

# Mechanistic Insights into the Directing Effect of Thr303 in Ethanol Oxidation by Cytochrome P450 2E1

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## References

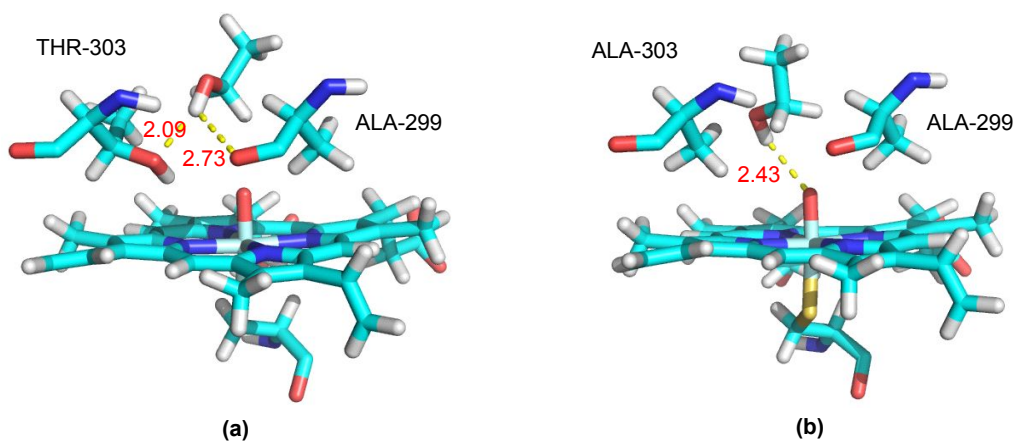


Figure S1. The docking of ethanol in the active cavity of CYP2E1 and its T303A mutant.

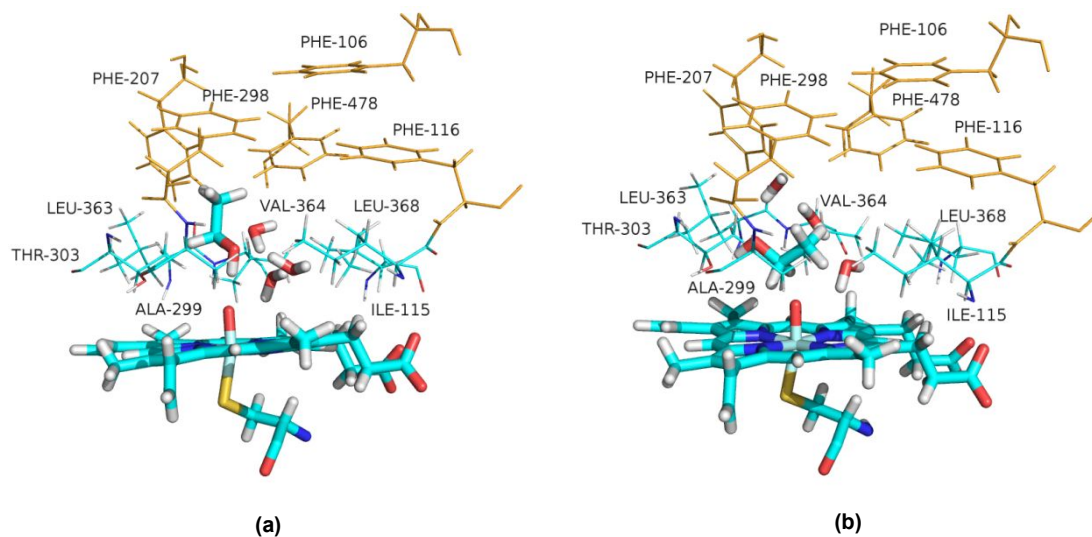


Figure S2. The three water molecules in the binding pocket of CYP2E1 after the solvation of the enzyme.

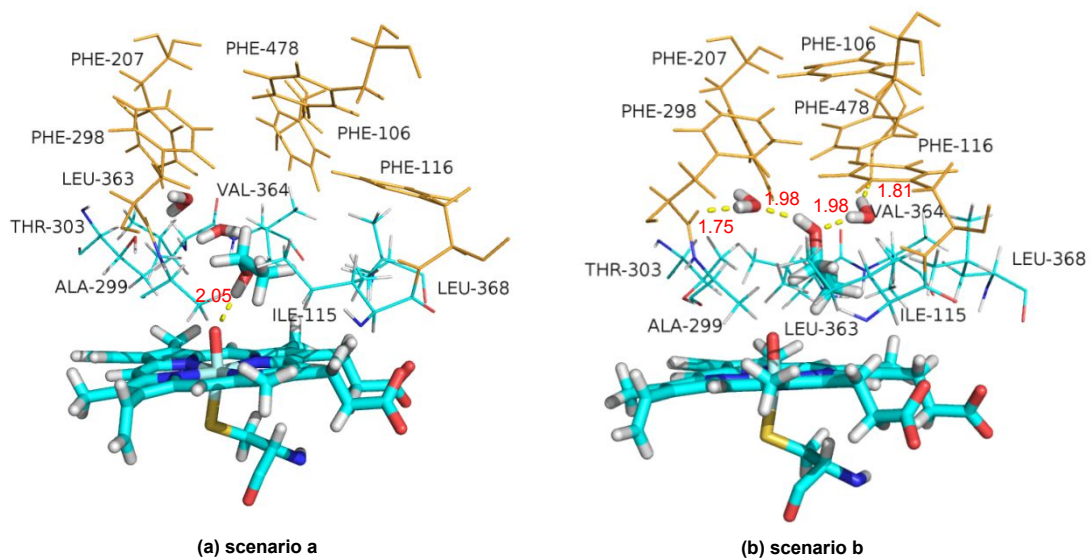


Figure S3. Two representative snapshots in the MD simulation starting from pose-A.

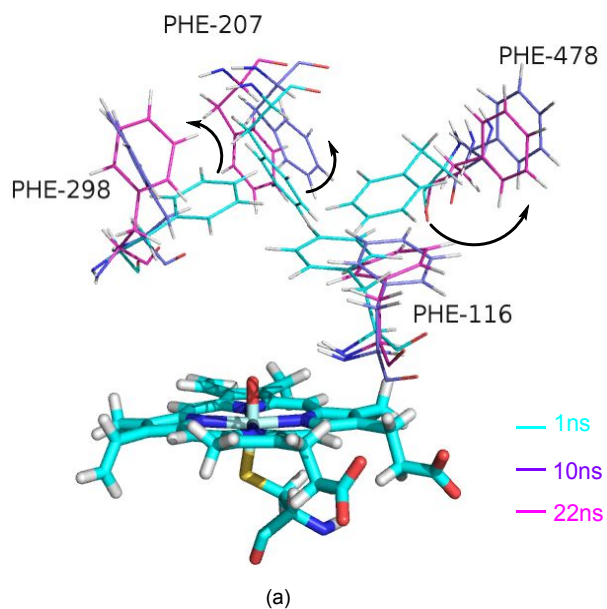


Figure S4. The deformation of the dome region of CYP2E1

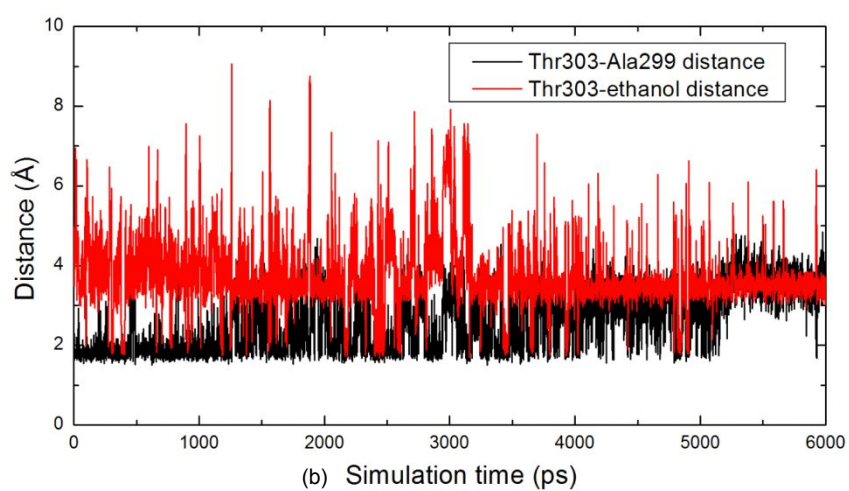
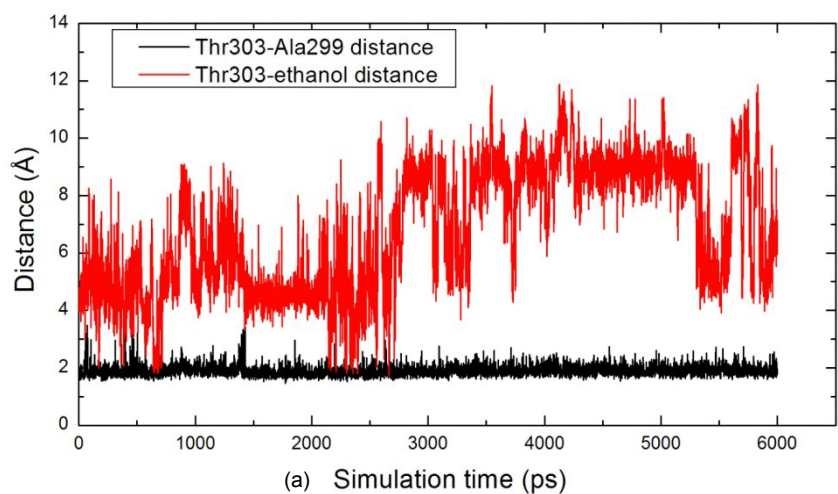


Figure S5. (a) Variations of Thr303(H)-Ala299(O) distances and Thr303(O)-ethanol(H) distances in the earlier 6ns of the first MD simulation. (b) Variations of Thr303(H)-Ala299(O) distances and Thr303(O)-ethanol(H) distances in the earlier 6ns of the second MD simulation.

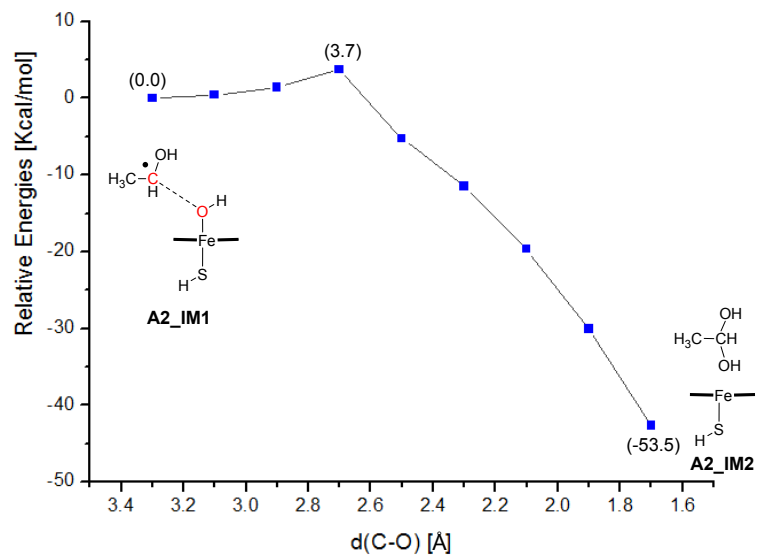


Figure S6. The relaxed energy scan of OH-rebound of **A2\_IM1** in the quartet state.

