

Oxygen Activation in Extradial Catecholase Dioxygenases – A Density Functional Study

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Supplementary Information

Table 1 Calculated Mössbauer parameters for the native enzyme and substrate with different protonation states of the O₂-adduct.

		Spin	Prot.	δ , mm s ⁻¹	ΔE_Q , mm s ⁻¹
<i>O₂ adduct</i>	WT with native substrate	HS	PII	0.63	0.94
		IS	PI	0.57	1.44
			PII	0.60	0.83
			PIII	0.65	-1.16
			PIV	0.66	-1.23

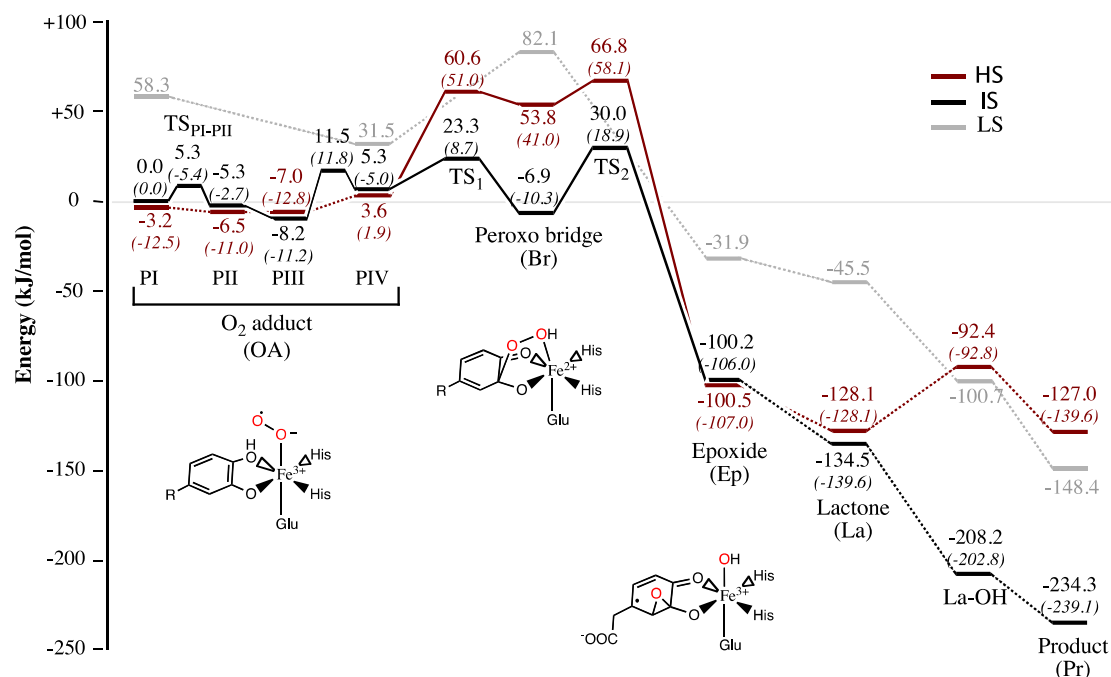


Figure 1 Calculated reaction profile for high, intermediate and low spin states without Van der Waals corrections. Free energies shown in parenthesis.

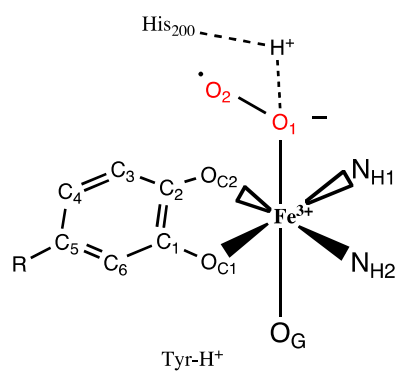


Figure 2 Labelling Scheme.

Table 2 Löwdin unpaired spin densities intermediate spin.

	Rx	O ₂ (pI)	O ₂ (pII)	O ₂ (pIII)	O ₂ (pIV)	4NC	Br
Fe		4.177	4.172	4.072	4.108	4.210	
3O ₂		-0.535	-0.532	-0.468	-0.573	-0.530	
ΣO ₂		-0.754	-0.818	-0.792	-0.864	-0.798	
O _{c1}		0.189	0.171	0.175	0.198	0.155	
O _{c2}		0.059	0.166	0.206	0.190	0.135	
ΣO _{subs}		0.248	0.337	0.380	0.388	0.290	
O _G		0.092	0.076	0.074	0.082	0.087	
N _{H1}		0.052	0.044	0.041	0.038	0.049	
N _{H2}		0.064	0.053	0.048	0.049	0.060	
C _{c1}		-0.005	0.013	0.031	0.012	0.004	
ΣC _{ring}		0.061	0.082	0.126	0.141	0.043	

Table 3 Löwdin unpaired spin densities – 4NC intermediate spin

	Rx	O ₂ (p2)	O ₂ (p3)	Mut O ₂	Native geom
Fe	4.172	4.208		4.202	4.210
O ₁	-0.286	-0.262		-0.304	-0.267
O ₂	-0.532	-0.534		-0.522	-0.530
ΣO ₂	-0.818	-0.796		-0.826	-0.798
O _{c1} (attacked)	0.171	0.158		0.163	0.155
O _{c2}	0.166	0.121		0.160	0.135

ΣO_{subs}	0.337	0.278		0.323	0.290
O_G	0.076	0.092		0.079	0.087
N_{H1} (trans to O_{C1})	0.044	0.051		0.051	0.049
N_{H2}	0.053	0.059		0.048	0.060
C_{C1}	0.013	0.004		0.009	0.004
ΣC_{ring}	0.082	0.043		0.056	0.043

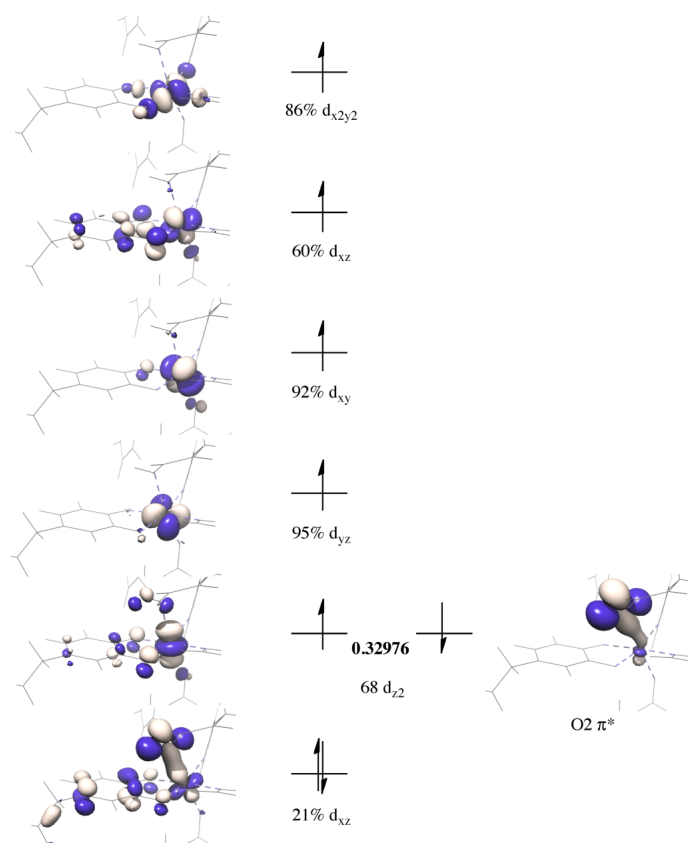


Figure 3 Molecular orbital analysis for the oxygen adduct with a small model lacking Arg243 and with Tyr257 truncated to H_2O .

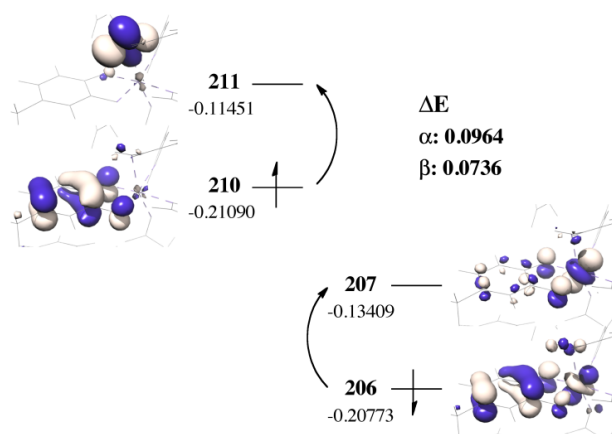


Figure 4 Canonical orbitals for the O₂ adduct (OA⁵) showing the α and β donor and acceptor orbitals for the two electron oxidation of the substrate. Note that this is the O₂ adduct and not the peroxo bridge, (Br⁵) B)

