.72929800	-1.77931600
H	2.58730000	-2.45320300	-1.64343500
C	5.41843200	-0.48571700	0.12297100
H	4.01593900	-0.26066600	1.75658900
C	5.62902900	-1.01822200	-1.14988700
H	4.75791800	-2.14577100	-2.77127100
H	6.21251500	0.06405300	0.62161700
H	6.58457500	-0.88226400	-1.64937300

15

Fe	-0.01755200	0.31883200	1.05270600
C	0.01227400	-0.99393700	-0.83318900
O	0.00765400	-2.24751700	-0.91759700
H	-0.19126900	-3.09786400	0.55567300
C	-1.17256700	-0.11556500	-0.69652000

C	-0.67716000	1.23360200	-0.71076600
C	-1.44898200	2.52348500	-0.83169100
H	-2.35330400	2.50055000	-0.21740300
H	-1.79320400	2.60960200	-1.87359000
C	-0.58441500	3.74679700	-0.48960500
H	-1.13137700	4.66184700	-0.74454200
H	-0.39813500	3.77839300	0.59290100
C	0.74925800	3.69112200	-1.24361800
H	1.32747900	4.60766200	-1.07961500
H	0.54356300	3.63932700	-2.32225800
C	1.59372000	2.47342700	-0.82443500
H	2.38212100	2.30092200	-1.56552900
H	2.11334800	2.68763300	0.11661300
C	0.76292800	1.21296200	-0.69827700
C	1.21263800	-0.14837700	-0.64689200
Si	-2.93643900	-0.81222000	-0.86548200
C	-2.95858500	-1.90134100	-2.41140900
H	-2.75040800	-1.31639400	-3.31589400
H	-3.93903700	-2.37658300	-2.54033500
H	-2.19878300	-2.68501700	-2.33551300
C	-4.21510900	0.57373300	-1.08789600
H	-3.99979700	1.21845800	-1.94765000
H	-4.31425900	1.21062200	-0.20115300
H	-5.19662600	0.11472300	-1.26420500
C	-3.41382000	-1.81001000	0.66599800
H	-3.56753700	-1.15345700	1.53160000
H	-2.64589200	-2.54444000	0.93045500
H	-4.35474400	-2.34693700	0.49029900
Si	2.95521700	-0.88608900	-0.79930700
C	3.14495700	-1.46881600	-2.59049300
H	4.12713400	-1.92884000	-2.75573600
H	3.04157700	-0.63960800	-3.30102200
H	2.37677900	-2.21299900	-2.82807400
C	4.29758500	0.39313000	-0.39599600
H	5.27421300	-0.10770700	-0.38924300
H	4.15838300	0.84596800	0.59264800
H	4.35380000	1.20136300	-1.13304800
C	3.19047300	-2.35275900	0.37209200
H	4.12202700	-2.87784700	0.12549300
H	2.36844400	-3.06986800	0.28912500
H	3.26736900	-2.03022200	1.41761000

C	-1.34703400	0.99011900	2.02701400
O	-2.22569300	1.45998600	2.60757600
C	1.27906300	0.93913900	2.10441800
O	2.13993600	1.38229700	2.73194000
H	-0.22446700	-1.25851300	1.94786300
C	0.07741600	-2.30404900	2.30828500
H	-0.38347900	-2.37415800	3.29801800
H	1.16978800	-2.30136600	2.40210000
O	-0.42265700	-3.30283200	1.49795400

16

Fe	0.22420700	-0.18420800	0.72061100
C	1.07726700	0.23765100	-1.35061400
O	0.65379500	-0.23221800	-2.43809300
H	-1.03216800	-0.55536100	-2.36657200
C	0.56510900	1.44286600	-0.65074900
C	1.35417000	1.58440000	0.53756100
C	1.39510000	2.74114700	1.50430200
H	0.39106900	3.13821800	1.68858600
H	1.95913700	3.55339800	1.02265500
C	2.09340500	2.36725800	2.82066500
H	2.24300200	3.27085900	3.42287400
H	1.45197900	1.69682300	3.40848500
C	3.43824300	1.68673000	2.53680200
H	3.98423000	1.50270000	3.46921100
H	4.05906000	2.37050600	1.94055800
C	3.26654200	0.35782700	1.77540700
H	4.22637500	0.06475600	1.33414100
H	3.00525000	-0.44267000	2.47729800
C	2.23010700	0.45237800	0.67371600
C	2.02132200	-0.43900100	-0.43519400
Si	-0.58344500	2.75364900	-1.42663200
C	-0.97920600	2.34955100	-3.22739200
H	-0.08054100	2.08261400	-3.79161100
H	-1.43691600	3.22784300	-3.70120500
H	-1.68151500	1.51561900	-3.30662500
C	0.35132800	4.41054600	-1.41044300
H	1.32679300	4.32598700	-1.90512600
H	0.51876900	4.80190400	-0.40109100
H	-0.22908800	5.16326900	-1.95911600