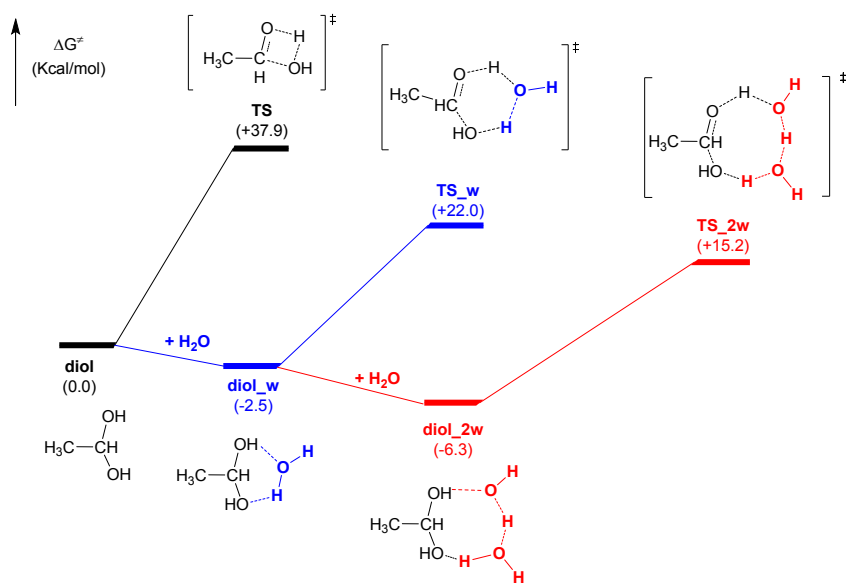


Figure S7. Energy profiles of water-assisted dehydration of gem-diol intermediate calculated at B3LYP<sup>1</sup>/6-31G(d) level of theory using Gaussian 09 package.<sup>2</sup>

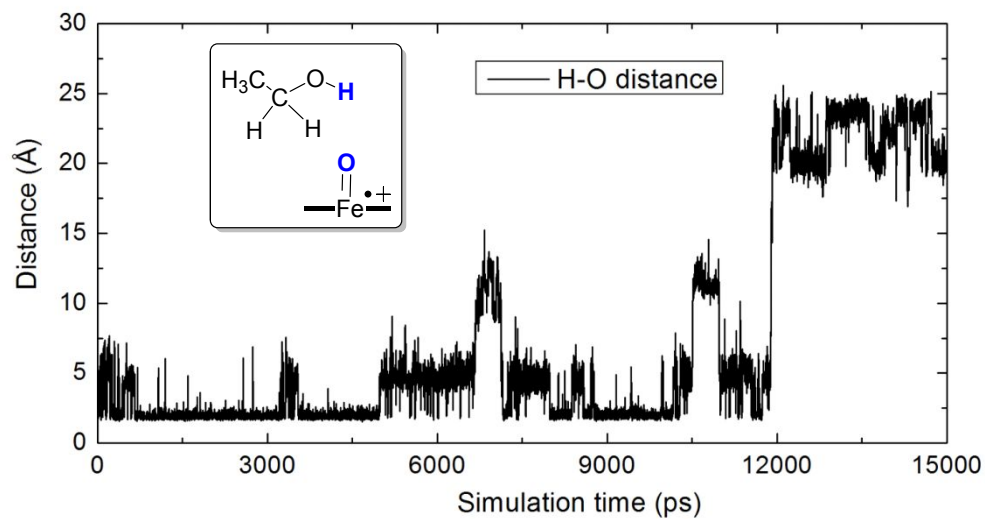


Figure S8. The MD results with a protonated Glu302 based on pose-B.

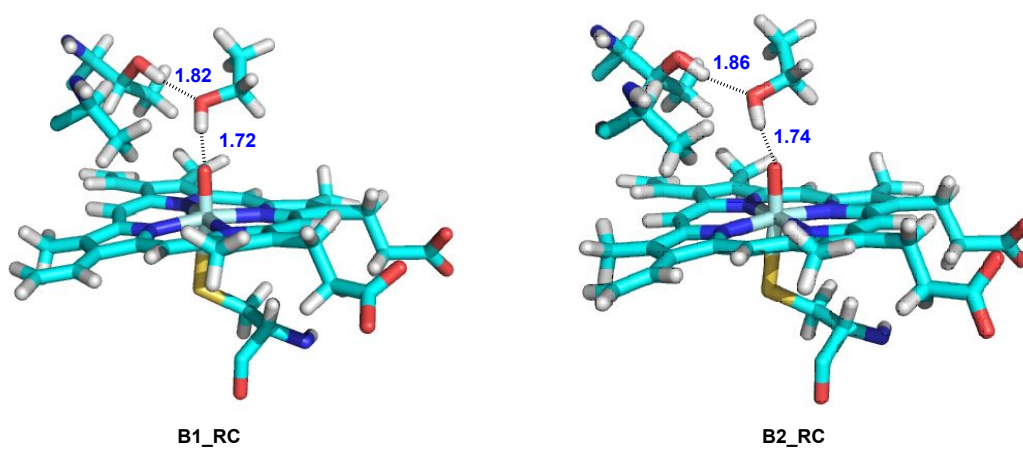


Figure S9. The QM/MM optimized structures of B1\_RC and B2\_RC.

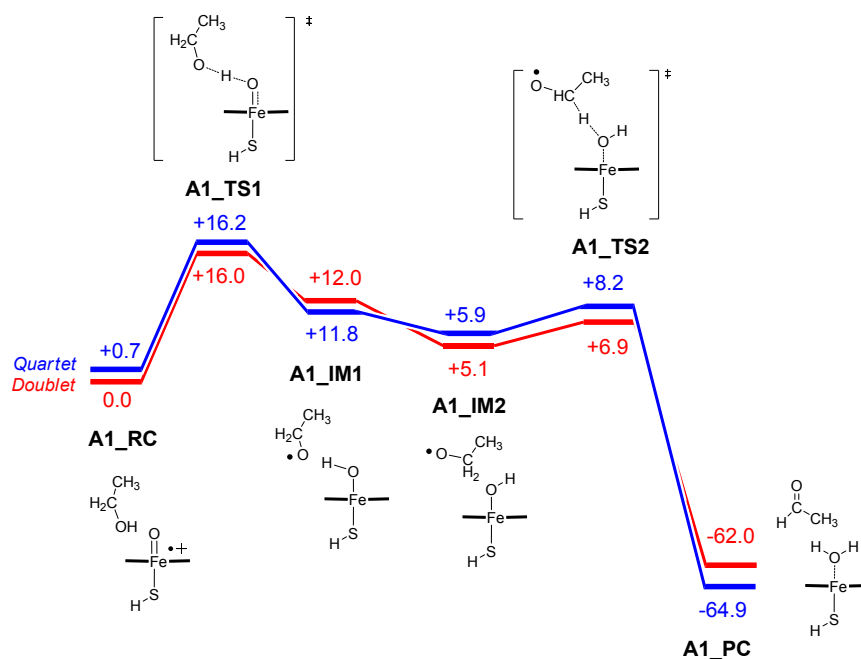


Figure S10. Energy profiles (kcal/mol) for ethanol oxidation by the HA\_O mechanism.

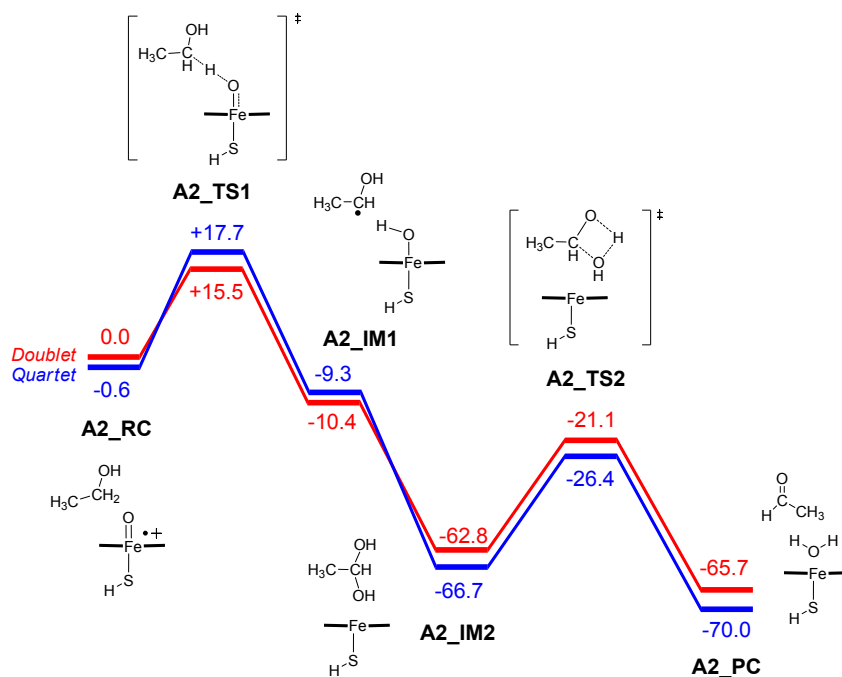


Figure S11. Energy profiles (kcal/mol) for ethanol oxidation by the gem-diol mechanism.



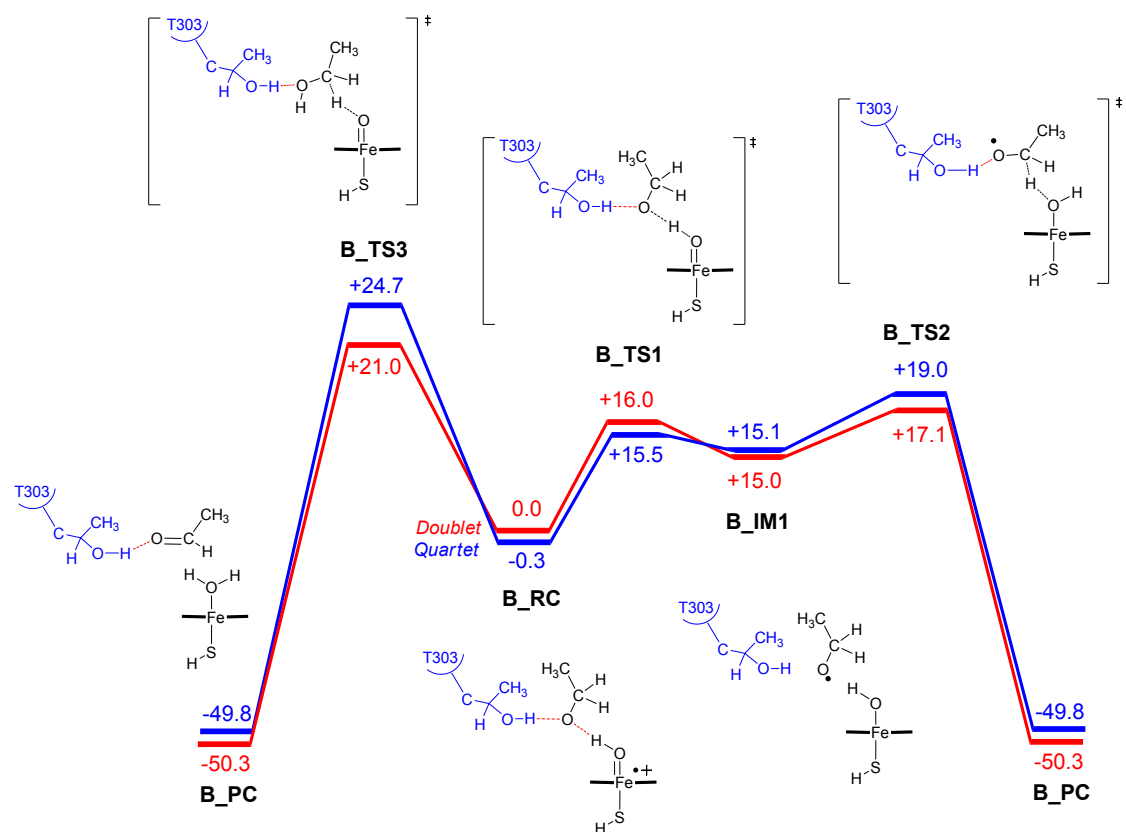


Figure S12. Energy profiles (kcal/mol) for ethanol oxidation in the presence of Thr303 effect.

Table S1. Spin density distributions of intermediates and transition states in dual hydrogen abstraction mechanism on the doublet surface.

	<b>FE</b>	<b>Oxo</b>	<b>SH</b>	<b>Por</b>	<b>H<sub>abst1</sub></b>	<b>H<sub>abst2</sub></b>	<b>Ethanol- H<sub>abst1</sub></b>	<b>Ethanol-H<sub>abst1</sub> - H<sub>abst2</sub></b>
<b>A1_RC</b>	1.35	0.77	-0.33	-0.79	/	/	/	/
<b>A1_TS1</b>	1.80	0.35	-0.13	-0.56	0.01	/	-0.47	/
<b>A1_IM1</b>	1.92	0.22	-0.01	-0.14	0.01	/	-1.00	/
<b>A1_IM2</b>	2.00	0.19	-0.09	-0.12	0.01	/	-0.99	/
<b>A1_TS2</b>	1.70	0.15	-0.06	-0.05	/	-0.15	/	-0.59
<b>A1_PC</b>	1.05	/	0.02	-0.07	/	/	/	/
<b>B_RC</b>	1.37	0.76	-0.30	-0.83	/	/	/	/
<b>B_TS1</b>	1.78	0.39	-0.12	-0.58	0.01	/	-0.48	/
<b>B_IM1</b>	1.88	0.27	-0.02	-0.26	0.01	/	-0.88	/
<b>B_TS2</b>	1.89	0.10	-0.06	-0.30	/	-0.15	/	-0.68
<b>B_PC</b>	1.05	0.00	0.02	-0.07	/	/	/	/
<b>B_TS3</b>	1.84	-0.23	-0.06	-0.21	0.01	/	-0.35	/

Table S2. Spin density distributions of intermediates and transition states in the gem-diol mechanism.