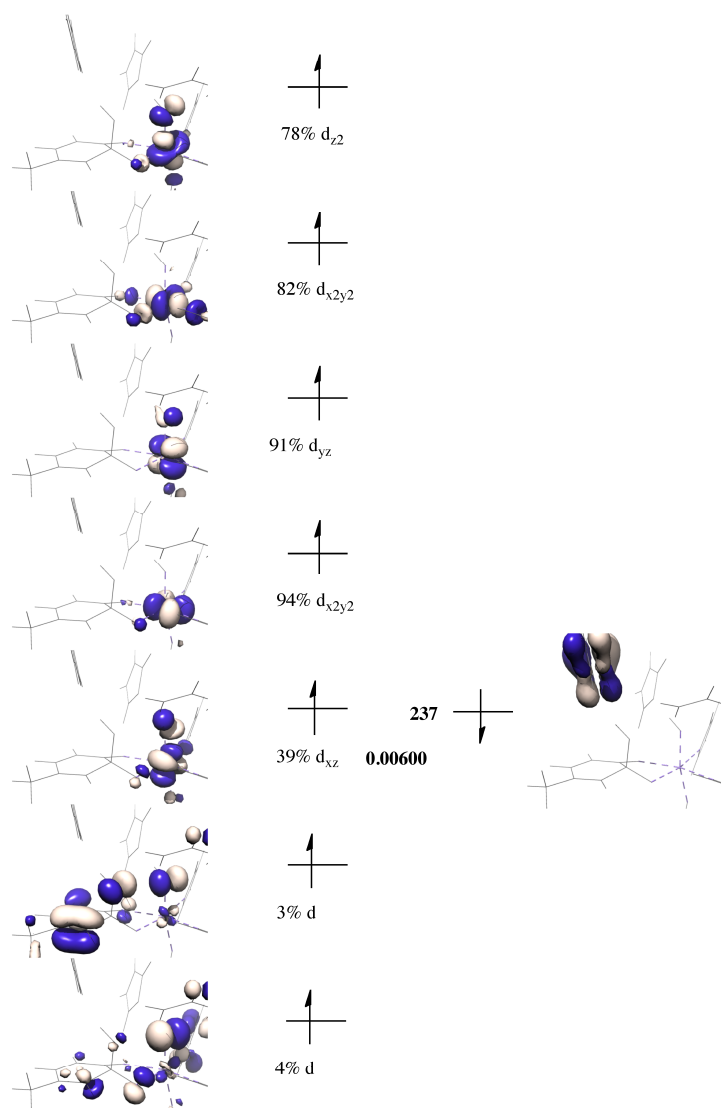


Figure 5 Molecular orbital diagram of the gem-diol intermediate for the model including Tryptophan.

Cartesian Coordinates for Optimised Geometries

O₂ adduct PI

Fe	-1.129795	0.547320	-1.013701
O	-2.661051	1.486835	-0.114846
N	-2.534800	-0.866527	-1.737623
N	-1.152078	2.213105	-2.373487
O	-0.630273	-0.774076	0.312458
O	0.702320	1.410884	-0.153109
C	1.321060	0.490872	0.674368
C	0.579942	-0.690825	0.888166

C	1.100643	-1.704875	1.698430
C	2.328087	-1.536088	2.356862
C	3.038034	-0.340525	2.158916
C	2.545768	0.669057	1.310015
C	-1.821280	3.347130	-2.203793
N	-1.540968	4.204792	-3.206035
C	-0.649593	3.594836	-4.068821
C	-0.414907	2.354737	-3.536238
C	-2.240034	-2.160224	-1.749785
N	-3.260445	-2.859702	-2.274308
C	-4.265765	-1.980171	-2.617880
C	-3.802001	-0.733080	-2.271240
C	-3.264533	1.673365	1.012253
O	-2.706659	1.683986	2.121972
C	2.860722	-2.646626	3.255249
C	1.763426	-3.258204	4.141655
O	1.442406	-2.612688	5.205893
C	-4.762774	1.958941	0.914721
O	1.216077	-4.324861	3.783602
N	2.290669	2.810083	-1.735190
C	3.074123	2.453598	-2.816952
C	3.609158	3.586962	-3.392909
N	3.126273	4.636175	-2.635436
C	2.342815	4.128522	-1.653885
O	-1.910088	-1.992918	2.244042
C	-3.248205	-2.158355	2.409076
C	-4.193862	-1.828373	1.424648
C	-5.552449	-2.065786	1.667411
C	-5.976125	-2.622882	2.881032
C	-5.027384	-2.930632	3.865663
C	-3.671403	-2.697466	3.634676
N	0.628419	-0.107019	4.903019
C	1.043966	1.148490	5.291863
C	0.266472	2.048955	4.607585
N	-0.596065	1.307127	3.822640
C	-0.359281	0.009323	4.017006
N	-1.208723	-5.038176	4.987102
C	-1.560429	-4.410403	6.107970
N	-0.723016	-3.528627	6.652565
N	-2.761089	-4.642707	6.680119
C	-1.044277	-2.359249	-4.775854
C	-0.524826	-3.499451	-3.918330
N	0.676457	-3.294320	-3.326053
O	-1.157619	-4.551616	-3.766629
H	0.228866	1.561400	-3.889327
H	-1.935256	5.134561	-3.311559
H	-2.498022	3.554412	-1.384512
H	-1.059054	-1.424399	-4.200210
H	-2.052119	-2.600927	-5.128884

H	1.019623	-4.007781	-2.687896
H	1.090721	-2.363861	-3.246207
H	3.189165	1.413217	-3.102209
H	3.335830	5.619308	-2.777999
H	1.838821	4.742148	-0.913779
H	-4.276185	0.237275	-2.354935
H	-3.229597	-3.857008	-2.474134
H	-1.311638	-2.588660	-1.396652
H	-3.000177	-4.201985	7.562096
H	-0.299343	-4.809243	4.520840
H	-1.885448	-5.595202	4.476439
H	-0.950844	-3.081604	7.533683
H	0.139989	-3.220836	6.140056
H	0.251055	3.131664	4.612537
H	1.063969	-1.041245	5.137361
H	-1.321240	1.633693	3.150906
H	-0.883221	-0.805259	3.522486
H	-6.282539	-1.813485	0.897102
H	-5.346085	-3.354621	4.819443
H	-3.865699	-1.393606	0.480639
H	-2.919397	-2.925741	4.386511
H	-1.650987	-1.544973	1.389173
H	-5.176074	2.167259	1.908025
H	-4.918731	2.833566	0.266259
H	0.517856	-2.614358	1.835565
H	3.108647	1.589880	1.156140
H	3.990648	-0.186192	2.667119
H	3.658768	-2.253552	3.898598
H	3.287610	-3.451577	2.639872
H	1.367019	1.922851	-0.781074
H	4.275095	3.761153	-4.240894
H	-0.270200	4.082700	-4.958800
H	-0.389400	-2.199101	-5.642801
H	-5.190900	-2.322200	-3.064101
H	-5.325799	1.123600	0.465897
H	-3.352102	-5.417098	6.393199
H	1.839000	1.274602	6.019601
H	-7.029002	-2.820797	3.066701
O	0.087249	-0.307194	-2.447123
O	1.366869	-0.521449	-2.236384

TS PI-PII

Fe	-1.071124	0.520565	-1.039481
O	-2.622384	1.460748	-0.132647
N	-2.524961	-0.889313	-1.733132
N	-1.120201	2.198014	-2.379795
O	-0.615766	-0.827940	0.284425

O	0.778769	1.290152	-0.317583
C	1.372200	0.399903	0.537939
C	0.610077	-0.758363	0.826333
C	1.118928	-1.752974	1.666410
C	2.361147	-1.590784	2.298409
C	3.094685	-0.421203	2.038472
C	2.614229	0.563661	1.153343
C	-1.726687	3.356102	-2.153995
N	-1.451550	4.224583	-3.149118
C	-0.631070	3.593574	-4.064475
C	-0.432415	2.330945	-3.571719
C	-2.237969	-2.183753	-1.755203
N	-3.263708	-2.875698	-2.281330
C	-4.264188	-1.988048	-2.616860
C	-3.792068	-0.745787	-2.262807
C	-3.239917	1.645671	0.984431
O	-2.703273	1.634291	2.106676
C	2.885111	-2.680032	3.229138
C	1.782385	-3.280219	4.117178
O	1.472140	-2.636360	5.186055
C	-4.733213	1.964793	0.867086
O	1.219815	-4.338612	3.757350
N	2.273919	2.643007	-1.825476
C	3.046928	2.350819	-2.935182
C	3.604504	3.520302	-3.407437
N	3.142889	4.509836	-2.558825
C	2.350184	3.950350	-1.623296
O	-1.908284	-2.001789	2.229336
C	-3.245836	-2.163171	2.397257
C	-4.193872	-1.842452	1.411659
C	-5.552222	-2.078157	1.658633
C	-5.975635	-2.623956	2.877796
C	-5.024747	-2.921831	3.863719
C	-3.668942	-2.690688	3.628443
N	0.671500	-0.129780	4.882153
C	1.055353	1.133335	5.280395
C	0.264794	2.018360	4.589945
N	-0.573312	1.260533	3.792726
C	-0.309461	-0.032074	3.986263
N	-1.210966	-5.051129	4.968673
C	-1.558107	-4.414477	6.086064
N	-0.717951	-3.528010	6.618974
N	-2.755959	-4.641327	6.667161
C	-1.114275	-2.488512	-4.871223
C	-0.553188	-3.566476	-3.961977
N	0.673908	-3.321862	-3.441129
O	-1.181471	-4.600418	-3.703267
H	0.154142	1.515999	-3.972426
H	-1.810614	5.171756	-3.219700