C	-2.19068400	2.95087000	-0.44726700
H	-2.01909600	3.22998400	0.59857200
H	-2.77483900	2.02407800	-0.45786600
H	-2.80670400	3.73829400	-0.90032100
Si	3.09436400	-1.90766000	-0.98221900
C	4.47247200	-1.16551100	-2.05403700
H	5.15225200	-1.94439000	-2.42173400
H	5.07389700	-0.43531200	-1.49854300
H	4.04745900	-0.65373400	-2.92541700
C	3.86735700	-2.81716700	0.49297200
H	4.39939000	-3.70292600	0.12236500
H	3.11313800	-3.16684600	1.20712700
H	4.59452300	-2.20974600	1.04209400
C	2.12602700	-3.16618200	-2.00200400
H	2.81807100	-3.87938700	-2.46762700
H	1.55660300	-2.66625100	-2.79046600
H	1.42994600	-3.74168100	-1.38146200
C	-0.95601100	0.58106800	1.81702500
O	-1.64836900	1.11527600	2.56700800
C	0.51493900	-1.57557900	1.78587200
O	0.75232400	-2.46468500	2.48273900
H	-1.14763700	-1.02936000	-0.16083800
C	-1.96549200	-1.41649400	-0.88330300
O	-1.96608500	-0.64313600	-2.03539000
C	-1.61657100	-2.88114400	-1.17612500
H	-1.55078700	-3.47581600	-0.25910800
H	-2.39685700	-3.30844200	-1.81481900
H	-0.66203300	-2.93768500	-1.70405800
C	-3.28365600	-1.26343300	-0.14351100
C	-3.45282400	-1.82291700	1.13106300
C	-4.35856400	-0.59040100	-0.73578500
C	-4.67024500	-1.71145000	1.80147100
H	-2.62707300	-2.34689500	1.60748000
C	-5.57933400	-0.48179300	-0.06504200
H	-4.22934300	-0.15987000	-1.72195800
C	-5.73974900	-1.03951900	1.20365900
H	-4.78303000	-2.14734400	2.79062400
H	-6.40603100	0.04203800	-0.53789200
H	-6.68915000	-0.95173200	1.72503300

17

Fe	0.00139500	0.02410600	0.53280800
C	1.42517900	0.06905800	-1.23659200
O	1.02600500	-0.02426000	-2.43619200
H	-0.61446000	-0.10816400	-1.87270400
C	1.41800600	1.30557100	-0.43303600
C	1.87383600	0.94425900	0.88629300
C	2.25849600	1.84676000	2.03281600
H	1.54731900	2.67006400	2.14399300
H	3.22508800	2.31190600	1.78451500
C	2.40075900	1.07030800	3.35107900
H	2.84235700	1.72254600	4.11363900
H	1.40644800	0.77918300	3.71754200
C	3.26490500	-0.18090900	3.15124800
H	3.44718100	-0.68407400	4.10801700
H	4.24777600	0.12752800	2.76690800
C	2.62029000	-1.17367600	2.16526600
H	3.37618300	-1.89182200	1.82631800
H	1.85588300	-1.76720300	2.68028900
C	2.03278100	-0.47705900	0.95404100
C	1.66831100	-1.05581000	-0.31611400
Si	1.18117800	2.98901300	-1.26749000
C	-0.41510900	3.03538200	-2.28029000
H	-0.39950400	2.26539800	-3.05730500
H	-0.52960800	4.01360400	-2.76430300
H	-1.29500000	2.86458800	-1.64998300
C	2.66535000	3.25353500	-2.41484200
H	2.72647800	2.43936700	-3.14543700
H	3.60955900	3.27761800	-1.85704300
H	2.57913200	4.19872800	-2.96544000
C	1.11556300	4.40264400	-0.00140100
H	2.04347700	4.50099900	0.57290500
H	0.28713400	4.28948700	0.70779500
H	0.96027900	5.35069300	-0.53255300
Si	1.87465200	-2.83027300	-0.94295700
C	3.56847100	-2.91679200	-1.79159400
H	3.76138700	-3.91830000	-2.19624400
H	4.38367200	-2.67497100	-1.09859300
H	3.61475300	-2.20345800	-2.62260900
C	1.81174600	-4.09770000	0.46868700