	<b>FE</b>	<b>Oxo</b>	<b>SH</b>	<b>Por</b>	<b>H<sub>abst1</sub></b>	<b>Ethanol-H abst1</b>	<b>diol</b>
<b>A2_RC</b>	1.27	0.85	-0.40	-0.72	/	/	/
<b>A2_TS1</b>	1.77	0.06	-0.22	-0.27	-0.01	-0.33	/
<b>A2_IM1</b>	1.88	0.20	0.01	-0.13	-0.01	-0.95	/
<b>A2_IM2</b>	1.18	/	-0.06	-0.12	/	/	0.0
<b>A2_TS2</b>	1.18	/	-0.06	-0.12	/	/	0.0
<b>A2_PC</b>	1.18	/	-0.06	-0.12	/	/	0.0

Table S3. Energies of intermediates and transition states on doublet surface.

	MM energy (Hartree)	QM energy at UB3LYP/B1 level (Hartree)	QM energy at UB3LYP/B2 level (Hartree)	ZPE (J/mol)
<b>A1_RC</b>	-116.693624	-2879.471855	-2880.958355	756979.9749
<b>A1_TS1</b>	-116.692732	-2879.443736	-2880.928267	742469.5809
<b>A1_IM1</b>	-116.694656	-2879.450575	-2880.935797	750738.4235
<b>A1_IM2</b>	-116.692913	-2879.459198	-2880.947741	748409.7693
<b>A1_TS2</b>	-116.691801	-2879.455101	-2880.940905	735065.0334
<b>A1_PC</b>	-116.688722	-2879.577957	-2881.063306	759980.4688
<b>A2_RC</b>	-116.812232	-2879.479261	-2880.969484	762585.9493
<b>A2_TS1</b>	-116.811302	-2879.452566	-2880.940037	747522.2984
<b>A2_IM1</b>	-116.823929	-2879.480987	-2880.970194	751273.0003
<b>A2_IM2</b>	-116.82336	-2879.570034	-2881.060009	766719.1126
<b>A2_TS2</b>	-116.822579	-2879.498374	-2880.988837	752262.4803
<b>A2_PC</b>	-116.821155	-2879.566672	-2881.064832	761569.1865
<b>B_RC</b>	-117.852815	-2879.484459	-2880.971715	758725.0057
<b>B_TS1</b>	-117.853491	-2879.453911	-2880.939951	743624.1859
<b>B_IM1</b>	-117.853432	-2879.459105	-2880.944322	751062.0923
<b>B_TS2</b>	-117.851048	-2879.453038	-2880.939574	741399.2350
<b>B_PC</b>	-117.851978	-2879.5677	-2881.051977	756578.5299
<b>B_TS3</b>	-117.851181	-2879.448159	-2880.93397	743143.6759

## References:

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**Cartesian coordinates (Å) of QM region for intermediates and transition states on doublet surface**

**A1\_RC**

S	3.102073	0.354050	5.389137
O	3.014547	-1.176687	1.544459
Fe	2.981448	-0.644509	3.094631
N	1.704612	-2.100386	3.715587
N	1.403730	0.599032	2.730159
N	4.281543	0.916445	2.780350
N	4.549210	-1.831696	3.628459
C	2.017672	-3.371459	4.133393
C	0.816963	-4.126962	4.464162
C	-0.239623	-3.279812	4.223203
C	0.337064	-2.030078	3.746611
C	0.077725	0.300772	2.844965
C	-0.758407	1.428489	2.432524
C	0.104900	2.441913	2.066187
C	1.453929	1.892256	2.290191
C	3.952013	2.194488	2.446273
C	5.134687	3.048676	2.339556
C	6.221480	2.228696	2.574131
C	5.652626	0.900560	2.860622
C	5.876681	-1.524958	3.498537
C	6.706665	-2.699248	3.722009
C	5.841739	-3.728857	4.020376
C	4.503183	-3.166546	3.956185
C	3.320538	-3.863067	4.210839
H	3.422686	-4.904762	4.518615
C	-0.402138	-0.914656	3.345252
H	-1.485570	-1.013829	3.435147
C	2.642698	2.621146	2.201961
H	2.535228	3.667963	1.925590
C	6.367905	-0.251606	3.188807
H	7.458243	-0.180055	3.186015
C	1.078465	-2.795188	-0.708469
O	1.503864	-3.281538	0.538538
H	2.108820	-2.613996	0.924269
H	0.609821	-1.790935	-0.618926
H	0.282570	-3.476009	-1.065618
C	2.202217	-2.733970	-1.742654
H	2.993092	-2.040477	-1.412840
H	1.835736	-2.383563	-2.722963
H	2.657186	-3.729787	-1.875114

H	2.678663	-0.534616	6.356267
H	0.796168	-5.162766	4.802899
H	-1.309765	-3.466868	4.311930
H	-1.847338	1.381387	2.441294
H	-0.058680	3.454186	1.696575
H	5.071130	4.118539	2.141010
H	7.297201	2.404269	2.566104
H	7.787881	-2.728393	3.587143
H	6.081837	-4.764319	4.261700

### A1\_TS1

S	3.033973	0.347838	5.370467
O	3.079618	-1.175901	1.543712
Fe	3.006354	-0.622351	3.166713
N	1.732360	-2.095064	3.708178
N	1.428451	0.617705	2.769070
N	4.305024	0.924455	2.802850
N	4.576196	-1.832374	3.649830
C	2.046285	-3.368686	4.115743
C	0.843909	-4.120426	4.442266
C	-0.213058	-3.268855	4.215309
C	0.356982	-2.014282	3.750277
C	0.105365	0.321446	2.885960
C	-0.727688	1.449549	2.468233
C	0.136054	2.458336	2.091412
C	1.486599	1.910328	2.312327
C	3.976980	2.196274	2.444145
C	5.162378	3.043141	2.327556
C	6.247563	2.226047	2.586176
C	5.677348	0.903951	2.892504
C	5.899812	-1.519090	3.521758
C	6.730166	-2.697457	3.723862
C	5.865823	-3.732994	4.004294
C	4.526428	-3.172083	3.948792
C	3.344681	-3.871545	4.190644
H	3.441678	-4.916331	4.488221
C	-0.382293	-0.897499	3.376196
H	-1.464940	-0.993106	3.474760
C	2.670807	2.629986	2.194621
H	2.569270	3.669687	1.892693
C	6.393772	-0.241950	3.234579
H	7.483431	-0.168567	3.239304
C	1.254145	-2.997404	-0.249239
O	1.858384	-3.191122	0.967702

H	2.600731	-2.133502	1.305290
H	0.552692	-2.125541	-0.181050
H	0.586425	-3.860070	-0.478243
C	2.233747	-2.751902	-1.402690
H	2.860745	-1.871027	-1.191197
H	1.703680	-2.581925	-2.355412
H	2.902397	-3.619935	-1.527012
H	2.621900	-0.554956	6.329375
H	0.820872	-5.156543	4.779901
H	-1.282585	-3.455382	4.312194
H	-1.816749	1.405954	2.478894
H	-0.029060	3.468755	1.717440
H	5.100215	4.110485	2.115476
H	7.323180	2.402404	2.582876
H	7.810999	-2.725627	3.585753
H	6.106493	-4.769328	4.241269

**A1\_IM1**

S	3.046219	0.343001	5.351842
O	3.101377	-1.238226	1.537041
Fe	3.017870	-0.648279	3.228790
N	1.738325	-2.128246	3.766793
N	1.436584	0.555222	2.749587
N	4.309025	0.904591	2.852556
N	4.581903	-1.858773	3.658210
C	2.062284	-3.407715	4.157659
C	0.859110	-4.162949	4.476552
C	-0.200025	-3.309726	4.259857
C	0.369099	-2.049039	3.807976
C	0.106350	0.264575	2.909059
C	-0.723614	1.393565	2.498563
C	0.137679	2.396586	2.096267
C	1.489929	1.851150	2.298828
C	3.968455	2.170804	2.467034
C	5.151151	3.024336	2.363166
C	6.237482	2.219414	2.650218
C	5.674740	0.893305	2.960948
C	5.907886	-1.531238	3.554310
C	6.737712	-2.709341	3.753511
C	5.874779	-3.750641	4.018125
C	4.532255	-3.199378	3.959500
C	3.360150	-3.907706	4.221061
H	3.466530	-4.950516	4.522706
C	-0.378774	-0.936133	3.425485

H	-1.459961	-1.030627	3.535657
C	2.670344	2.585096	2.184417
H	2.560479	3.621935	1.876609
C	6.401060	-0.249529	3.303524
H	7.490085	-0.169251	3.319484
C	1.494225	-2.867321	-1.087064
O	0.926930	-1.880465	-0.338831
H	2.284488	-1.068394	1.029281
H	0.812608	-3.172821	-1.916343
H	1.472798	-3.752233	-0.396369
C	2.923352	-2.616792	-1.565843
H	2.953001	-1.783908	-2.286507
H	3.323868	-3.512438	-2.069041
H	3.567345	-2.362463	-0.710470
H	2.636372	-0.542557	6.327628
H	0.837665	-5.200471	4.809952
H	-1.269992	-3.495208	4.353843
H	-1.812302	1.354658	2.534782
H	-0.032247	3.404233	1.717006
H	5.087315	4.090805	2.147211
H	7.311676	2.403692	2.664923
H	7.820275	-2.732796	3.628724
H	6.120429	-4.786470	4.252182

#### A1\_IM2

S	3.126441	0.360592	5.291599
O	3.260527	-1.025027	1.370287
Fe	3.152401	-0.580665	3.126494
N	1.909286	-2.097194	3.587622
N	1.558777	0.639584	2.704039
N	4.418501	0.994005	2.810440
N	4.734181	-1.779703	3.584224
C	2.240394	-3.374455	3.998939
C	1.042028	-4.135264	4.319356
C	-0.022624	-3.287139	4.101495
C	0.533903	-2.026494	3.641825
C	0.238045	0.310261	2.810828
C	-0.611414	1.425645	2.393814
C	0.234520	2.451876	2.023602
C	1.595158	1.934236	2.255325
C	4.062312	2.273165	2.470068
C	5.232390	3.137825	2.405841
C	6.331662	2.329445	2.636171
C	5.788603	0.994509	2.913597



C	6.057483	-1.430742	3.487805
C	6.906209	-2.595377	3.689063
C	6.059688	-3.650974	3.945277
C	4.706704	-3.122887	3.873955
C	3.542164	-3.857132	4.098074
H	3.661301	-4.899124	4.399776
C	-0.228118	-0.916848	3.281949
H	-1.308459	-1.034309	3.375550
C	2.767109	2.683525	2.162018
H	2.669653	3.713222	1.821017
C	6.531462	-0.145061	3.228439
H	7.618493	-0.043843	3.237279
C	1.811568	-2.896810	-0.788340
O	0.687492	-2.583524	-1.466318
H	3.667919	-0.315940	0.826813
H	1.661265	-3.784814	-0.126046
H	1.955344	-2.072740	-0.028811
C	3.090621	-3.009364	-1.620811
H	3.041483	-3.868333	-2.310973
H	3.964948	-3.142808	-0.963474
H	3.236864	-2.100739	-2.226723
H	2.689211	-0.547759	6.233977
H	1.012609	-5.169888	4.661048
H	-1.088863	-3.480084	4.219706
H	-1.699324	1.358581	2.398590
H	0.051904	3.460865	1.653929
H	5.160759	4.219174	2.289142
H	7.402047	2.533792	2.611974
H	7.990101	-2.604695	3.574352
H	6.319882	-4.682677	4.181825

#### A1\_TS2

S	3.135926	0.342832	5.239006
O	3.268857	-1.003255	1.306881
Fe	3.138219	-0.613154	3.130459
N	1.899218	-2.120037	3.564068
N	1.545932	0.607778	2.676855
N	4.414559	0.966766	2.766327
N	4.717698	-1.807423	3.542716
C	2.226922	-3.398293	3.982329
C	1.027697	-4.154854	4.311416
C	-0.035769	-3.306530	4.094427
C	0.520356	-2.048505	3.625599
C	0.225261	0.287367	2.791900

C	-0.623393	1.406659	2.385152
C	0.224566	2.430987	2.013246
C	1.584362	1.906606	2.235075
C	4.056335	2.246337	2.440981
C	5.223476	3.119248	2.387850
C	6.323553	2.313621	2.617774
C	5.780535	0.974191	2.883501
C	6.043904	-1.452842	3.460852
C	6.892328	-2.614028	3.673904
C	6.046730	-3.671495	3.929447
C	4.693999	-3.148450	3.845752
C	3.528344	-3.881074	4.077040
H	3.648377	-4.920770	4.386753
C	-0.240847	-0.940590	3.265286
H	-1.321148	-1.056158	3.362973
C	2.757174	2.654489	2.140486
H	2.656912	3.687039	1.808606
C	6.519750	-0.166347	3.205913
H	7.606970	-0.064159	3.227199
C	2.009491	-2.711946	-0.414357
O	0.878757	-2.230496	-0.804632
H	3.641935	-0.293736	0.736772
H	1.958467	-3.533090	0.350337
H	2.474438	-1.866630	0.402366
C	3.131669	-2.909602	-1.438172
H	2.894091	-3.758325	-2.103905
H	4.089911	-3.126395	-0.937822
H	3.242902	-2.013373	-2.070357
H	2.692364	-0.556337	6.187212
H	0.999945	-5.187844	4.658156
H	-1.102053	-3.496490	4.216987
H	-1.711535	1.344133	2.395437
H	0.043756	3.441582	1.647084
H	5.147021	4.201111	2.279249
H	7.393843	2.519118	2.600003
H	7.977144	-2.619704	3.568034
H	6.309984	-4.700747	4.173175