H	-2.355909	3.573840	-1.300248
H	-1.335645	-1.589440	-4.279874
H	-2.029615	-2.854912	-5.347139
H	1.026441	-3.969307	-2.740468
H	1.073083	-2.380984	-3.438433
H	3.128584	1.334354	-3.301159
H	3.373589	5.497288	-2.617800
H	1.856824	4.500109	-0.829142
H	-4.260745	0.227937	-2.339115
H	-3.235116	-3.871065	-2.490697
H	-1.309525	-2.619402	-1.412067
H	-2.987729	-4.191639	7.546524
H	-0.305071	-4.822390	4.496504
H	-1.890891	-5.608680	4.462831
H	-0.939403	-3.077133	7.499793
H	0.149325	-3.231478	6.106808
H	0.224811	3.100446	4.599042
H	1.116730	-1.058554	5.119538
H	-1.301837	1.571935	3.114744
H	-0.815161	-0.855332	3.487231
H	-6.282769	-1.833182	0.886298
H	-5.341401	-3.336995	4.822115
H	-3.867179	-1.416130	0.463495
H	-2.916332	-2.912124	4.381859
H	-1.640997	-1.567780	1.367599
H	-5.140405	2.237433	1.847569
H	-4.866197	2.805538	0.170942
H	0.514534	-2.640173	1.849416
H	3.200391	1.462574	0.958242
H	4.059070	-0.268853	2.525444
H	3.675063	-2.270063	3.872069
H	3.322079	-3.497155	2.636758
H	1.532373	1.883243	-1.073064
H	4.275095	3.761153	-4.240894
H	-0.270200	4.082700	-4.958800
H	-0.389400	-2.199101	-5.642801
H	-5.190900	-2.322200	-3.064101
H	-5.325799	1.123600	0.465897
H	-3.352102	-5.417098	6.393199
H	1.839000	1.274602	6.019601
H	-7.029002	-2.820797	3.066701
O	0.006472	-0.431759	-2.552803
O	1.321073	-0.429398	-2.610329

O₂ adduct PII

Fe	-1.062675	0.516072	-0.961361
O	-2.679133	1.429958	-0.127006
N	-2.514067	-0.903912	-1.725388
N	-1.111767	2.201202	-2.361686
O	-0.646385	-0.940547	0.306962
O	0.626943	1.281382	-0.150138
C	1.231716	0.407478	0.683038
C	0.556333	-0.825835	0.891418
C	1.111263	-1.820840	1.699661
C	2.314164	-1.592948	2.388994
C	2.958772	-0.356690	2.218706
C	2.434714	0.631100	1.363185
C	-1.619779	3.393213	-2.085450
N	-1.336432	4.264245	-3.079379
C	-0.614851	3.596912	-4.051636
C	-0.483974	2.311078	-3.589319
C	-2.229703	-2.197465	-1.764357
N	-3.256587	-2.884426	-2.298263
C	-4.258733	-1.992418	-2.620707
C	-3.782291	-0.755178	-2.251527
C	-3.249034	1.667078	1.002768
O	-2.663703	1.746556	2.099448
C	2.876502	-2.677290	3.301172
C	1.793274	-3.292117	4.201921
O	1.456753	-2.630087	5.251671
C	-4.754520	1.940175	0.939471
O	1.268159	-4.378295	3.868410
N	2.257759	2.545845	-1.934923
C	3.042811	2.289796	-3.040838
C	3.594590	3.485885	-3.432202
N	3.114200	4.431420	-2.543147
C	2.310263	3.841811	-1.648584
O	-1.895712	-2.060985	2.280312
C	-3.234340	-2.206921	2.436109
C	-4.168013	-1.881108	1.437647
C	-5.530952	-2.100927	1.671278
C	-5.972764	-2.634682	2.889122
C	-5.037263	-2.934801	3.888597
C	-3.676877	-2.719642	3.667094
N	0.657467	-0.125229	4.891242
C	1.056198	1.136234	5.279218
C	0.282228	2.024890	4.575021
N	-0.560870	1.271260	3.779696
C	-0.315481	-0.022881	3.987125
N	-1.185590	-5.058411	5.018833
C	-1.547614	-4.425929	6.133556
N	-0.708819	-3.552500	6.689777

N	-2.757135	-4.649651	6.690381
C	-1.065574	-2.437683	-4.812114
C	-0.475086	-3.519672	-3.926697
N	0.750641	-3.254038	-3.410067
O	-1.073079	-4.575745	-3.689393
H	0.015267	1.462116	-4.036998
H	-1.636518	5.233648	-3.116040
H	-2.185891	3.637686	-1.194698
H	-1.206607	-1.517340	-4.229274
H	-2.025726	-2.778089	-5.212913
H	1.121339	-3.902027	-2.719364
H	1.116704	-2.301203	-3.386304
H	3.128197	1.290246	-3.446744
H	3.342940	5.421914	-2.552090
H	1.794697	4.332624	-0.831582
H	-4.251165	0.219722	-2.309424
H	-3.232101	-3.878283	-2.512828
H	-1.303536	-2.637381	-1.421277
H	-3.010292	-4.198238	7.562791
H	-0.266132	-4.838297	4.567271
H	-1.862546	-5.601652	4.493796
H	-0.949799	-3.095286	7.562104
H	0.154421	-3.239619	6.179019
H	0.257574	3.107439	4.572672
H	1.092131	-1.055827	5.141529
H	-1.280509	1.590677	3.094270
H	-0.825531	-0.846718	3.493100
H	-6.250679	-1.853216	0.889643
H	-5.369950	-3.339929	4.845973
H	-3.825817	-1.462723	0.491206
H	-2.934559	-2.943109	4.430017
H	-1.618224	-1.659494	1.401079
H	-5.152164	2.112352	1.946087
H	-4.922719	2.840938	0.330059
H	0.569074	-2.757096	1.826207
H	2.950382	1.585065	1.239331
H	3.886063	-0.154075	2.757349
H	3.668319	-2.256574	3.934897
H	3.316243	-3.487211	2.701229
H	1.662413	1.868812	-1.373702
H	4.275095	3.761153	-4.240893
H	-0.270200	4.082700	-4.958800
H	-0.389400	-2.199101	-5.642801
H	-5.190900	-2.322200	-3.064101
H	-5.325799	1.123600	0.465897
H	-3.352103	-5.417099	6.393198
H	1.838999	1.274601	6.019601
H	-7.029002	-2.820797	3.066700
O	0.062080	-0.408948	-2.477219

O	1.373906	-0.290966	-2.556121
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TS PII-PIII

Fe	-1.074776	0.519367	-0.932638
O	-2.695239	1.430290	-0.114685
N	-2.518282	-0.902933	-1.716658
N	-1.117788	2.200571	-2.357839
O	-0.651260	-0.966834	0.310975
O	0.573007	1.287792	-0.083281
C	1.185644	0.416979	0.739246
C	0.540614	-0.839308	0.912600
C	1.110621	-1.836702	1.707358
C	2.298888	-1.591334	2.415862
C	2.914443	-0.335637	2.278451
C	2.376149	0.656389	1.438124
C	-1.622384	3.394324	-2.084364
N	-1.335670	4.264144	-3.078912
C	-0.614587	3.594942	-4.050475
C	-0.488311	2.308479	-3.585374
C	-2.231723	-2.195808	-1.761075
N	-3.256961	-2.882757	-2.298672
C	-4.260427	-1.991393	-2.618031
C	-3.786586	-0.754773	-2.243276
C	-3.259322	1.662209	1.019332
O	-2.670235	1.733575	2.114212
C	2.872396	-2.676025	3.319930
C	1.795261	-3.294992	4.224790
O	1.452923	-2.628981	5.270128
C	-4.764176	1.932381	0.962211
O	1.279575	-4.387774	3.898222
N	2.333297	2.276517	-2.047008
C	3.112002	2.151594	-3.176866
C	3.614679	3.397565	-3.454793
N	3.110724	4.237220	-2.475980
C	2.336378	3.538122	-1.635411
O	-1.891711	-2.081354	2.293219
C	-3.231342	-2.222096	2.446683
C	-4.161109	-1.889553	1.446837
C	-5.525346	-2.103888	1.676685
C	-5.971866	-2.638633	2.892238
C	-5.040364	-2.945058	3.893460
C	-3.678527	-2.735353	3.675572
N	0.649650	-0.125263	4.899486
C	1.053846	1.136020	5.282177
C	0.282870	2.025258	4.575716
N	-0.563972	1.272283	3.784302
C	-0.323398	-0.022115	3.995432