H	1.84251500	-5.10975700	0.04491200
H	0.88989100	-4.01714500	1.05616400
H	2.65755000	-4.00904200	1.15879100
C	0.53903400	-3.28298300	-2.20328300
H	0.78659200	-4.23481300	-2.69007600
H	0.46831100	-2.50717800	-2.97102500
H	-0.44500600	-3.40281500	-1.73456800
C	-0.88024700	1.30060400	1.41013000
O	-1.38460900	2.15474800	1.99775900
C	-0.64207200	-1.31041700	1.51914100
O	-0.98509000	-2.18524600	2.19001600
H	-2.06117400	-1.96403300	-1.06416500
C	-2.38164000	-0.94460700	-1.31373400
O	-1.26375200	-0.04876300	-1.11162000
C	-2.79306000	-0.89681400	-2.78794200
H	-3.63551300	-1.57381200	-2.96337200
H	-3.09903100	0.11599500	-3.06933800
H	-1.96264400	-1.20621400	-3.43266900
C	-3.50792500	-0.54476600	-0.38340200
C	-4.17881500	-1.51611500	0.36797400
C	-3.92343400	0.79104100	-0.29133200
C	-5.24819100	-1.16430800	1.19477300
H	-3.86114900	-2.55495900	0.30952800
C	-4.98605800	1.14552400	0.53915000
H	-3.40260100	1.55242000	-0.86488600
C	-5.65275800	0.16821500	1.28356500
H	-5.75760500	-1.93007100	1.77354400
H	-5.29400600	2.18553300	0.60673600
H	-6.48050500	0.44556300	1.93065800

CH_2O

C	0.000006	0.528957	0.000000
H	-0.937930	1.123590	0.000000
H	0.937845	1.123754	0.000000
O	0.000006	-0.677636	0.000000

CO

C	0.000000	0.000000	-0.650255
O	0.000000	0.000000	0.487691

CH_3OH

C	0.653076	0.036855	0.000000
H	1.102508	-0.959887	0.000000
H	1.010828	0.572644	0.893153
H	1.010828	0.572644	-0.893153
O	-0.753189	-0.150100	0.000000
H	-1.166187	0.726174	0.000000

$PhCOCH_3$

C	-0.43253000	1.19585400	-0.00000100
C	-1.82499100	1.27750100	0.00000400
C	-2.59291700	0.11168900	0.00002000
C	-1.96589900	-1.13829300	0.00000000
C	-0.57712000	-1.21967900	-0.00005800
C	0.20520600	-0.05388100	-0.00000900
H	0.15303100	2.11021200	0.00002200
H	-2.30989300	2.24989200	-0.00001800
H	-3.67784700	0.17629900	0.00004800
H	-2.56289200	-2.04628300	0.00007200
H	-0.06786100	-2.17789400	-0.00009800
C	1.69775800	-0.20355200	-0.00002200
C	2.56207800	1.04745200	-0.00001600
H	2.36197700	1.66520400	0.88354800
H	3.61097700	0.74633600	-0.00007100
H	2.36202500	1.66583700	-0.88326400
O	2.21262100	-1.31151700	0.00003200

$PhCH(OH)CH_3$

C	0.69400200	-1.20909300	-0.37935400
C	2.07438400	-1.09105200	-0.21462800
C	2.63260000	0.13809400	0.14131300
C	1.80110900	1.24360200	0.32963800
C	0.41991500	1.12264000	0.16964200
C	-0.14677100	-0.10704500	-0.18450500
H	0.26586200	-2.16730200	-0.66817200
H	2.71342800	-1.95603500	-0.37280000
H	3.70814400	0.23464500	0.26454200
H	2.22908000	2.20593700	0.59915500
H	-0.22802200	1.98261700	0.30178500

C	-1.65036900	-0.26866900	-0.31153300
C	-2.28138000	-0.74266400	1.00600100
H	-2.09613700	-0.00827500	1.79691500
H	-3.36688200	-0.86995200	0.89361300
H	-1.86287200	-1.70451100	1.32098400
O	-2.20089000	0.98664000	-0.71342000
H	-1.85019300	-1.02774900	-1.08635300
H	-3.16623200	0.90262400	-0.68174800