#### A1\_PC

S	3.075744	0.341887	5.320054
O	3.389305	-1.111593	1.218331
Fe	3.170348	-0.541060	3.251806
N	1.913724	-2.113615	3.587131
N	1.595822	0.631227	2.671367

N	4.441393	1.006390	2.824682
N	4.737759	-1.769777	3.629100
C	2.236687	-3.388642	3.995808
C	1.034152	-4.155579	4.311955
C	-0.024717	-3.304830	4.092194
C	0.546352	-2.041345	3.635032
C	0.269638	0.308138	2.796405
C	-0.580713	1.430274	2.398311
C	0.263921	2.461989	2.034763
C	1.624857	1.934703	2.241171
C	4.098611	2.278865	2.457710
C	5.271713	3.149934	2.403511
C	6.362084	2.347926	2.677882
C	5.805683	1.014395	2.969094
C	6.060507	-1.413840	3.578675
C	6.912132	-2.577424	3.785480
C	6.063692	-3.642864	3.996175
C	4.710943	-3.118444	3.901718
C	3.543610	-3.861648	4.100026
H	3.666983	-4.906110	4.394480
C	-0.201777	-0.919463	3.269031
H	-1.283603	-1.027940	3.364740
C	2.802228	2.683014	2.138533
H	2.702346	3.716842	1.807468
C	6.535423	-0.120159	3.331391
H	7.621612	-0.012574	3.380427
C	1.740788	-2.611243	-1.590501
O	1.354878	-2.182063	-0.524922
H	3.738168	-0.357510	0.692581
H	0.989727	-2.998809	-2.327674
H	2.576712	-1.416391	0.763658
C	3.169972	-2.649862	-2.036699
H	3.407704	-3.624308	-2.494074
H	3.836319	-2.443458	-1.188352
H	3.318602	-1.888322	-2.825064
H	2.660666	-0.582708	6.256634
H	1.004424	-5.189329	4.656258
H	-1.092249	-3.490687	4.210094
H	-1.668985	1.372307	2.417571
H	0.079143	3.479469	1.690294
H	5.200873	4.230462	2.278986
H	7.433186	2.549931	2.678622
H	7.999036	-2.588438	3.704337
H	6.324954	-4.677600	4.217831

**A2\_RC**

S	3.062452	0.460339	5.570844
O	2.903357	-1.124125	1.718129
Fe	2.864718	-0.587806	3.256957
N	1.607187	-2.054562	3.915274
N	1.280948	0.647739	2.936702
N	4.155058	0.970619	2.920061
N	4.444807	-1.774147	3.774800
C	1.926944	-3.336519	4.289856
C	0.728373	-4.108069	4.603008
C	-0.332144	-3.256740	4.399459
C	0.240375	-1.989071	3.967808
C	-0.037377	0.353780	3.114872
C	-0.889194	1.479320	2.737018
C	-0.045231	2.483627	2.307105
C	1.314325	1.934049	2.475281
C	3.816871	2.241265	2.563136
C	4.997005	3.099253	2.450202
C	6.086689	2.291536	2.713660
C	5.525694	0.962751	3.005635
C	5.768538	-1.466416	3.612202
C	6.604817	-2.645103	3.785288
C	5.747774	-3.680296	4.080576
C	4.407008	-3.117340	4.070160
C	3.233823	-3.825170	4.332756
H	3.347671	-4.874851	4.607940
C	-0.506039	-0.865224	3.616204
H	-1.585749	-0.965047	3.741991
C	2.502536	2.655280	2.321854
H	2.389873	3.687210	1.997007
C	6.251052	-0.189442	3.313194
H	7.340903	-0.117376	3.287156
C	1.730717	-2.859377	-1.008059
O	1.022493	-2.817227	-2.240891
H	1.603024	-2.368401	-2.891687
H	2.194590	-1.883037	-0.777665
H	2.561339	-3.597109	-1.055409
C	0.783122	-3.236081	0.116366
H	0.356885	-4.241508	-0.034002
H	-0.051238	-2.517084	0.164522
H	1.313007	-3.205579	1.079777
H	2.614420	-0.392749	6.558698
H	0.712628	-5.148091	4.928849

H	-1.403347	-3.442904	4.476500
H	-1.973338	1.409928	2.825801
H	-0.223466	3.486942	1.920248
H	4.939591	4.168818	2.248208
H	7.160447	2.477448	2.737036
H	7.683040	-2.667174	3.627125
H	5.993632	-4.720373	4.294726

### A2\_TS1

S	3.022065	0.372341	5.394130
O	2.931659	-1.040256	1.548522
Fe	2.803426	-0.667468	3.199644
N	1.552692	-2.122565	3.818477
N	1.215326	0.586145	2.881869
N	4.097762	0.896295	2.827527
N	4.382920	-1.870019	3.647504
C	1.878653	-3.403526	4.217136
C	0.680149	-4.152616	4.567732
C	-0.380111	-3.296784	4.369335
C	0.183551	-2.039508	3.907235
C	-0.102486	0.300975	3.087832
C	-0.946604	1.442485	2.742037
C	-0.100936	2.443328	2.308617
C	1.258531	1.881273	2.441411
C	3.751508	2.171401	2.483328
C	4.934209	3.026726	2.381440
C	6.022856	2.218215	2.647932
C	5.463644	0.885277	2.928875
C	5.705490	-1.541943	3.516725
C	6.545146	-2.715372	3.714752
C	5.691197	-3.754305	4.006229
C	4.345341	-3.203719	3.965027
C	3.176227	-3.907809	4.251470
H	3.287476	-4.949139	4.555313
C	-0.572331	-0.916527	3.578975
H	-1.648252	-1.011597	3.731236
C	2.443133	2.599310	2.269629
H	2.333499	3.639918	1.974424
C	6.191954	-0.261381	3.254964
H	7.281328	-0.182821	3.259781
C	1.966302	-2.809779	-0.113516
O	1.433111	-2.339923	-1.298532
H	2.135406	-1.984825	-1.894370
H	2.261519	-1.900202	0.648577

H	2.960243	-3.284120	-0.242618
C	0.970572	-3.698696	0.597643
H	0.737302	-4.588529	-0.014935
H	0.028421	-3.155069	0.775279
H	1.363571	-4.028437	1.569086
H	2.577019	-0.461353	6.399731
H	0.661790	-5.185944	4.914089
H	-1.450128	-3.474425	4.476918
H	-2.029255	1.388006	2.855903
H	-0.276020	3.453060	1.937329
H	4.870925	4.096069	2.180030
H	7.096484	2.404228	2.675998
H	7.626078	-2.729326	3.575265
H	5.942490	-4.786916	4.248368

### A2\_IM1

S	3.045753	0.483855	5.546432
O	2.988384	-1.096254	1.723625
Fe	2.950314	-0.528544	3.438437
N	1.660345	-1.997260	3.993391
N	1.375888	0.701283	2.985929
N	4.248392	1.002260	3.037115
N	4.493426	-1.771392	3.806980
C	1.965911	-3.293844	4.339362
C	0.751617	-4.047050	4.627455
C	-0.295973	-3.176621	4.428864
C	0.292218	-1.904256	4.034813
C	0.048508	0.442956	3.214493
C	-0.769660	1.594818	2.853960
C	0.089318	2.559099	2.360557
C	1.437535	1.985882	2.502081
C	3.921975	2.267431	2.633305
C	5.114024	3.105779	2.541289
C	6.190158	2.287712	2.832586
C	5.614711	0.971485	3.137842
C	5.822677	-1.467979	3.660774
C	6.636238	-2.664147	3.801929
C	5.763833	-3.693909	4.074356
C	4.430457	-3.117292	4.081067
C	3.256754	-3.814063	4.362589
H	3.356270	-4.867666	4.625145
C	-0.441845	-0.765143	3.709260
H	-1.520357	-0.858039	3.834088
C	2.630915	2.686980	2.320324

H	2.546884	3.694325	1.917668
C	6.331949	-0.191575	3.426819
H	7.422178	-0.131437	3.395429
C	1.511786	-2.537667	-0.820464
O	1.130686	-2.704902	-2.120025
H	1.782617	-2.249517	-2.705884
H	2.337585	-0.605654	1.194009
H	2.545021	-2.225423	-0.629976
C	0.736133	-3.286363	0.199253
H	0.871352	-4.387524	0.115042
H	-0.350220	-3.105011	0.097229
H	1.055345	-2.981476	1.206099
H	2.592758	-0.361422	6.538726
H	0.719147	-5.091190	4.938557
H	-1.369148	-3.359358	4.483365
H	-1.847494	1.634089	3.011435
H	-0.083568	3.554173	1.950673
H	5.079995	4.184097	2.385924
H	7.264839	2.468304	2.855263
H	7.714159	-2.696486	3.643482
H	5.999307	-4.737459	4.283213

## A2\_IM2

S	2.967550	0.521365	5.619486
O	2.288820	-1.798421	0.065756
Fe	2.793606	-0.496097	3.637895
N	1.522143	-2.024007	4.007044
N	1.247032	0.663653	3.046061
N	4.081443	0.949749	2.977639
N	4.325677	-1.796800	3.760464
C	1.822852	-3.328821	4.345630
C	0.615344	-4.088728	4.644078
C	-0.434143	-3.220037	4.458498
C	0.151640	-1.943288	4.072343
C	-0.078492	0.420482	3.315163
C	-0.906996	1.573814	2.985389
C	-0.069551	2.512960	2.416588
C	1.281102	1.942416	2.532021
C	3.761738	2.222381	2.580276
C	4.949829	3.065345	2.472955
C	6.028163	2.249971	2.756169
C	5.452644	0.936152	3.076883
C	5.664612	-1.494648	3.632023
C	6.483685	-2.682815	3.786286

C	5.615318	-3.716900	4.062326
C	4.282376	-3.146431	4.056618
C	3.113298	-3.845579	4.350066
H	3.219374	-4.898488	4.613107
C	-0.578507	-0.792517	3.785457
H	-1.661995	-0.870005	3.896887
C	2.463723	2.641372	2.296227
H	2.366384	3.644230	1.882869
C	6.170743	-0.218632	3.386442
H	7.261630	-0.154438	3.369178
C	2.064027	-2.989748	-0.651355
O	1.355578	-2.783421	-1.851375
H	1.954330	-2.306604	-2.470972
H	2.943898	-1.258867	-0.399252
H	3.044500	-3.463020	-0.885916
C	1.240725	-3.902557	0.234440
H	1.042021	-4.858019	-0.273754
H	0.277455	-3.416002	0.454032
H	1.759413	-4.087640	1.185734
H	2.550345	-0.364189	6.592152
H	0.594019	-5.132156	4.958512
H	-1.507290	-3.399976	4.522097
H	-1.955404	1.636602	3.276878
H	-0.271822	3.480755	1.957756
H	4.911043	4.144046	2.321408
H	7.103229	2.429667	2.759190
H	7.562683	-2.713867	3.635072
H	5.861350	-4.756657	4.277822

#### A2\_TS2

S	3.019011	0.530293	5.644762
O	1.831227	-2.040405	-0.636297
Fe	2.846716	-0.483844	3.662606
N	1.571720	-2.014200	4.014861
N	1.306180	0.677633	3.063144
N	4.135921	0.956835	2.985644
N	4.373783	-1.786142	3.774797
C	1.869525	-3.320563	4.354754
C	0.659590	-4.081318	4.637562
C	-0.389138	-3.212229	4.446469
C	0.199761	-1.935032	4.069238
C	-0.022870	0.430064	3.314921
C	-0.849710	1.578986	2.973013
C	-0.009622	2.521253	2.413167