N	-1.176498	-5.063291	5.036554
C	-1.544626	-4.429560	6.148557
N	-0.707874	-3.558123	6.711144
N	-2.758436	-4.651247	6.696725
C	-1.054842	-2.410442	-4.795675
C	-0.485347	-3.517785	-3.927508
N	0.730330	-3.272630	-3.377730
O	-1.089564	-4.579188	-3.734040
H	0.004034	1.455717	-4.034392
H	-1.631556	5.234862	-3.115362
H	-2.188198	3.642067	-1.194166
H	-1.148266	-1.485878	-4.210624
H	-2.035384	-2.714874	-5.175658
H	1.088234	-3.949489	-2.708271
H	1.103807	-2.324362	-3.312787
H	3.232145	1.197981	-3.674946
H	3.304263	5.231848	-2.392586
H	1.801545	3.920622	-0.774393
H	-4.257351	0.219396	-2.298915
H	-3.230293	-3.875597	-2.517541
H	-1.305693	-2.635864	-1.417969
H	-3.016801	-4.201064	7.568179
H	-0.253686	-4.844887	4.590621
H	-1.851793	-5.604609	4.507385
H	-0.956887	-3.098255	7.579881
H	0.155523	-3.241245	6.203292
H	0.262822	3.107873	4.569217
H	1.082648	-1.056152	5.151628
H	-1.280988	1.591989	3.096308
H	-0.834951	-0.846102	3.503033
H	-6.242396	-1.851202	0.894196
H	-5.377279	-3.350749	4.849114
H	-3.814632	-1.470112	0.502424
H	-2.939043	-2.963473	4.439808
H	-1.616166	-1.681690	1.412668
H	-5.164841	2.076724	1.971922
H	-4.936218	2.847301	0.375182
H	0.590310	-2.788110	1.811053
H	2.868500	1.625338	1.339103
H	3.829470	-0.121943	2.833545
H	3.666024	-2.254284	3.950683
H	3.310895	-3.483156	2.715502
H	1.774117	1.525464	-1.590307
H	4.275095	3.761154	-4.240893
H	-0.270200	4.082700	-4.958800
H	-0.389400	-2.199102	-5.642801
H	-5.190900	-2.322200	-3.064101
H	-5.325799	1.123600	0.465897
H	-3.352103	-5.417099	6.393198

H	1.838999	1.274601	6.019601
H	-7.029002	-2.820797	3.066700
O	0.074335	-0.397216	-2.451201
O	1.395379	-0.378587	-2.426602

O₂ adduct PIII

Fe	-1.097634	0.541955	-0.909607
O	-2.724049	1.427952	-0.100876
N	-2.522151	-0.888545	-1.722396
N	-1.143704	2.190641	-2.367224
O	-0.657807	-0.983848	0.294105
O	0.481223	1.317586	0.022827
C	1.128640	0.435584	0.787488
C	0.524395	-0.851890	0.901101
C	1.118666	-1.863258	1.662274
C	2.288689	-1.606759	2.392686
C	2.870697	-0.327025	2.305174
C	2.311767	0.681310	1.503736
C	-1.746798	3.351301	-2.155794
N	-1.460398	4.218081	-3.152735
C	-0.634041	3.584045	-4.061744
C	-0.446978	2.319063	-3.556611
C	-2.235221	-2.181744	-1.759786
N	-3.259771	-2.872430	-2.294174
C	-4.263318	-1.983801	-2.618946
C	-3.790809	-0.744787	-2.249939
C	-3.271979	1.655574	1.042375
O	-2.668689	1.728169	2.128911
C	2.871662	-2.697634	3.282025
C	1.798017	-3.313319	4.195008
O	1.472566	-2.650380	5.247062
C	-4.777912	1.913257	1.004446
O	1.269458	-4.399082	3.865632
N	2.590995	1.653245	-2.370472
C	3.405428	1.844868	-3.467065
C	3.676784	3.185239	-3.540812
N	3.006564	3.765450	-2.477487
C	2.350996	2.821173	-1.786960
O	-1.889123	-2.104410	2.288031
C	-3.229982	-2.238680	2.443907
C	-4.158729	-1.902660	1.444493
C	-5.523680	-2.110923	1.675580
C	-5.971312	-2.642787	2.891846
C	-5.040534	-2.951674	3.892965
C	-3.677952	-2.747952	3.673871
N	0.665629	-0.139860	4.898137
C	1.057161	1.125682	5.280641

C	0.279028	2.006695	4.571623
N	-0.558805	1.245429	3.779162
C	-0.306742	-0.046326	3.991864
N	-1.179646	-5.074481	5.024688
C	-1.540127	-4.436949	6.136956
N	-0.702884	-3.557178	6.685758
N	-2.745824	-4.662617	6.699953
C	-1.038705	-2.343687	-4.768210
C	-0.579760	-3.549902	-3.967676
N	0.581175	-3.405547	-3.281775
O	-1.220616	-4.607705	-3.950083
H	0.125906	1.491626	-3.954866
H	-1.814907	5.166799	-3.227208
H	-2.382486	3.576111	-1.307791
H	-0.990367	-1.431206	-4.161240
H	-2.064124	-2.511017	-5.114201
H	0.871735	-4.177722	-2.687255
H	0.989353	-2.489591	-3.079946
H	3.720935	1.020565	-4.094925
H	3.011203	4.754172	-2.242779
H	1.715322	2.951016	-0.916725
H	-4.263233	0.228302	-2.310367
H	-3.237747	-3.866634	-2.507075
H	-1.308893	-2.619690	-1.415866
H	-3.004449	-4.199039	7.564144
H	-0.261674	-4.855790	4.569724
H	-1.854464	-5.628486	4.508340
H	-0.941177	-3.098568	7.558101
H	0.163827	-3.252189	6.177167
H	0.248826	3.089077	4.563830
H	1.105275	-1.066838	5.148612
H	-1.276881	1.560567	3.089050
H	-0.809958	-0.875513	3.499773
H	-6.240244	-1.855771	0.893503
H	-5.378578	-3.354572	4.849384
H	-3.811583	-1.485163	0.499402
H	-2.938806	-2.977801	4.437799
H	-1.619346	-1.709136	1.406184
H	-5.177931	2.001273	2.020711
H	-4.961355	2.855937	0.466500
H	0.623290	-2.831056	1.729969
H	2.772728	1.668788	1.453369
H	3.773275	-0.109451	2.878633
H	3.673692	-2.282353	3.906105
H	3.298738	-3.503687	2.668394
H	2.146720	0.714606	-2.102383
H	4.275095	3.761153	-4.240893
H	-0.270200	4.082700	-4.958800
H	-0.389400	-2.199101	-5.642801

H	-5.190900	-2.322200	-3.064101
H	-5.325799	1.123600	0.465897
H	-3.352103	-5.417099	6.393198
H	1.838999	1.274601	6.019601
H	-7.029002	-2.820797	3.066700
O	0.128656	-0.400527	-2.387071
O	1.406243	-0.699938	-2.192742

TS PIII-PIV

Fe	-1.062366	0.520124	-0.943552
O	-2.711284	1.391229	-0.138879
N	-2.479727	-0.913455	-1.772200
N	-1.144697	2.169267	-2.389287
O	-0.629964	-0.980578	0.263995
O	0.480112	1.351538	0.052656
C	1.122708	0.465042	0.810919
C	0.537766	-0.836236	0.894335
C	1.131235	-1.850775	1.652806
C	2.285325	-1.591313	2.404563
C	2.851460	-0.301600	2.343849
C	2.292608	0.711686	1.550836
C	-1.565354	3.381754	-2.060861
N	-1.263627	4.264331	-3.039276
C	-0.622560	3.584568	-4.058801
C	-0.560010	2.278373	-3.638459
C	-2.241433	-2.216205	-1.734815
N	-3.285394	-2.897428	-2.246058
C	-4.252395	-1.992447	-2.631428
C	-3.736259	-0.753368	-2.324470
C	-3.251557	1.635102	1.003416
O	-2.645375	1.703438	2.089547
C	2.867711	-2.686564	3.288595
C	1.792767	-3.305915	4.197620
O	1.464131	-2.645095	5.250313
C	-4.754031	1.920031	0.969527
O	1.266215	-4.391656	3.865406
N	2.311779	1.912488	-2.368277
C	3.105208	1.993267	-3.493027
C	3.607912	3.267988	-3.535474
N	3.090331	3.916287	-2.426517
C	2.304684	3.078911	-1.735264
O	-1.893105	-2.088960	2.257638
C	-3.233624	-2.227913	2.418413
C	-4.170517	-1.881080	1.430318
C	-5.533855	-2.093651	1.670130
C	-5.972198	-2.640525	2.883510
C	-5.032426	-2.961295	3.872597

C	-3.671793	-2.753811	3.644906
N	0.660467	-0.136044	4.898205
C	1.055972	1.128231	5.280750
C	0.282830	2.011451	4.568734
N	-0.555023	1.252824	3.773983
C	-0.308116	-0.039675	3.988130
N	-1.176193	-5.075592	5.031867
C	-1.544555	-4.430837	6.137583
N	-0.710609	-3.549042	6.687856
N	-2.755978	-4.650993	6.691193
C	-0.883204	-2.215607	-4.660497
C	-0.522030	-3.507830	-3.947749
N	0.532251	-3.451556	-3.098545
O	-1.146297	-4.555075	-4.153719
H	-0.133104	1.413519	-4.129892
H	-1.497265	5.252476	-3.032989
H	-2.077760	3.634869	-1.140200
H	-0.577920	-1.327469	-4.095710
H	-1.966757	-2.192136	-4.827959
H	0.768969	-4.299769	-2.589832
H	0.927643	-2.565495	-2.755863
H	3.245133	1.147459	-4.154497
H	3.284015	4.877765	-2.159092
H	1.749123	3.283418	-0.827038
H	-4.172334	0.231334	-2.441919
H	-3.313074	-3.903480	-2.384906
H	-1.341919	-2.671554	-1.344919
H	-3.015404	-4.190199	7.556756
H	-0.257561	-4.855648	4.578237
H	-1.848332	-5.631978	4.514505
H	-0.957855	-3.082400	7.553448
H	0.157062	-3.243184	6.180887
H	0.257118	3.093925	4.559642
H	1.097544	-1.064277	5.149799
H	-1.267941	1.567352	3.078746
H	-0.810635	-0.866604	3.491619
H	-6.256727	-1.828851	0.897137
H	-5.361902	-3.376531	4.826708
H	-3.831600	-1.449958	0.487845
H	-2.926232	-2.993743	4.399453
H	-1.625202	-1.694643	1.377198
H	-5.141848	2.051692	1.985946
H	-4.924952	2.845853	0.399412
H	0.646473	-2.825355	1.696737
H	2.742049	1.705313	1.522801
H	3.742532	-0.081899	2.934362
H	3.668910	-2.274818	3.916103
H	3.295219	-3.489878	2.671837
H	1.729437	1.102195	-2.097757