C	1.340182	1.953882	2.539451
C	3.818504	2.232416	2.595883
C	5.006468	3.075052	2.490516
C	6.084490	2.257546	2.766252
C	5.507746	0.942713	3.080126
C	5.712547	-1.491624	3.619417
C	6.526974	-2.683802	3.759837
C	5.659250	-3.712927	4.054970
C	4.329229	-3.137172	4.069923
C	3.160515	-3.835924	4.366477
H	3.267860	-4.888880	4.629452
C	-0.526768	-0.784304	3.776942
H	-1.611036	-0.866450	3.873676
C	2.522925	2.651832	2.304631
H	2.429193	3.651656	1.883022
C	6.222977	-0.218433	3.368656
H	7.313397	-0.160029	3.331764
C	1.364580	-3.602986	-0.881390
O	0.389964	-3.272167	-1.705168
H	0.934094	-2.091109	-1.368545
H	2.630891	-1.837428	-1.156792
H	2.280048	-4.070267	-1.317076
C	1.008564	-4.156268	0.477068
H	0.605917	-5.171936	0.328722
H	0.218812	-3.541792	0.933461
H	1.876792	-4.204789	1.151153
H	2.580069	-0.351373	6.611375
H	0.636288	-5.125767	4.948447
H	-1.462553	-3.392342	4.504829
H	-1.902538	1.639606	3.248597
H	-0.209894	3.491552	1.958771
H	4.963912	4.154452	2.345081
H	7.159208	2.439300	2.770011
H	7.604262	-2.717039	3.597318
H	5.902172	-4.753088	4.272043

#### A2\_PC

S	2.955505	0.547479	5.666307
O	3.067852	-2.070700	-0.782977
Fe	2.791686	-0.472433	3.689426
N	1.522655	-2.008366	4.039427
N	1.240336	0.670727	3.067610
N	4.072432	0.971564	3.015501
N	4.323522	-1.771753	3.794131

C	1.826881	-3.313244	4.380014
C	0.621822	-4.077110	4.672697
C	-0.431352	-3.211817	4.483843
C	0.149749	-1.933334	4.101165
C	-0.087565	0.426637	3.336445
C	-0.918028	1.575525	3.000881
C	-0.081230	2.515983	2.431742
C	1.270421	1.951443	2.553305
C	3.749795	2.241572	2.609821
C	4.936215	3.085326	2.491740
C	6.016715	2.273408	2.774606
C	5.444528	0.961028	3.106970
C	5.662292	-1.468510	3.660444
C	6.483489	-2.655838	3.808047
C	5.618076	-3.691733	4.084778
C	4.284498	-3.123301	4.088300
C	3.119102	-3.825254	4.385907
H	3.228955	-4.878019	4.647278
C	-0.584464	-0.786185	3.809571
H	-1.667748	-0.867133	3.919899
C	2.451289	2.654967	2.321829
H	2.351288	3.655929	1.904849
C	6.165595	-0.191596	3.416243
H	7.256070	-0.126168	3.394360
C	0.325931	-2.801024	-0.232312
O	-0.368362	-2.867154	-1.224711
H	3.137476	-1.865775	-1.746419
H	3.262207	-1.221027	-0.362292
H	0.596140	-1.808599	0.201338
C	0.877325	-3.982469	0.509403
H	1.975953	-3.906626	0.460809
H	0.528758	-4.922514	0.056162
H	0.587497	-3.933724	1.573138
H	2.541499	-0.345675	6.633375
H	0.601968	-5.121158	4.985163
H	-1.503882	-3.395794	4.546280
H	-1.967965	1.635447	3.287425
H	-0.285886	3.481058	1.968264
H	4.896207	4.162310	2.328731
H	7.091613	2.454057	2.769517
H	7.561839	-2.684913	3.651896
H	5.865529	-4.732848	4.291931

**B\_RC**

S	2.784336	0.454316	5.298022
O	2.696297	-1.412135	1.549686
Fe	2.815903	-0.832613	3.073984
N	1.604585	-2.258616	3.880984
N	1.212068	0.424350	2.874369
N	4.071795	0.701858	2.593111
N	4.425267	-2.010114	3.502399
C	1.954979	-3.528780	4.284182
C	0.778921	-4.278224	4.706635
C	-0.291226	-3.426369	4.554083
C	0.243788	-2.181181	4.024290
C	-0.107095	0.121847	3.105162
C	-0.972633	1.229844	2.711781
C	-0.148555	2.234615	2.246049
C	1.218416	1.706682	2.370103
C	3.714209	1.972903	2.267658
C	4.883466	2.826444	2.080093
C	5.986313	2.014979	2.243242
C	5.444553	0.688959	2.573635
C	5.725447	-1.728346	3.184836
C	6.571819	-2.898623	3.358754
C	5.752965	-3.896960	3.839566
C	4.414142	-3.326862	3.895396
C	3.261948	-4.017231	4.275124
H	3.401917	-5.053420	4.586311
C	-0.536852	-1.079228	3.663288
H	-1.603190	-1.179364	3.865081
C	2.392839	2.405476	2.105474
H	2.289846	3.429876	1.744113
C	6.191373	-0.464700	2.805946
H	7.272223	-0.389458	2.675581
C	0.431487	-2.881468	-0.409515
O	0.766257	-1.513523	-0.399707
H	1.482716	-1.372621	0.257935
H	0.063513	-3.211903	0.584370
H	1.317229	-3.511364	-0.637722
C	-0.645250	-3.121134	-1.457643
H	-1.541221	-2.517946	-1.236592
H	-0.941185	-4.183046	-1.488472
H	-0.286592	-2.824074	-2.457036
H	2.475227	-0.369672	6.360962
H	0.773912	-5.315688	5.040864
H	-1.350056	-3.589667	4.754783
H	-2.059789	1.177098	2.769893

H	-0.351556	3.231109	1.853804
H	4.801695	3.908077	1.973092
H	7.055356	2.213715	2.167622
H	7.626460	-2.941378	3.086779
H	6.036040	-4.899141	4.161386

**B\_TS<sub>OH</sub>**

S	2.922244	0.352519	5.183520
O	2.665435	-1.412703	1.467614
Fe	2.782687	-0.809168	3.088530
N	1.575107	-2.263575	3.833092
N	1.174004	0.412940	2.772901
N	4.040718	0.714582	2.580699
N	4.392008	-2.008928	3.459636
C	1.924622	-3.524315	4.242878
C	0.750694	-4.269722	4.676473
C	-0.320716	-3.417179	4.523259
C	0.210703	-2.176441	3.980390
C	-0.130562	0.115446	3.019555
C	-1.000650	1.229536	2.647702
C	-0.176964	2.236351	2.184523
C	1.189143	1.697990	2.290580
C	3.682075	1.983373	2.248680
C	4.853829	2.837206	2.075707
C	5.956283	2.026881	2.244763
C	5.416444	0.698526	2.568647
C	5.691388	-1.721448	3.155805
C	6.540836	-2.889969	3.338541
C	5.725657	-3.890043	3.819616
C	4.381628	-3.328986	3.862617
C	3.235431	-4.018271	4.237490
H	3.373340	-5.052823	4.554313
C	-0.563659	-1.080099	3.607737
H	-1.628195	-1.168443	3.824855
C	2.363169	2.409540	2.056696
H	2.261973	3.436718	1.703210
C	6.161435	-0.455478	2.785459
H	7.242328	-0.380767	2.657670
C	0.443972	-2.792019	-0.274867
O	0.769474	-1.467125	-0.118952
H	1.803792	-1.340976	0.849044
H	0.106976	-3.247498	0.688570
H	1.360101	-3.379608	-0.539187
C	-0.609714	-3.023201	-1.360154

H	-1.526572	-2.456628	-1.128260
H	-0.875071	-4.091387	-1.443422
H	-0.244360	-2.673051	-2.339370
H	2.552952	-0.435097	6.254795
H	0.748208	-5.305382	5.016280
H	-1.377959	-3.578611	4.733604
H	-2.086764	1.181386	2.725833
H	-0.378033	3.240461	1.811159
H	4.770980	3.918881	1.969957
H	7.025573	2.226587	2.175458
H	7.596902	-2.929684	3.071684
H	6.012324	-4.889814	4.145726

**B\_TS<sub>CH</sub>**

S	2.989628	0.413126	5.257584
O	2.941650	-1.265523	1.540592
Fe	2.842365	-0.779829	3.188560
N	1.634664	-2.231370	3.884942
N	1.227207	0.419363	2.806420
N	4.103512	0.744056	2.671050
N	4.458568	-1.974767	3.583954
C	1.988413	-3.501432	4.299409
C	0.811157	-4.240638	4.726274
C	-0.258096	-3.381874	4.582566
C	0.270647	-2.140977	4.045141
C	-0.082322	0.129979	3.067189
C	-0.949333	1.226835	2.643207
C	-0.121743	2.214808	2.146478
C	1.246361	1.688209	2.293514
C	3.733643	2.004191	2.296688
C	4.906240	2.854809	2.115204
C	6.009484	2.053027	2.320107
C	5.474923	0.730238	2.671029
C	5.760881	-1.679990	3.274116
C	6.603395	-2.858717	3.427768
C	5.784889	-3.864400	3.888550
C	4.442979	-3.298427	3.951132
C	3.292393	-3.996570	4.306851
H	3.429290	-5.032920	4.616628
C	-0.513092	-1.045079	3.681872
H	-1.574247	-1.127692	3.915036
C	2.421337	2.412460	2.072592
H	2.316576	3.434726	1.706035
C	6.228331	-0.419159	2.908753

H	7.308675	-0.340216	2.779800
C	1.446604	-2.378465	-0.130091
O	1.373022	-1.305323	-1.004864
H	2.236931	-0.849241	-1.065112
H	2.005946	-1.975430	0.877465
H	2.155989	-3.163369	-0.466625
C	0.071170	-2.911756	0.172233
H	-0.546480	-2.140380	0.659505
H	0.130066	-3.790950	0.831056
H	-0.432869	-3.210109	-0.765389
H	2.605739	-0.381308	6.318644
H	0.801037	-5.280555	5.052673
H	-1.316038	-3.544265	4.788609
H	-2.035908	1.178543	2.714547
H	-0.321963	3.200466	1.726409
H	4.826905	3.932897	1.975563
H	7.079006	2.254011	2.258499
H	7.657134	-2.899091	3.151962
H	6.066948	-4.872036	4.193803

Cartesian coordinates (Å) of QM region for species on quartet surface

**A1\_RC**

S	3.102073	0.354050	5.389137
O	3.014547	-1.176687	1.544459
Fe	2.981448	-0.644509	3.094631
N	1.704612	-2.100386	3.715587
N	1.403730	0.599032	2.730159
N	4.281543	0.916445	2.780350
N	4.549210	-1.831696	3.628459
C	2.017672	-3.371459	4.133393
C	0.816963	-4.126962	4.464162
C	-0.239623	-3.279812	4.223203
C	0.337064	-2.030078	3.746611
C	0.077725	0.300772	2.844965
C	-0.758407	1.428489	2.432524
C	0.104900	2.441913	2.066187
C	1.453929	1.892256	2.290191
C	3.952013	2.194488	2.446273
C	5.134687	3.048676	2.339556
C	6.221480	2.228696	2.574131
C	5.652626	0.900560	2.860622
C	5.876681	-1.524958	3.498537
C	6.706665	-2.699248	3.722009

C	5.841739	-3.728857	4.020376
C	4.503183	-3.166546	3.956185
C	3.320538	-3.863067	4.210839
H	3.422686	-4.904762	4.518615
C	-0.402138	-0.914656	3.345252
H	-1.485570	-1.013829	3.435147
C	2.642698	2.621146	2.201961
H	2.535228	3.667963	1.925590
C	6.367905	-0.251606	3.188807
H	7.458243	-0.180055	3.186015
C	1.078465	-2.795188	-0.708469
O	1.503864	-3.281538	0.538538
H	2.108820	-2.613996	0.924269
H	0.609821	-1.790935	-0.618926
H	0.282570	-3.476009	-1.065618
C	2.202217	-2.733970	-1.742654
H	2.993092	-2.040477	-1.412840
H	1.835736	-2.383563	-2.722963
H	2.657186	-3.729787	-1.875114
H	2.678663	-0.534616	6.356267
H	0.796168	-5.162766	4.802899
H	-1.309765	-3.466868	4.311930
H	-1.847338	1.381387	2.441294
H	-0.058680	3.454186	1.696575
H	5.071130	4.118539	2.141010
H	7.297201	2.404269	2.566104
H	7.787881	-2.728393	3.587143
H	6.081837	-4.764319	4.261700

#### Al\_TS1

S	3.002177	0.338598	5.368369
O	3.048500	-1.188203	1.559236
Fe	3.028463	-0.606580	3.177165
N	1.734371	-2.096534	3.709598
N	1.436946	0.626569	2.767077
N	4.306649	0.923714	2.799471
N	4.585884	-1.823473	3.650162
C	2.046961	-3.366810	4.114534
C	0.845398	-4.120939	4.442101
C	-0.210790	-3.268016	4.216520
C	0.363650	-2.013417	3.752574
C	0.113338	0.325275	2.886419
C	-0.723442	1.450872	2.467676
C	0.137056	2.461662	2.089539