H	4.275095	3.761153	-4.240893
H	-0.270200	4.082700	-4.958800
H	-0.389400	-2.199101	-5.642801
H	-5.190900	-2.322200	-3.064101
H	-5.325799	1.123600	0.465897
H	-3.352103	-5.417099	6.393198
H	1.838999	1.274601	6.019601
H	-7.029002	-2.820797	3.066700
O	0.345719	-0.171706	-2.342779
O	1.434593	-0.880834	-2.032569

O₂ adduct PIV

C	-0.572057	3.589597	-4.034485
N	-0.841948	4.305760	-2.883223
C	-0.743375	2.270024	-3.684750
C	-1.160736	3.435255	-1.899706
N	-1.102332	2.191333	-2.350253
C	-0.926569	-2.240956	-4.683502
C	-0.649134	-3.584680	-4.028456
O	-1.279409	-4.598821	-4.343915
N	0.347542	-3.604995	-3.109843
C	3.593784	3.232215	-3.583968
N	3.274242	3.686750	-2.316570
C	2.884006	2.074299	-3.758130
C	2.403385	2.840383	-1.744022
N	2.163283	1.859931	-2.604077
C	-4.251889	-1.992367	-2.634451
N	-3.303671	-2.900125	-2.211543
C	-3.722275	-0.752975	-2.356929
C	-2.257328	-2.220843	-1.703227
N	-2.475233	-0.915546	-1.782193
N	-2.758909	-4.650628	6.695445
C	-1.547876	-4.424062	6.144340
N	-1.169895	-5.074515	5.045307
N	-0.722966	-3.531297	6.690683
C	1.049085	1.146118	5.284853
N	0.637755	-0.108777	4.889054
C	0.281008	2.046932	4.589699
C	-0.335242	0.009250	3.986547
N	-0.570280	1.307329	3.791351
C	-5.972519	-2.637935	2.887435
C	-5.533170	-2.081918	1.678826
C	-5.035018	-2.964601	3.876630
C	-4.169643	-1.866069	1.443521
C	-3.674283	-2.754228	3.653252
C	-3.234949	-2.219573	2.431248
O	-1.894092	-2.076538	2.274160

C	-4.777090	1.921731	0.989606
C	-3.271454	1.667303	1.014264
O	-2.745415	1.384958	-0.128007
O	-2.647589	1.788738	2.084302
Fe	-1.109487	0.527677	-0.909237
C	2.267626	-1.572431	2.415361
C	1.122721	-1.843533	1.653165
C	0.517342	-0.830624	0.903543
C	1.074617	0.483192	0.845181
C	2.236030	0.742057	1.594548
C	2.810937	-0.272513	2.374411
C	2.857558	-2.666591	3.294964
C	1.785541	-3.287481	4.206421
O	1.275448	-4.384842	3.887823
O	1.441750	-2.615279	5.247258
O	-0.646225	-0.985796	0.265109
O	0.413402	1.369030	0.103067
H	-0.616422	1.373839	-4.281135
H	-0.834434	5.317261	-2.794047
H	-1.417687	3.721669	-0.886193
H	-0.608769	-1.392222	-4.066479
H	-2.000161	-2.160960	-4.892725
H	0.533308	-4.483658	-2.632668
H	0.710104	-2.740077	-2.688168
H	2.832198	1.394663	-4.599893
H	3.648123	4.521790	-1.874091
H	1.952834	2.917273	-0.759917
H	-4.142716	0.234046	-2.507965
H	-3.354847	-3.909790	-2.310599
H	-1.374963	-2.678714	-1.279637
H	-3.027996	-4.183239	7.554404
H	-0.250612	-4.852866	4.594307
H	-1.831946	-5.649165	4.535082
H	-0.981430	-3.052865	7.546492
H	0.141670	-3.220979	6.181544
H	0.266913	3.129645	4.594265
H	1.070193	-1.043774	5.128358
H	-1.279523	1.639524	3.103027
H	-0.850250	-0.807680	3.485867
H	-6.255201	-1.812112	0.906841
H	-5.366530	-3.386847	4.826910
H	-3.829339	-1.426576	0.505266
H	-2.929457	-2.999106	4.406841
H	-1.628758	-1.690091	1.389701
H	-5.166648	2.023078	2.008757
H	-4.966588	2.857076	0.441267
H	0.654917	-2.826888	1.682904
H	2.664109	1.745374	1.589347
H	3.694102	-0.044428	2.973412

H	3.659146	-2.253083	3.920846
H	3.284959	-3.468260	2.676289
H	1.429574	1.080681	-2.457200
H	4.275095	3.761153	-4.240894
H	-0.270200	4.082700	-4.958800
H	-0.389400	-2.199100	-5.642800
H	-5.190900	-2.322200	-3.064101
H	-5.325796	1.123604	0.465899
H	-3.352102	-5.417098	6.393199
H	1.839001	1.274602	6.019600
H	-7.029002	-2.820793	3.066700
O	0.449877	-0.097234	-2.322292
O	1.321398	-1.072264	-2.069910

TS PIII-OOH

C	-0.672418	3.573719	-4.084256
N	-1.652121	4.136551	-3.286966
C	-0.396397	2.356170	-3.511444
C	-1.937787	3.275954	-2.285675
N	-1.190332	2.185295	-2.389640
C	-0.863020	-2.191028	-4.652245
C	-0.452112	-3.442506	-3.897905
O	-1.094489	-4.494212	-3.981797
N	0.674320	-3.349423	-3.147675
C	3.710671	3.154736	-3.537672
N	3.038411	3.705424	-2.463205
C	3.483081	1.802361	-3.455786
C	2.432050	2.716628	-1.774713
N	2.691538	1.553389	-2.352059
C	-4.257720	-1.973229	-2.633193
N	-3.252875	-2.854590	-2.291088
C	-3.780466	-0.726332	-2.295113
C	-2.224872	-2.152716	-1.777182
N	-2.509157	-0.858555	-1.768694
N	-2.736187	-4.669152	6.698164
C	-1.535253	-4.448454	6.122267
N	-1.204931	-5.056244	4.983787
N	-0.672829	-3.601550	6.683537
C	1.053250	1.123230	5.286235
N	0.655675	-0.143211	4.913363
C	0.276004	2.002752	4.574781
C	-0.319790	-0.051640	4.009834
N	-0.566617	1.239872	3.789992
C	-5.971358	-2.645229	2.894157
C	-5.519161	-2.138567	1.669066
C	-5.046920	-2.931572	3.907329
C	-4.153312	-1.934756	1.441111
C	-3.683248	-2.731481	3.691683

C	-3.231197	-2.249736	2.453020
O	-1.888488	-2.119216	2.297256
C	-4.788294	1.900188	1.030370
C	-3.285692	1.638993	1.047768
O	-2.758788	1.429105	-0.110798
O	-2.666332	1.680119	2.124814
Fe	-1.123631	0.585918	-0.905101
C	2.264904	-1.574698	2.367890
C	1.110230	-1.840520	1.626960
C	0.488150	-0.815818	0.899749
C	1.059487	0.498388	0.833461
C	2.251692	0.743323	1.545879
C	2.825569	-0.275439	2.312098
C	2.858512	-2.666578	3.247297
C	1.784834	-3.294997	4.155253
O	1.240628	-4.364099	3.800402
O	1.477490	-2.655222	5.226361
O	-0.684201	-0.950994	0.299416
O	0.377472	1.386416	0.131036
H	0.309418	1.593294	-3.810051
H	-2.095146	5.038883	-3.430772
H	-2.674250	3.453289	-1.511374
H	-0.566638	-1.274135	-4.130474
H	-1.949435	-2.199075	-4.796712
H	0.953483	-4.161071	-2.602763
H	1.095583	-2.455490	-2.903410
H	3.828223	1.001956	-4.100866
H	3.004165	4.691856	-2.224809
H	1.801097	2.846168	-0.901185
H	-4.252878	0.245268	-2.376153
H	-3.236839	-3.854338	-2.474326
H	-1.301960	-2.585232	-1.417353
H	-2.962747	-4.238245	7.588182
H	-0.294428	-4.833446	4.518296
H	-1.901941	-5.571299	4.456609
H	-0.887041	-3.167740	7.574736
H	0.184331	-3.287378	6.165350
H	0.250593	3.085167	4.559385
H	1.096534	-1.069022	5.163124
H	-1.284326	1.553429	3.100130
H	-0.826119	-0.881661	3.522135
H	-6.232395	-1.900352	0.878752
H	-5.390701	-3.313029	4.870352
H	-3.800964	-1.536891	0.489004
H	-2.948533	-2.941151	4.465612
H	-1.631760	-1.724954	1.415868
H	-5.184792	1.951757	2.050338
H	-4.977282	2.858928	0.523831
H	0.636318	-2.820227	1.667035

H	2.692102	1.740269	1.524138
H	3.724457	-0.060603	2.891787
H	3.658740	-2.251953	3.873461
H	3.288265	-3.464780	2.625566
H	2.123753	0.402078	-2.017446
H	4.275095	3.761153	-4.240894
H	-0.270200	4.082700	-4.958800
H	-0.389400	-2.199100	-5.642801
H	-5.190900	-2.322200	-3.064101
H	-5.325795	1.123604	0.465900
H	-3.352100	-5.417099	6.393198
H	1.839003	1.274601	6.019599
H	-7.029000	-2.820794	3.066700
O	0.265263	-0.256044	-2.237427
O	1.507977	-0.593688	-1.842174

Hydroperoxo

C	-0.689279	3.547358	-4.106957
N	-1.819809	3.988555	-3.441337
C	-0.312951	2.396833	-3.457969
C	-2.094222	3.126561	-2.439493
N	-1.198178	2.147813	-2.420242
C	-0.785877	-2.126798	-4.621050
C	-0.369113	-3.367900	-3.853942
O	-0.983773	-4.435813	-3.966140
N	0.722209	-3.246761	-3.060034
C	3.783133	3.122717	-3.516979
N	3.091354	3.633842	-2.438379
C	3.674130	1.755980	-3.401924
C	2.594209	2.593347	-1.724608
N	2.934176	1.443574	-2.279964
C	-4.260194	-1.990095	-2.617529
N	-3.258594	-2.881113	-2.290823
C	-3.783338	-0.751698	-2.252778
C	-2.230069	-2.193247	-1.761328
N	-2.514111	-0.899320	-1.727135
N	-2.715302	-4.710018	6.747646
C	-1.505901	-4.499033	6.187844
N	-1.203239	-5.037108	5.007481
N	-0.607737	-3.733439	6.808019
C	1.035041	1.084378	5.314795
N	0.631999	-0.201137	5.018767
C	0.243050	1.922762	4.570524
C	-0.360124	-0.159135	4.128387
N	-0.611777	1.118275	3.841723
C	-5.966236	-2.670464	2.911764
C	-5.484764	-2.203017	1.682755

C	-5.067806	-2.947318	3.949790
C	-4.112259	-2.030337	1.476246
C	-3.696411	-2.777806	3.755159
C	-3.216864	-2.337133	2.512936
O	-1.867099	-2.232482	2.371882
C	-4.741330	1.907635	0.975073
C	-3.255991	1.555913	1.047247
O	-2.666587	1.411353	-0.086636
O	-2.703718	1.463652	2.160482
Fe	-1.073048	0.518689	-0.983101
C	2.246558	-1.580077	2.468263
C	1.113818	-1.866348	1.721179
C	0.475621	-0.846902	0.981683
C	1.041355	0.504786	0.936306
C	2.229576	0.760165	1.682431
C	2.796674	-0.252275	2.430788
C	2.867473	-2.650551	3.347091
C	1.802609	-3.311762	4.247345
O	1.260639	-4.367959	3.857525
O	1.506805	-2.703988	5.337392
O	-0.657613	-1.000186	0.373751
O	0.396140	1.375055	0.247440
H	0.516376	1.726044	-3.640080
H	-2.360423	4.817923	-3.667168
H	-2.923431	3.223198	-1.749193
H	-0.422601	-1.203946	-4.154322
H	-1.880207	-2.100961	-4.693047
H	0.996875	-4.059061	-2.513441
H	1.101774	-2.339700	-2.773850
H	4.078371	0.984246	-4.049565
H	2.969232	4.616946	-2.218258
H	1.970347	2.705124	-0.843673
H	-4.251809	0.222751	-2.319784
H	-3.243873	-3.877010	-2.494547
H	-1.305659	-2.634017	-1.415000
H	-2.926876	-4.335929	7.666754
H	-0.284532	-4.826062	4.555785
H	-1.923687	-5.478044	4.445577
H	-0.806489	-3.352063	7.726502
H	0.243217	-3.395128	6.300074
H	0.216867	3.002632	4.494797
H	1.084368	-1.108710	5.302378
H	-1.342672	1.393844	3.143027
H	-0.867056	-1.012992	3.683950
H	-6.179726	-1.971486	0.874558
H	-5.437469	-3.295674	4.915593
H	-3.734536	-1.660183	0.522921
H	-2.981260	-2.976364	4.550077
H	-1.613763	-1.844680	1.493344

H	-5.151104	2.058528	1.980059
H	-4.865564	2.830806	0.390060
H	0.664475	-2.857447	1.745095
H	2.658009	1.761227	1.665939
H	3.690943	-0.044386	3.018996
H	3.655389	-2.217443	3.974893
H	3.317599	-3.432501	2.719241
H	2.119486	0.020794	-1.886805
H	4.275095	3.761153	-4.240894
H	-0.270200	4.082700	-4.958800
H	-0.389400	-2.199100	-5.642801
H	-5.190900	-2.322200	-3.064101
H	-5.325795	1.123604	0.465900
H	-3.352100	-5.417099	6.393198
H	1.839003	1.274601	6.019599
H	-7.029000	-2.820794	3.066700
O	0.249283	-0.172243	-2.195147
O	1.467572	-0.729450	-1.671024

TS1

C	-0.597029	3.609117	-4.034630
N	-1.061591	4.350293	-2.964437
C	-0.641584	2.300546	-3.615186
C	-1.366299	3.503323	-1.957502
N	-1.120727	2.251243	-2.316718
C	-0.050866	-1.866082	-4.651038
C	1.271303	-1.137160	-4.801947
O	1.412631	-0.236190	-5.633103
N	2.290947	-1.552482	-4.003584
C	3.623910	3.224100	-3.560433
N	3.358337	3.682354	-2.285195
C	2.912593	2.053322	-3.683386
C	2.518501	2.801633	-1.686584
N	2.234788	1.805862	-2.506209
C	-4.247389	-1.953997	-2.670262
N	-3.180765	-2.798819	-2.431212
C	-3.807652	-0.702622	-2.304477
C	-2.156307	-2.066693	-1.940276
N	-2.503069	-0.791575	-1.855707
N	-2.714048	-4.688573	6.698656
C	-1.533485	-4.482910	6.077761
N	-1.291891	-5.032970	4.889226
N	-0.606574	-3.710060	6.643328
C	1.077848	1.094311	5.268121
N	0.710554	-0.180250	4.887455
C	0.288460	1.957845	4.550979
C	-0.264338	-0.103959	3.978593

N	-0.531558	1.182570	3.756887
C	-5.964625	-2.675202	2.906475
C	-5.473505	-2.312847	1.645799
C	-5.072179	-2.850563	3.972379
C	-4.099899	-2.145229	1.437204
C	-3.700453	-2.682596	3.777089
C	-3.210398	-2.346226	2.505607
O	-1.861408	-2.237729	2.365467
C	-4.826010	1.433854	1.389722
C	-3.321048	1.576942	1.207483
O	-2.867644	1.500423	0.010605
O	-2.628864	1.784469	2.228465
Fe	-1.250714	0.666156	-0.862273
C	2.248835	-1.719187	2.225392
C	1.104377	-1.931490	1.504641
C	0.475758	-0.851536	0.784788
C	1.093664	0.497419	0.812177
C	2.344357	0.650717	1.512163
C	2.871993	-0.408180	2.200725
C	2.828889	-2.819524	3.098727
C	1.743771	-3.395707	4.029550
O	1.145689	-4.435013	3.674853
O	1.489885	-2.743130	5.103076
O	-0.757663	-0.902008	0.417145
O	0.452194	1.442364	0.271527
H	-0.336728	1.404794	-4.144624
H	-1.175515	5.358670	-2.941545
H	-1.761678	3.810632	-0.995726
H	-0.794947	-1.163758	-4.252742
H	0.006994	-2.728765	-3.977334
H	3.127209	-0.973441	-3.989994
H	2.077273	-2.010046	-3.119619
H	2.808979	1.396619	-4.542072
H	3.730885	4.527515	-1.864533
H	2.123674	2.917840	-0.683257
H	-4.328750	0.247457	-2.315858
H	-3.168684	-3.801840	-2.587024
H	-1.195777	-2.470575	-1.643551
H	-2.878030	-4.309129	7.625270
H	-0.390184	-4.833293	4.397971
H	-2.049361	-5.446651	4.356042
H	-0.742933	-3.346467	7.580185
H	0.227690	-3.387873	6.097300
H	0.238913	3.039576	4.541686
H	1.151861	-1.100580	5.136301
H	-1.276085	1.504915	3.085396
H	-0.764043	-0.946233	3.504467
H	-6.161922	-2.156496	0.814248
H	-5.447133	-3.115807	4.962137