C	1.488836	1.916112	2.309876
C	3.978064	2.198120	2.439206
C	5.164070	3.044065	2.325154
C	6.249391	2.227989	2.583513
C	5.682080	0.905127	2.888909
C	5.908603	-1.516053	3.523438
C	6.736236	-2.696491	3.724068
C	5.868749	-3.729892	4.003139
C	4.530258	-3.165603	3.948431
C	3.349686	-3.866111	4.187871
H	3.448699	-4.912179	4.480430
C	-0.373085	-0.893218	3.375856
H	-1.455982	-0.988100	3.471362
C	2.674877	2.634419	2.187756
H	2.574544	3.674032	1.885037
C	6.400979	-0.236779	3.235194
H	7.490671	-0.162021	3.241460
C	1.241674	-2.994645	-0.258473
O	1.829504	-3.204512	0.964786
H	2.580725	-2.140122	1.316758
H	0.550050	-2.116079	-0.186863
H	0.573100	-3.851737	-0.504960
C	2.237391	-2.745859	-1.397560
H	2.869058	-1.870699	-1.177767
H	1.715984	-2.568326	-2.353577
H	2.896724	-3.620602	-1.520989
H	2.604250	-0.566778	6.330811
H	0.823016	-5.157117	4.779594
H	-1.280652	-3.453272	4.312145
H	-1.812415	1.405330	2.479124
H	-0.030330	3.471759	1.715702
H	5.102091	4.111491	2.113430
H	7.324937	2.404800	2.580987
H	7.817033	-2.726530	3.586073
H	6.106783	-4.766737	4.240539

#### A1\_IM1

S	3.045818	0.343884	5.349930
O	3.096869	-1.234841	1.534549
Fe	3.014696	-0.647885	3.229162
N	1.734503	-2.127612	3.766852
N	1.434005	0.554702	2.746878
N	4.305587	0.904523	2.851610
N	4.577315	-1.860009	3.654138



C	2.057877	-3.406706	4.159336
C	0.854353	-4.161655	4.477726
C	-0.204386	-3.308344	4.259832
C	0.365230	-2.047871	3.807943
C	0.103474	0.263863	2.904435
C	-0.725888	1.391054	2.488102
C	0.135871	2.392416	2.082476
C	1.487702	1.849081	2.291395
C	3.965377	2.170903	2.466123
C	5.148356	3.024039	2.362760
C	6.234601	2.217391	2.645433
C	5.671614	0.891206	2.954643
C	5.903549	-1.534263	3.544468
C	6.732564	-2.713030	3.741806
C	5.869478	-3.753211	4.010818
C	4.527455	-3.200395	3.956997
C	3.355472	-3.907416	4.222012
H	3.461609	-4.949834	4.524800
C	-0.382180	-0.935215	3.424069
H	-1.463505	-1.029394	3.532932
C	2.667633	2.584230	2.180601
H	2.556944	3.619979	1.869917
C	6.397534	-0.253445	3.291754
H	7.486758	-0.175678	3.302033
C	1.512792	-2.952755	-0.905133
O	0.915412	-1.893342	-0.292732
H	2.297668	-1.011883	1.020145
H	0.817123	-3.441224	-1.627815
H	1.605591	-3.701470	-0.074427
C	2.892400	-2.686095	-1.507357
H	2.824497	-1.956763	-2.330792
H	3.321955	-3.616643	-1.913800
H	3.565948	-2.283531	-0.735927
H	2.634950	-0.541015	6.325886
H	0.832405	-5.199320	4.810648
H	-1.274397	-3.493693	4.353590
H	-1.814630	1.352555	2.523099
H	-0.033447	3.397368	1.695864
H	5.085861	4.091412	2.150921
H	7.309001	2.400648	2.657555
H	7.814750	-2.737705	3.614014
H	6.114886	-4.789011	4.245253

A1\_IM2

S	3.126146	0.362019	5.293931
O	3.260405	-1.023801	1.372177
Fe	3.157476	-0.576592	3.128083
N	1.914471	-2.094740	3.589372
N	1.563009	0.641652	2.704085
N	4.422402	0.997545	2.810496
N	4.739683	-1.775199	3.586331
C	2.246297	-3.371346	4.001246
C	1.048362	-4.133427	4.320396
C	-0.016807	-3.286331	4.100883
C	0.539229	-2.025262	3.641663
C	0.242463	0.310839	2.809009
C	-0.607439	1.425484	2.390751
C	0.238010	2.452558	2.021993
C	1.598757	1.936140	2.255765
C	4.065588	2.277093	2.470759
C	5.235274	3.142136	2.406693
C	6.335033	2.333932	2.636591
C	5.792700	0.998522	2.913005
C	6.062734	-1.426683	3.487108
C	6.911853	-2.591351	3.687462
C	6.065659	-3.646453	3.946746
C	4.712563	-3.118218	3.876951
C	3.548475	-3.852800	4.101571
H	3.668263	-4.894322	4.404331
C	-0.223318	-0.916578	3.279537
H	-1.303711	-1.034807	3.371549
C	2.770193	2.686232	2.162653
H	2.670925	3.715289	1.820930
C	6.536125	-0.141036	3.226686
H	7.623126	-0.039927	3.234606
C	1.802002	-2.906792	-0.827170
O	0.679099	-2.602364	-1.514193
H	3.670770	-0.315333	0.830208
H	1.653525	-3.800803	-0.172795
H	1.927407	-2.086190	-0.063450
C	3.088825	-3.002346	-1.649312
H	3.051345	-3.853875	-2.349323
H	3.957738	-3.137969	-0.985320
H	3.235691	-2.086271	-2.243725
H	2.689371	-0.546706	6.236159
H	1.019300	-5.168151	4.661818
H	-1.083065	-3.480096	4.217562
H	-1.695303	1.357568	2.393477

H	0.054963	3.461266	1.651765
H	5.166578	4.223467	2.288079
H	7.405410	2.538274	2.612034
H	7.995469	-2.600219	3.570139
H	6.325598	-4.678020	4.184165

#### A1\_TS2

S	3.106604	0.368589	5.318446
O	3.219738	-1.059645	1.304517
Fe	3.153536	-0.567741	3.144360
N	1.904625	-2.096908	3.586082
N	1.557992	0.641610	2.697135
N	4.415099	0.984906	2.785276
N	4.732086	-1.779227	3.568018
C	2.234999	-3.372088	4.001966
C	1.037185	-4.131623	4.325922
C	-0.027388	-3.283812	4.104601
C	0.529876	-2.025490	3.640528
C	0.236494	0.310580	2.804917
C	-0.613248	1.424761	2.386437
C	0.231772	2.451336	2.014267
C	1.592009	1.934489	2.244979
C	4.058948	2.269213	2.452052
C	5.227986	3.133234	2.395692
C	6.328076	2.324113	2.624509
C	5.787307	0.988137	2.893224
C	6.056773	-1.434451	3.470554
C	6.902263	-2.599008	3.677331
C	6.053351	-3.651978	3.940035
C	4.701842	-3.122381	3.867543
C	3.537792	-3.854102	4.099720
H	3.657738	-4.894610	4.405864
C	-0.230455	-0.915254	3.276960
H	-1.310954	-1.031905	3.367689
C	2.764833	2.682257	2.146614
H	2.667082	3.711932	1.806251
C	6.531614	-0.149790	3.208206
H	7.618469	-0.048109	3.219017
C	2.024108	-2.767904	-0.424292
O	0.872729	-2.310270	-0.819702
H	3.643355	-0.355615	0.761965
H	1.982362	-3.589871	0.341495
H	2.475863	-1.911556	0.354801
C	3.115648	-2.995312	-1.476636

H	2.855524	-3.854051	-2.121249
H	4.089079	-3.207375	-1.003854
H	3.214405	-2.111326	-2.127625
H	2.677580	-0.548641	6.255982
H	1.008492	-5.165989	4.668458
H	-1.094024	-3.477058	4.218666
H	-1.701069	1.356164	2.388782
H	0.048828	3.459809	1.643349
H	5.159682	4.215217	2.282936
H	7.398175	2.530463	2.605187
H	7.986138	-2.610240	3.562628
H	6.313023	-4.682989	4.180148

### A1\_PC

S	2.994105	0.450164	5.593056
O	2.957945	-1.036304	0.527529
Fe	3.123322	-0.538806	3.429659
N	1.877468	-2.106013	3.690709
N	1.545504	0.572759	2.674086
N	4.392831	0.942637	2.851282
N	4.697972	-1.805452	3.622589
C	2.201478	-3.387512	4.092824
C	1.002158	-4.154373	4.391940
C	-0.061631	-3.308651	4.163443
C	0.500805	-2.045881	3.716003
C	0.210408	0.267571	2.813750
C	-0.628890	1.383423	2.396556
C	0.224443	2.402954	2.010614
C	1.577958	1.879148	2.232902
C	4.044135	2.219347	2.482343
C	5.212433	3.086665	2.412425
C	6.310730	2.283136	2.659622
C	5.765598	0.952901	2.953776
C	6.027811	-1.471494	3.518180
C	6.869209	-2.640347	3.709021
C	6.017181	-3.689290	3.977290
C	4.669243	-3.150819	3.925403
C	3.503913	-3.873987	4.178530
H	3.622372	-4.916742	4.478136
C	-0.258553	-0.943486	3.322827
H	-1.339367	-1.055316	3.419928
C	2.753766	2.626368	2.151925
H	2.662043	3.655955	1.807974
C	6.508487	-0.185805	3.268605

H	7.596181	-0.088712	3.274498
C	0.521094	-3.552219	-1.851226
O	0.057436	-4.642533	-1.610497
H	3.549557	-0.334382	0.179967
H	-0.164865	-2.686758	-2.064457
H	2.249352	-0.532116	0.960799
C	1.981692	-3.222072	-1.887705
H	2.231067	-2.507370	-1.078774
H	2.227948	-2.718080	-2.839253
H	2.582299	-4.135834	-1.772168
H	2.604151	-0.529180	6.483655
H	0.974306	-5.192149	4.724073
H	-1.129287	-3.506025	4.259466
H	-1.717454	1.333398	2.420895
H	0.046078	3.411671	1.638132
H	5.136772	4.167630	2.294712
H	7.380896	2.488998	2.638800
H	7.952522	-2.653398	3.589314
H	6.274928	-4.721202	4.215598

#### A2\_RC

S	3.062452	0.460339	5.570844
O	2.903357	-1.124125	1.718129
Fe	2.864718	-0.587806	3.256957
N	1.607187	-2.054562	3.915274
N	1.280948	0.647739	2.936702
N	4.155058	0.970619	2.920061
N	4.444807	-1.774147	3.774800
C	1.926944	-3.336519	4.289856
C	0.728373	-4.108069	4.603008
C	-0.332144	-3.256740	4.399459
C	0.240375	-1.989071	3.967808
C	-0.037377	0.353780	3.114872
C	-0.889194	1.479320	2.737018
C	-0.045231	2.483627	2.307105
C	1.314325	1.934049	2.475281
C	3.816871	2.241265	2.563136
C	4.997005	3.099253	2.450202
C	6.086689	2.291536	2.713660
C	5.525694	0.962751	3.005635
C	5.768538	-1.466416	3.612202
C	6.604817	-2.645103	3.785288
C	5.747774	-3.680296	4.080576
C	4.407008	-3.117340	4.070160

C	3.233823	-3.825170	4.332756
H	3.347671	-4.874851	4.607940
C	-0.506039	-0.865224	3.616204
H	-1.585749	-0.965047	3.741991
C	2.502536	2.655280	2.321854
H	2.389873	3.687210	1.997007
C	6.251052	-0.189442	3.313194
H	7.340903	-0.117376	3.287156
C	1.730717	-2.859377	-1.008059
O	1.022493	-2.817227	-2.240891
H	1.603024	-2.368401	-2.891687
H	2.194590	-1.883037	-0.777665
H	2.561339	-3.597109	-1.055409
C	0.783122	-3.236081	0.116366
H	0.356885	-4.241508	-0.034002
H	-0.051238	-2.517084	0.164522
H	1.313007	-3.205579	1.079777
H	2.614420	-0.392749	6.558698
H	0.712628	-5.148091	4.928849
H	-1.403347	-3.442904	4.476500
H	-1.973338	1.409928	2.825801
H	-0.223466	3.486942	1.920248
H	4.939591	4.168818	2.248208
H	7.160447	2.477448	2.737036
H	7.683040	-2.667174	3.627125
H	5.993632	-4.720373	4.294726

## A2\_TS1

S	2.950785	0.369441	5.436560
O	2.809721	-1.162949	1.613859
Fe	2.859953	-0.610558	3.236245
N	1.579968	-2.109552	3.854532
N	1.257995	0.624069	2.916698
N	4.125217	0.909810	2.846829
N	4.420591	-1.837893	3.669834
C	1.903316	-3.387786	4.234116
C	0.703947	-4.147657	4.571364
C	-0.354959	-3.289783	4.377519
C	0.218524	-2.027152	3.931627
C	-0.061465	0.324504	3.117743
C	-0.913142	1.459421	2.762360
C	-0.073644	2.464961	2.328227
C	1.288687	1.910554	2.466122
C	3.781906	2.190476	2.495012