H	-3.717294	-1.855336	0.457397
H	-2.993242	-2.797622	4.595665
H	-1.607047	-1.833625	1.489420
H	-5.024114	0.692807	2.175236
H	-5.243244	2.394757	1.725434
H	0.598504	-2.895566	1.522356
H	2.815133	1.632673	1.528181
H	3.793812	-0.269789	2.767168
H	3.654386	-2.427256	3.705089
H	3.219082	-3.633574	2.472864
H	1.229880	0.633116	-2.156519
H	4.275095	3.761153	-4.240894
H	-0.270200	4.082700	-4.958800
H	-0.389400	-2.199100	-5.642799
H	-5.190900	-2.322199	-3.064101
H	-5.325798	1.123605	0.465898
H	-3.352103	-5.417094	6.393199
H	1.839000	1.274606	6.019599
H	-7.029003	-2.820791	3.066699
O	0.602691	-0.164243	-1.904860
O	1.429741	-0.973147	-1.102576

Peroxo bridge

C	-0.605622	3.633015	-4.024716
N	-1.098186	4.400455	-2.987628
C	-0.657237	2.335662	-3.566983
C	-1.424956	3.578582	-1.964036
N	-1.167322	2.318139	-2.281301
C	-0.707315	-2.025603	-4.604457
C	-0.374726	-3.261896	-3.789039
O	-1.016701	-4.309079	-3.911278
N	0.681017	-3.157258	-2.944387
C	3.605904	3.262685	-3.546292
N	3.025772	3.924529	-2.482582
C	3.145822	1.968927	-3.459727
C	2.255135	3.041715	-1.801671
N	2.308949	1.849281	-2.368590
C	-4.280635	-1.935264	-2.620519
N	-3.252056	-2.770840	-2.243471
C	-3.861742	-0.666078	-2.286568
C	-2.268230	-2.018525	-1.706113
N	-2.603435	-0.736672	-1.719570
N	-2.726652	-4.678523	6.697961
C	-1.541343	-4.468855	6.089514
N	-1.267938	-5.056968	4.925679
N	-0.640607	-3.658575	6.644318
C	1.050841	1.111618	5.290387

N	0.666054	-0.157978	4.912427
C	0.254942	1.983388	4.588779
C	-0.318702	-0.073511	4.015443
N	-0.581560	1.215718	3.802641
C	-5.966816	-2.632949	2.893424
C	-5.511353	-2.099960	1.678956
C	-5.031850	-2.927282	3.896601
C	-4.145319	-1.881103	1.451431
C	-3.669015	-2.711464	3.681571
C	-3.212419	-2.204914	2.451926
O	-1.867784	-2.066883	2.305352
C	-4.922408	1.706888	1.304123
C	-3.400005	1.716378	1.278598
O	-2.861046	1.736846	0.113249
O	-2.776931	1.745349	2.361644
Fe	-1.355988	0.759172	-0.780692
C	2.235064	-1.606844	2.252963
C	1.270571	-1.830705	1.332811
C	0.667197	-0.729119	0.508569
C	1.105928	0.697221	0.910833
C	2.219900	0.853472	1.826483
C	2.731402	-0.239423	2.455195
C	2.792814	-2.736341	3.107554
C	1.702493	-3.327275	4.022187
O	1.104572	-4.356946	3.645781
O	1.456107	-2.699181	5.112977
O	-0.671472	-0.784784	0.390471
O	0.477413	1.645021	0.417685
H	-0.353949	1.421125	-4.062469
H	-1.221722	5.407920	-2.997088
H	-1.848495	3.909167	-1.022105
H	-0.226078	-1.118713	-4.219019
H	-1.795119	-1.882491	-4.607981
H	0.887252	-3.945749	-2.336846
H	1.058890	-2.253712	-2.672284
H	3.360289	1.124509	-4.106673
H	3.164887	4.900422	-2.240381
H	1.672423	3.292710	-0.921561
H	-4.372855	0.283180	-2.399697
H	-3.186948	-3.769065	-2.422377
H	-1.343509	-2.411190	-1.306931
H	-2.914810	-4.277209	7.610580
H	-0.381683	-4.824527	4.420411
H	-2.007379	-5.513636	4.401942
H	-0.813149	-3.248673	7.555690
H	0.197104	-3.339118	6.102466
H	0.213059	3.065495	4.582883
H	1.108243	-1.082027	5.151732
H	-1.344656	1.534705	3.148060

H	-0.822246	-0.908589	3.528832
H	-6.223405	-1.848987	0.891497
H	-5.366527	-3.326548	4.855851
H	-3.802762	-1.463805	0.504943
H	-2.935478	-2.924884	4.455593
H	-1.561449	-1.605375	1.461982
H	-5.292660	1.305222	2.253930
H	-5.283669	2.741477	1.196239
H	0.866454	-2.827881	1.157816
H	2.581436	1.859173	2.036098
H	3.542054	-0.103871	3.172950
H	3.619598	-2.371018	3.728985
H	3.175259	-3.537790	2.463554
H	1.327563	0.643137	-1.995173
H	4.275095	3.761153	-4.240894
H	-0.270200	4.082700	-4.958800
H	-0.389400	-2.199100	-5.642800
H	-5.190900	-2.322200	-3.064101
H	-5.325797	1.123603	0.465899
H	-3.352102	-5.417098	6.393199
H	1.839001	1.274602	6.019600
H	-7.029002	-2.820794	3.066700
O	0.640715	-0.114736	-1.808516
O	1.331376	-0.942216	-0.827022

TS2

C	-0.668314	3.599302	-4.067354
N	-1.408679	4.284310	-3.120630
C	-0.580961	2.314222	-3.590218
C	-1.742642	3.425458	-2.131250
N	-1.251463	2.220476	-2.382256
C	-0.778587	-2.053955	-4.624169
C	-0.325788	-3.227939	-3.774218
O	-0.785227	-4.360438	-3.941427
N	0.633266	-2.958378	-2.854938
C	3.618823	3.240877	-3.546456
N	3.088199	3.867604	-2.436601
C	3.136011	1.952025	-3.495250
C	2.324420	2.971448	-1.765644
N	2.334013	1.801124	-2.380455
C	-4.257109	-1.992988	-2.622855
N	-3.355584	-2.887384	-2.082381
C	-3.697811	-0.751172	-2.436912
C	-2.307936	-2.198134	-1.592530
N	-2.481006	-0.899109	-1.798258
N	-2.680710	-4.777479	6.803562
C	-1.513440	-4.495722	6.189209

N	-1.153816	-5.151209	5.088066
N	-0.702658	-3.567715	6.695965
C	1.050640	1.108021	5.291606
N	0.640455	-0.164708	4.954962
C	0.285904	1.972139	4.547528
C	-0.328189	-0.090067	4.039470
N	-0.557059	1.196262	3.776223
C	-5.962367	-2.655790	2.896906
C	-5.498896	-2.001072	1.746636
C	-5.029269	-3.102010	3.844135
C	-4.127750	-1.802336	1.529028
C	-3.662188	-2.909100	3.638230
C	-3.197377	-2.268570	2.475280
O	-1.852845	-2.143219	2.338107
C	-4.805339	1.666917	1.267050
C	-3.282241	1.632338	1.136810
O	-2.802234	1.488466	-0.040031
O	-2.610977	1.806621	2.180060
Fe	-1.206569	0.570652	-0.962531
C	2.233938	-1.595023	2.367271
C	1.252218	-1.830393	1.464554
C	0.659579	-0.742180	0.608220
C	1.108796	0.693208	0.981140
C	2.221343	0.857246	1.897372
C	2.731944	-0.227752	2.542361
C	2.808701	-2.715746	3.221760
C	1.736034	-3.327829	4.142721
O	1.178208	-4.386965	3.786229
O	1.462762	-2.688434	5.220571
O	-0.700233	-0.772837	0.502482
O	0.511856	1.635209	0.442493
H	-0.074492	1.457626	-4.016771
H	-1.674654	5.263243	-3.164440
H	-2.328218	3.687510	-1.257597
H	-0.433742	-1.086944	-4.239154
H	-1.874795	-2.050600	-4.680599
H	0.911302	-3.703775	-2.222252
H	0.820747	-2.005008	-2.548786
H	3.313561	1.130985	-4.182323
H	3.251820	4.830638	-2.160251
H	1.777567	3.198589	-0.856406
H	-4.078135	0.229315	-2.697326
H	-3.445119	-3.898957	-2.076603
H	-1.458428	-2.638568	-1.088615
H	-3.011776	-4.204002	7.571721
H	-0.269153	-4.900418	4.587154
H	-1.796377	-5.793588	4.637486
H	-0.952323	-3.079335	7.548611
H	0.162630	-3.276966	6.182802

H	0.272339	3.053839	4.498923
H	1.075499	-1.085416	5.221025
H	-1.283304	1.514231	3.079516
H	-0.838746	-0.932517	3.574385
H	-6.209170	-1.634649	1.004132
H	-5.371246	-3.602946	4.751898
H	-3.777566	-1.283495	0.635975
H	-2.925972	-3.246787	4.363776
H	-1.538980	-1.607696	1.532661
H	-5.105291	1.257840	2.238916
H	-5.131005	2.718436	1.230193
H	0.845643	-2.828594	1.304119
H	2.589683	1.863940	2.089509
H	3.548099	-0.081808	3.251850
H	3.630967	-2.336587	3.841010
H	3.204004	-3.510394	2.576748
H	1.286507	0.621231	-1.976175
H	4.275095	3.761153	-4.240894
H	-0.270200	4.082700	-4.958800
H	-0.389400	-2.199100	-5.642800
H	-5.190900	-2.322200	-3.064101
H	-5.325797	1.123603	0.465899
H	-3.352102	-5.417098	6.393199
H	1.839001	1.274602	6.019600
H	-7.029002	-2.820794	3.066700
O	0.528812	-0.057920	-1.769335
O	1.329490	-1.017744	-0.643229