C	4.966479	3.039883	2.384192
C	6.054493	2.232410	2.657153
C	5.496469	0.902648	2.947710
C	5.742569	-1.522507	3.538258
C	6.577564	-2.700356	3.725835
C	5.717944	-3.735333	4.014720
C	4.374475	-3.176694	3.983566
C	3.206863	-3.884229	4.265923
H	3.321973	-4.928247	4.560769
C	-0.530041	-0.893905	3.604915
H	-1.607178	-0.988612	3.750818
C	2.477155	2.623763	2.280412
H	2.369072	3.661651	1.974800
C	6.227931	-0.240849	3.272209
H	7.317278	-0.162600	3.272855
C	1.993021	-2.850086	-0.155461
O	1.446004	-2.345332	-1.313959
H	2.147373	-1.970702	-1.900510
H	2.292920	-1.939691	0.683398
H	2.998917	-3.291406	-0.303989
C	1.020121	-3.755148	0.560915
H	0.787664	-4.645374	-0.052676
H	0.076185	-3.222164	0.760819
H	1.430650	-4.082502	1.526294
H	2.528860	-0.479817	6.439100
H	0.686911	-5.183289	4.910839
H	-1.425539	-3.467994	4.478352
H	-1.995951	1.397802	2.870963
H	-0.252962	3.472680	1.953509
H	4.904058	4.107201	2.172053
H	7.128051	2.418510	2.687258
H	7.657897	-2.719471	3.582370
H	5.965355	-4.770708	4.248928

#### A2\_IM1

S	3.042609	0.489753	5.548891
O	2.984855	-1.091633	1.726384
Fe	2.951281	-0.528164	3.442805
N	1.662444	-1.997134	3.998508
N	1.375030	0.702032	2.990855
N	4.249003	1.005504	3.039505
N	4.493848	-1.769222	3.809939
C	1.968305	-3.293880	4.343810
C	0.754276	-4.047917	4.630255

C	-0.293478	-3.177948	4.431500
C	0.294004	-1.904720	4.039152
C	0.048304	0.442580	3.220246
C	-0.770327	1.593924	2.860078
C	0.088043	2.558610	2.366135
C	1.436614	1.986454	2.507433
C	3.922039	2.269957	2.632511
C	5.114897	3.107553	2.534572
C	6.190669	2.291507	2.833529
C	5.615011	0.975205	3.140049
C	5.823056	-1.464326	3.663243
C	6.637040	-2.659833	3.802921
C	5.765591	-3.690683	4.075422
C	4.431990	-3.115793	4.083300
C	3.259201	-3.813596	4.365252
H	3.359941	-4.867001	4.627675
C	-0.440911	-0.766340	3.714099
H	-1.519321	-0.859871	3.838755
C	2.629402	2.688400	2.325463
H	2.539166	3.697316	1.930018
C	6.331884	-0.187948	3.429605
H	7.422061	-0.129273	3.398727
C	1.506410	-2.557417	-0.851676
O	1.089612	-2.707581	-2.147769
H	1.736197	-2.257277	-2.741457
H	2.324799	-0.614954	1.197099
H	2.563493	-2.314955	-0.690865
C	0.734408	-3.303077	0.175825
H	0.838082	-4.406524	0.076207
H	-0.348685	-3.092302	0.100156
H	1.080266	-3.019381	1.180357
H	2.591537	-0.355951	6.541697
H	0.722671	-5.092383	4.940350
H	-1.366580	-3.361732	4.483875
H	-1.848725	1.631108	3.014160
H	-0.086436	3.552479	1.954009
H	5.084846	4.183099	2.360320
H	7.265442	2.470304	2.864515
H	7.714663	-2.692103	3.642441
H	6.002022	-4.734275	4.282988

## A2\_IM2

S	3.006289	0.587899	5.761961
O	2.363181	-1.834272	0.001494



Fe	2.855286	-0.483732	3.632962
N	1.574315	-2.017347	3.969150
N	1.295814	0.671387	3.003586
N	4.144732	0.935169	2.944154
N	4.392144	-1.809053	3.729542
C	1.875778	-3.319101	4.319475
C	0.666601	-4.070828	4.619673
C	-0.383115	-3.200521	4.423721
C	0.201561	-1.931315	4.026709
C	-0.028808	0.428651	3.264140
C	-0.849904	1.587084	2.939439
C	-0.006560	2.527880	2.381659
C	1.341204	1.949036	2.495981
C	3.822957	2.214072	2.559685
C	5.009894	3.053755	2.473802
C	6.089290	2.233033	2.751715
C	5.517927	0.916483	3.045653
C	5.728545	-1.515714	3.582576
C	6.540989	-2.707787	3.742917
C	5.667868	-3.732731	4.035707
C	4.337500	-3.153198	4.035046
C	3.164935	-3.842872	4.336463
H	3.264001	-4.892873	4.613149
C	-0.530885	-0.783285	3.733452
H	-1.614056	-0.862266	3.842738
C	2.529080	2.643218	2.270326
H	2.442016	3.648498	1.860683
C	6.239231	-0.242264	3.337689
H	7.329716	-0.179915	3.313197
C	2.160366	-2.993138	-0.773416
O	1.425194	-2.747972	-1.947973
H	2.011126	-2.253172	-2.566454
H	2.987421	-1.248915	-0.449962
H	3.149425	-3.425237	-1.047883
C	1.381445	-3.975121	0.077976
H	1.202334	-4.908476	-0.476756
H	0.409311	-3.531495	0.344416
H	1.926134	-4.195545	1.007128
H	2.567292	-0.323436	6.700628
H	0.637377	-5.112694	4.938622
H	-1.456195	-3.378623	4.493339
H	-1.898483	1.653469	3.229509
H	-0.202673	3.502882	1.935591
H	4.972780	4.135084	2.341831

H	7.163304	2.418112	2.769227
H	7.620197	-2.741120	3.593704
H	5.905356	-4.771791	4.263784

**A2\_TS2**

S	3.001093	0.595129	5.779578
O	1.852488	-2.060815	-0.621763
Fe	2.850863	-0.469678	3.655152
N	1.573556	-2.013011	3.972727
N	1.287814	0.675612	3.014144
N	4.135222	0.946707	2.957880
N	4.389040	-1.797510	3.735816
C	1.877652	-3.315066	4.324149
C	0.670634	-4.069846	4.621705
C	-0.381774	-3.202225	4.424863
C	0.199223	-1.931217	4.029826
C	-0.037761	0.429790	3.272518
C	-0.860989	1.586584	2.948409
C	-0.018555	2.529847	2.392754
C	1.330312	1.954505	2.507767
C	3.811258	2.224563	2.570652
C	4.997188	3.065050	2.478614
C	6.078200	2.246523	2.754924
C	5.509047	0.930200	3.054458
C	5.725221	-1.501858	3.586856
C	6.540310	-2.692300	3.743849
C	5.670236	-3.719551	4.037813
C	4.338689	-3.143046	4.040030
C	3.168227	-3.835549	4.342287
H	3.270745	-4.885193	4.618906
C	-0.536743	-0.784828	3.737956
H	-1.619619	-0.868293	3.845846
C	2.516699	2.651096	2.281731
H	2.427469	3.654677	1.868542
C	6.233010	-0.227088	3.344115
H	7.323200	-0.162796	3.317856
C	1.355790	-3.614569	-0.876069
O	0.386998	-3.258672	-1.695861
H	0.955169	-2.091223	-1.354062
H	2.650340	-1.873093	-1.150327
H	2.261365	-4.093007	-1.318637
C	0.993199	-4.181161	0.474993
H	0.560407	-5.181834	0.308010
H	0.222404	-3.551845	0.942993

H	1.862683	-4.268669	1.143709
H	2.565308	-0.320355	6.715701
H	0.643652	-5.112327	4.938838
H	-1.454275	-3.384142	4.493527
H	-1.910585	1.650455	3.235353
H	-0.216408	3.504814	1.947377
H	4.958198	4.145715	2.341834
H	7.152163	2.432414	2.765573
H	7.619099	-2.723339	3.591153
H	5.910676	-4.758776	4.262015

### A2\_PC

S	2.962614	0.604643	5.808799
O	3.069677	-2.074757	-0.798186
Fe	2.796856	-0.460982	3.689562
N	1.524668	-2.008100	4.009542
N	1.222919	0.671765	3.041614
N	4.069869	0.953852	2.969549
N	4.339055	-1.782927	3.765301
C	1.835946	-3.309450	4.358754
C	0.633706	-4.069303	4.659213
C	-0.423725	-3.205445	4.468544
C	0.149598	-1.931446	4.074285
C	-0.101839	0.425061	3.310356
C	-0.931240	1.576415	2.981818
C	-0.093759	2.516539	2.412385
C	1.257759	1.947647	2.525868
C	3.739008	2.227803	2.572830
C	4.921672	3.071471	2.466626
C	6.006904	2.259385	2.746019
C	5.444351	0.944215	3.062319
C	5.673411	-1.481902	3.615376
C	6.494184	-2.668952	3.772063
C	5.628727	-3.700343	4.063697
C	4.294797	-3.128968	4.067760
C	3.128226	-3.825460	4.371339
H	3.234597	-4.875988	4.642031
C	-0.593645	-0.788565	3.784924
H	-1.675524	-0.873816	3.901982
C	2.440962	2.646705	2.288680
H	2.344513	3.647435	1.870818
C	6.174149	-0.205812	3.365796
H	7.263842	-0.135952	3.341032
C	0.330159	-2.796393	-0.244080

O	-0.361181	-2.860664	-1.238571
H	3.138808	-1.865943	-1.760810
H	3.266421	-1.227399	-0.373868
H	0.599527	-1.804846	0.192157
C	0.878030	-3.979394	0.497957
H	1.976876	-3.905794	0.450553
H	0.528219	-4.918575	0.043978
H	0.587112	-3.930378	1.561299
H	2.538498	-0.316516	6.744715
H	0.612971	-5.112365	4.974902
H	-1.495254	-3.392325	4.539037
H	-1.979915	1.636552	3.272900
H	-0.296715	3.484784	1.954808
H	4.880777	4.150366	2.317025
H	7.080435	2.448045	2.748501
H	7.572817	-2.697377	3.617760
H	5.873843	-4.740180	4.279852

#### **B\_RC**

S	2.791786000	0.299173000	5.490747000
O	2.864994000	-1.140783000	1.609506000
Fe	2.817964000	-0.682599000	3.184482000
N	1.606146000	-2.207844000	3.761022000
N	1.193873000	0.523083000	2.882818000
N	4.055517000	0.927736000	2.929500000
N	4.429498000	-1.841138000	3.638976000
C	1.967143000	-3.482163000	4.120379000
C	0.796486000	-4.283890000	4.449427000
C	-0.290569000	-3.458884000	4.275938000
C	0.237219000	-2.175132000	3.834524000
C	-0.116489000	0.179033000	3.025300000
C	-0.997837000	1.294813000	2.687168000
C	-0.177864000	2.354071000	2.352845000
C	1.193110000	1.837135000	2.502734000
C	3.684649000	2.203568000	2.627680000
C	4.838717000	3.095809000	2.580767000
C	5.945115000	2.323246000	2.866723000
C	5.425059000	0.960325000	3.036143000
C	5.740171000	-1.493928000	3.463248000
C	6.615247000	-2.643534000	3.619880000
C	5.799094000	-3.708039000	3.923040000
C	4.439430000	-3.189243000	3.914978000
C	3.288849000	-3.937503000	4.155741000
H	3.438098000	-4.990058000	4.403930000

C	-0.544383000	-1.067844000	3.497456000
H	-1.620368000	-1.200783000	3.627849000
C	2.360943000	2.598742000	2.401268000
H	2.228581000	3.651170000	2.152329000
C	6.185722000	-0.192901000	3.217009000
H	7.271229000	-0.083438000	3.164385000
C	0.542703000	-2.273542000	-0.579965000
O	1.028593000	-0.969508000	-0.372279000
H	1.742656000	-0.995406000	0.302384000
H	0.296897000	-2.767093000	0.382926000
H	1.303874000	-2.916584000	-1.073653000
C	-0.701601000	-2.204650000	-1.453037000
H	-1.489573000	-1.616267000	-0.954382000
H	-1.099536000	-3.210488000	-1.667667000
H	-0.465344000	-1.704360000	-2.406540000
H	2.462685000	-0.623962000	6.462271000
H	0.822189000	-5.318831000	4.790457000
H	-1.352627000	-3.665046000	4.408591000
H	-2.083948000	1.203002000	2.686345000
H	-0.387559000	3.377737000	2.042678000
H	4.770668000	4.154159000	2.329110000
H	6.999943000	2.566407000	2.994308000
H	7.696240000	-2.613837000	3.483358000
H	6.087325000	-4.730376000	4.167616000

### **B\_TS1**

S	2.767247000	0.277815000	5.447613000
O	2.854594000	-1.104834000	1.570312000
Fe	2.817385000	-0.651710000	3.233758000
N	1.603743000	-2.191615000	3.757151000
N	1.203318000	0.555864000	2.905902000
N	4.060010000	0.951425000	2.953015000
N	4.423808000	-1.835215000	3.614673000
C	1.961478000	-3.461223000	4.121531000
C	0.786266000	-4.259707000	4.445459000
C	-0.299579000	-3.437502000	4.251831000
C	0.228458000	-2.153763000	3.808806000
C	-0.103507000	0.203350000	3.014250000
C	-0.981139000	1.326063000	2.687451000
C	-0.160078000	2.395427000	2.390948000
C	1.212183000	1.883090000	2.545449000
C	3.694485000	2.225811000	2.652460000
C	4.857466000	3.106824000	2.589157000
C	5.959838000	2.327464000	2.868603000

C	5.433435000	0.966372000	3.045905000
C	5.730517000	-1.488873000	3.441719000
C	6.602055000	-2.642654000	3.595882000
C	5.785376000	-3.705454000	3.902811000
C	4.425415000	-3.186619000	3.898191000
C	3.282012000	-3.928532000	4.157517000
H	3.426621000	-4.979685000	4.411750000
C	-0.546747000	-1.056816000	3.451695000
H	-1.624903000	-1.193690000	3.551558000
C	2.373036000	2.640222000	2.438793000
H	2.247997000	3.694107000	2.194223000
C	6.189352000	-0.185991000	3.216505000
H	7.275341000	-0.083519000	3.170499000
C	0.658015000	-2.192872000	-0.470691000
O	1.024124000	-0.935457000	-0.054851000
H	2.010794000	-0.976859000	0.916943000
H	0.520461000	-2.892647000	0.386574000
H	1.493510000	-2.641108000	-1.067342000
C	-0.595639000	-2.168069000	-1.348693000
H	-1.451663000	-1.777515000	-0.774162000
H	-0.853435000	-3.178950000	-1.707429000
H	-0.440397000	-1.505849000	-2.215558000
H	2.440801000	-0.643468000	6.421789000
H	0.808401000	-5.294089000	4.788431000
H	-1.362337000	-3.642498000	4.380629000
H	-2.067090000	1.233867000	2.670814000
H	-0.370321000	3.424817000	2.100741000
H	4.793238000	4.162850000	2.326956000
H	7.017293000	2.564253000	2.986017000
H	7.682729000	-2.614651000	3.456504000
H	6.073818000	-4.727016000	4.150356000

### **B\_IM1**

S	2.757336000	0.256212000	5.434831000
O	3.010035000	-1.189140000	1.586657000
Fe	2.869447000	-0.691745000	3.281660000
N	1.644669000	-2.239458000	3.761403000
N	1.240270000	0.481074000	2.844870000
N	4.095514000	0.919892000	2.988046000
N	4.466971000	-1.859640000	3.669480000
C	2.015123000	-3.513386000	4.131780000
C	0.839241000	-4.315033000	4.439727000
C	-0.249137000	-3.497034000	4.240254000
C	0.276415000	-2.211512000	3.801942000

C	-0.076403000	0.128806000	2.982997000
C	-0.948984000	1.248196000	2.644712000
C	-0.126771000	2.314687000	2.331564000
C	1.244633000	1.807029000	2.487437000
C	3.716158000	2.190173000	2.657564000
C	4.872104000	3.079486000	2.609686000
C	5.976274000	2.313214000	2.923032000
C	5.460429000	0.949978000	3.103542000
C	5.778653000	-1.498731000	3.499098000
C	6.649017000	-2.652135000	3.640503000
C	5.832828000	-3.720301000	3.934513000
C	4.472222000	-3.207717000	3.934528000
C	3.329603000	-3.966615000	4.185150000
H	3.483265000	-5.015141000	4.444099000
C	-0.514055000	-1.116871000	3.437261000
H	-1.590005000	-1.253745000	3.558235000
C	2.402834000	2.581557000	2.404162000
H	2.268942000	3.632390000	2.152780000
C	6.229638000	-0.198715000	3.288276000
H	7.314577000	-0.086545000	3.241428000
C	0.263995000	-2.029970000	-0.105120000
O	1.000298000	-0.899294000	-0.250658000
H	2.277037000	-0.892577000	0.997414000
H	-0.274686000	-1.921224000	0.879812000
H	0.936982000	-2.895631000	0.108271000
C	-0.718364000	-2.317204000	-1.237502000
H	-1.439502000	-1.491815000	-1.347872000
H	-1.274994000	-3.250251000	-1.051755000
H	-0.178173000	-2.419184000	-2.192552000
H	2.433534000	-0.666978000	6.408083000
H	0.862060000	-5.347434000	4.788574000
H	-1.311275000	-3.707192000	4.365805000
H	-2.035376000	1.160481000	2.633618000
H	-0.339540000	3.341634000	2.034623000
H	4.806697000	4.132528000	2.336025000
H	7.028384000	2.561320000	3.062945000
H	7.729658000	-2.622496000	3.501205000
H	6.122295000	-4.743064000	4.175825000

### **B\_TS2**

S	2.781371000	0.345347000	5.536014000
O	2.882040000	-1.021388000	1.608227000
Fe	2.812761000	-0.598953000	3.417920000
N	1.599717000	-2.127416000	3.850841000

N	1.200743000	0.610766000	3.012542000
N	4.060166000	0.994937000	3.062608000
N	4.403283000	-1.792949000	3.730639000
C	1.952135000	-3.421970000	4.183382000
C	0.770408000	-4.208384000	4.492442000
C	-0.308689000	-3.364783000	4.343417000
C	0.222479000	-2.075244000	3.937050000
C	-0.116478000	0.274118000	3.160655000
C	-0.980588000	1.389074000	2.788411000
C	-0.150007000	2.433738000	2.428266000
C	1.217476000	1.922716000	2.606047000
C	3.693405000	2.273650000	2.733486000
C	4.857811000	3.147515000	2.685322000
C	5.952476000	2.373970000	3.020949000
C	5.425886000	1.017946000	3.199480000
C	5.722922000	-1.433806000	3.580350000
C	6.585041000	-2.594891000	3.703698000
C	5.762269000	-3.665924000	3.966646000
C	4.404324000	-3.148292000	3.969889000
C	3.258600000	-3.901343000	4.205615000
H	3.400875000	-4.958278000	4.433156000
C	-0.558885000	-0.964585000	3.628780000
H	-1.633942000	-1.091244000	3.764644000
C	2.383774000	2.680254000	2.485699000
H	2.261068000	3.726169000	2.209487000
C	6.185372000	-0.136030000	3.393676000
H	7.271262000	-0.030241000	3.361798000
C	1.043801000	-2.300922000	0.061041000
O	0.877912000	-1.370902000	-0.840126000
H	2.800143000	-0.215191000	1.072274000
H	0.185013000	-2.449781000	0.766857000
H	1.830523000	-1.782321000	0.846099000
C	1.698237000	-3.616257000	-0.365824000
H	0.999750000	-4.208628000	-0.983186000
H	1.977736000	-4.222477000	0.510892000
H	2.599099000	-3.413639000	-0.966170000
H	2.451660000	-0.593828000	6.491831000
H	0.783979000	-5.252129000	4.806255000
H	-1.372918000	-3.567803000	4.462860000
H	-2.067616000	1.309329000	2.779694000
H	-0.352255000	3.446525000	2.079806000
H	4.807720000	4.195385000	2.389476000
H	7.003596000	2.617304000	3.175871000
H	7.666545000	-2.570630000	3.570185000



H	6.047721000	-4.694374000	4.187720000
<b>B_TS3</b>			
S	2.728275000	0.274458000	5.490906000
O	2.987591000	-1.043516000	1.653803000
Fe	2.778598000	-0.687551000	3.329685000
N	1.575370000	-2.225524000	3.791506000
N	1.153271000	0.498752000	2.948574000
N	4.023643000	0.914422000	3.004674000
N	4.398502000	-1.859634000	3.724845000
C	1.947331000	-3.507535000	4.149494000
C	0.776299000	-4.302690000	4.475762000
C	-0.313629000	-3.475299000	4.316823000
C	0.200840000	-2.186492000	3.887310000
C	-0.160347000	0.157616000	3.109310000
C	-1.032861000	1.271483000	2.747800000
C	-0.208683000	2.319926000	2.386310000
C	1.163550000	1.808729000	2.545285000
C	3.641280000	2.180807000	2.656414000
C	4.800130000	3.063336000	2.578908000
C	5.906477000	2.301065000	2.896903000
C	5.390417000	0.943752000	3.115087000
C	5.709384000	-1.496286000	3.557444000
C	6.582110000	-2.651926000	3.688192000
C	5.767359000	-3.724604000	3.962523000
C	4.405478000	-3.211578000	3.965832000
C	3.260455000	-3.970442000	4.189113000
H	3.408386000	-5.023962000	4.429454000
C	-0.593088000	-1.083806000	3.576950000
H	-1.666205000	-1.218646000	3.720913000
C	2.325701000	2.572110000	2.416426000
H	2.192091000	3.616499000	2.138827000
C	6.159552000	-0.199361000	3.329388000
H	7.244440000	-0.089591000	3.279123000
C	1.600691000	-1.976561000	-0.135304000
O	1.998277000	-0.856363000	-0.850585000
H	2.823299000	-0.548169000	-0.437135000
H	2.020283000	-1.759454000	0.988969000
H	2.180791000	-2.885868000	-0.398145000
C	0.110575000	-2.183150000	-0.162449000
H	-0.411493000	-1.309482000	0.257306000
H	-0.171757000	-3.073721000	0.419541000
H	-0.236368000	-2.319994000	-1.202662000
H	2.421550000	-0.663618000	6.455417000

H	0.800778000	-5.338778000	4.813383000
H	-1.374042000	-3.687962000	4.452344000
H	-2.119609000	1.187886000	2.755241000
H	-0.418714000	3.335976000	2.052250000
H	4.734498000	4.112736000	2.291646000
H	6.961422000	2.548447000	3.015051000
H	7.662739000	-2.621529000	3.548969000
H	6.057815000	-4.749717000	4.192401000

**B\_PC**

S	2.701262000	0.289896000	5.522651000
O	3.090701000	-1.174712000	1.415137000
Fe	2.839518000	-0.588830000	3.462844000
N	1.608327000	-2.174773000	3.773208000
N	1.251159000	0.572584000	2.912138000
N	4.101273000	0.964795000	3.016983000
N	4.427752000	-1.813504000	3.750545000
C	1.955040000	-3.461995000	4.117192000
C	0.768974000	-4.255424000	4.417362000
C	-0.306846000	-3.412580000	4.249246000
C	0.240475000	-2.121530000	3.843999000
C	-0.071533000	0.245720000	3.075219000
C	-0.932360000	1.374216000	2.727361000
C	-0.098219000	2.417664000	2.371076000
C	1.267184000	1.888649000	2.519378000
C	3.747153000	2.240178000	2.660506000
C	4.911564000	3.119856000	2.636939000
C	5.994875000	2.354705000	3.019523000
C	5.462563000	0.997576000	3.206902000
C	5.747806000	-1.455644000	3.648183000
C	6.610959000	-2.617509000	3.790945000
C	5.780551000	-3.691906000	4.011803000
C	4.422225000	-3.171795000	3.977478000
C	3.268519000	-3.929533000	4.171116000
H	3.410932000	-4.986792000	4.401583000
C	-0.525474000	-0.993740000	3.535003000
H	-1.601971000	-1.105465000	3.678532000
C	2.439667000	2.640658000	2.390781000
H	2.320704000	3.685707000	2.107537000
C	6.212894000	-0.152811000	3.455693000
H	7.299787000	-0.044712000	3.460371000
C	0.463339000	-2.078596000	-0.557930000
O	1.078539000	-1.034224000	-0.453943000
H	3.814643000	-0.591695000	1.141704000

H	-0.388622000	-2.131558000	-1.279953000
H	2.337676000	-0.947786000	0.824263000
C	0.751822000	-3.321838000	0.216941000
H	0.758284000	-4.188973000	-0.464487000
H	-0.068880000	-3.490833000	0.937763000
H	1.698241000	-3.244734000	0.768390000
H	2.407622000	-0.668972000	6.470646000
H	0.779460000	-5.292615000	4.752313000
H	-1.371027000	-3.607554000	4.381801000
H	-2.020500000	1.313066000	2.744049000
H	-0.296350000	3.440786000	2.051652000
H	4.864470000	4.166316000	2.335657000
H	7.040067000	2.601226000	3.206252000
H	7.696725000	-2.593468000	3.698200000
H	6.061006000	-4.723397000	4.224966000