Epoxide

Fe	-1.085809	0.442930	-1.044137
O	-2.646825	1.339044	-0.108484
N	-2.450243	-0.978554	-1.796904
N	-1.227593	2.170219	-2.412100
O	-0.702105	-0.933512	0.416123
O	0.495424	1.435819	0.375675
C	1.119132	0.511818	0.941189
C	0.579298	-0.896785	0.792377
C	1.244007	-1.969606	1.597580
C	2.339675	-1.623158	2.530511
C	2.843736	-0.319484	2.516165
C	2.286737	0.714828	1.753163
C	-1.845444	3.325751	-2.209892
N	-1.535162	4.200575	-3.192390
C	-0.675637	3.578017	-4.081456
C	-0.495512	2.312868	-3.579729
C	-2.281318	-2.285784	-1.644575
N	-3.345565	-2.944437	-2.138806

C	-4.248357	-2.021428	-2.626413
C	-3.676536	-0.792648	-2.404499
C	-3.218017	1.535370	1.026662
O	-2.643977	1.516028	2.133832
C	2.889947	-2.691682	3.430784
C	1.786452	-3.334116	4.308232
O	1.509881	-2.741455	5.407384
C	-4.708053	1.887064	0.971386
O	1.218237	-4.360119	3.882008
N	2.491847	1.715248	-2.324553
C	3.272266	1.903094	-3.446324
C	3.663804	3.220109	-3.527650
N	3.099715	3.833065	-2.427629
C	2.404083	2.893139	-1.735660
O	-1.862029	-2.152363	2.361467
C	-3.207731	-2.276007	2.500919
C	-4.122035	-1.900389	1.501325
C	-5.492959	-2.095959	1.710774
C	-5.964768	-2.655699	2.906100
C	-5.048496	-3.004791	3.907337
C	-3.679781	-2.813714	3.709847
N	0.658820	-0.233279	5.038247
C	1.062197	1.060119	5.289865
C	0.302946	1.867800	4.477884
N	-0.530654	1.036752	3.754095
C	-0.298744	-0.227877	4.108065
N	-1.191656	-5.060302	5.068216
C	-1.509698	-4.510428	6.238674
N	-0.617993	-3.750553	6.875437
N	-2.731811	-4.709550	6.771286
C	-0.728600	-2.084541	-4.603176
C	-0.069442	-3.161199	-3.752756
N	0.749953	-2.720908	-2.774101
O	-0.279699	-4.361464	-3.970264
H	0.110240	1.498484	-3.952564
H	-1.886125	5.150567	-3.266101
H	-2.504531	3.543163	-1.377769
H	-0.508877	-1.070361	-4.249575
H	-1.815930	-2.242981	-4.596532
H	1.140552	-3.408872	-2.134938
H	0.725548	-1.732366	-2.458035
H	3.502320	1.084430	-4.121412
H	3.194882	4.811190	-2.174228
H	1.841993	3.103206	-0.831174
H	-4.050883	0.200445	-2.621084
H	-3.452601	-3.954287	-2.156400
H	-1.422188	-2.752073	-1.182533
H	-2.954144	-4.362541	7.698469
H	-0.278135	-4.838546	4.611099

H	-1.903609	-5.518775	4.509300
H	-0.849495	-3.334232	7.770917
H	0.239018	-3.417149	6.379512
H	0.284074	2.943711	4.356530
H	1.097672	-1.126250	5.372097
H	-1.258228	1.298533	3.038933
H	-0.805076	-1.095341	3.686204
H	-6.196192	-1.806707	0.928510
H	-5.402755	-3.426431	4.849703
H	-3.758589	-1.458099	0.573185
H	-2.956000	-3.068929	4.480597
H	-1.579111	-1.677153	1.515314
H	-5.097673	2.039238	1.984252
H	-4.827654	2.819315	0.398991
H	0.664718	-2.870165	1.814430
H	2.694187	1.723208	1.807731
H	3.698593	-0.085522	3.152296
H	3.675917	-2.283514	4.076886
H	3.320450	-3.495072	2.812911
H	1.207636	0.502193	-2.109180
H	4.275095	3.761152	-4.240895
H	-0.270200	4.082700	-4.958800
H	-0.389400	-2.199102	-5.642801
H	-5.190900	-2.322200	-3.064101
H	-5.325799	1.123600	0.465897
H	-3.352101	-5.417098	6.393199
H	1.839001	1.274603	6.019600
H	-7.029002	-2.820797	3.066701
O	0.395052	-0.073028	-2.031991
O	1.530072	-1.789939	0.178919

TS Ep-La

Fe	-1.068024	0.445679	-1.057470
O	-2.646731	1.288002	-0.138714
N	-2.433045	-1.002966	-1.803472
N	-1.220687	2.135867	-2.435977
O	-0.633456	-1.146511	0.346464
O	0.395354	1.304619	0.368810
C	1.121343	0.373497	0.851354
C	0.611376	-1.011732	0.646196
C	1.511806	-2.245036	1.658264
C	2.447828	-1.691534	2.540077
C	2.962561	-0.377760	2.327077
C	2.346143	0.590644	1.549963
C	-1.847832	3.285762	-2.224427
N	-1.540376	4.170136	-3.197306

C	-0.673701	3.562487	-4.089655
C	-0.486031	2.293475	-3.600334
C	-2.253346	-2.314419	-1.707563
N	-3.323823	-2.961519	-2.202923
C	-4.242727	-2.027399	-2.635310
C	-3.673979	-0.803930	-2.377617
C	-3.213722	1.527719	0.993507
O	-2.637672	1.519301	2.096637
C	2.903953	-2.478044	3.759704
C	1.778217	-3.192659	4.532037
O	1.368967	-2.623128	5.605074
C	-4.695256	1.905526	0.924201
O	1.321975	-4.263486	4.080430
N	2.483419	1.666590	-2.384089
C	3.259595	1.885657	-3.503085
C	3.661887	3.201661	-3.541941
N	3.108227	3.781227	-2.418112
C	2.408453	2.823969	-1.754386
O	-1.843897	-2.217961	2.427784
C	-3.197124	-2.324130	2.549327
C	-4.086283	-2.017438	1.505990
C	-5.462233	-2.194846	1.698382
C	-5.960876	-2.666970	2.920092
C	-5.068083	-2.941869	3.964814
C	-3.694162	-2.768132	3.784942
N	0.624749	-0.159889	4.993079
C	1.081698	1.111107	5.258912
C	0.394322	1.956138	4.421784
N	-0.454482	1.165259	3.671864
C	-0.298535	-0.109288	4.032478
N	-1.173519	-4.937592	5.138290
C	-1.520590	-4.483434	6.341736
N	-0.640233	-3.791823	7.064581
N	-2.761751	-4.711445	6.818538
C	-0.747117	-2.124369	-4.606879
C	-0.060744	-3.201477	-3.779979
N	0.788472	-2.759013	-2.826818
O	-0.271559	-4.401662	-3.993165
H	0.126051	1.486767	-3.979489
H	-1.897209	5.118635	-3.262883
H	-2.510293	3.490966	-1.392105
H	-0.562793	-1.113412	-4.225012
H	-1.827895	-2.318754	-4.621328
H	1.206616	-3.446536	-2.204694
H	0.764635	-1.771136	-2.512600
H	3.479696	1.088355	-4.206405
H	3.214271	4.749046	-2.131477
H	1.850887	3.005356	-0.840263
H	-4.059864	0.194088	-2.545352

H	-3.423034	-3.970794	-2.259447
H	-1.383135	-2.795861	-1.284784
H	-3.007788	-4.430008	7.761977
H	-0.232916	-4.721281	4.737095
H	-1.877418	-5.319423	4.515216
H	-0.893369	-3.451416	7.986101
H	0.196724	-3.380647	6.590284
H	0.434662	3.031122	4.297733
H	0.985380	-1.067938	5.392204
H	-1.157825	1.449202	2.949772
H	-0.834317	-0.955198	3.605107
H	-6.147165	-1.961303	0.882087
H	-5.444019	-3.292051	4.927591
H	-3.701619	-1.641922	0.557009
H	-2.989339	-2.963760	4.590326
H	-1.561383	-1.838678	1.551715
H	-5.077663	2.121782	1.928196
H	-4.802029	2.804071	0.298243
H	0.958245	-3.152923	1.895843
H	2.742117	1.605629	1.541569
H	3.835170	-0.077197	2.909289
H	3.442867	-1.818614	4.449133
H	3.604731	-3.257422	3.420303
H	1.211192	0.462125	-2.135666
H	4.275095	3.761152	-4.240895
H	-0.270200	4.082700	-4.958800
H	-0.389400	-2.199102	-5.642801
H	-5.190900	-2.322200	-3.064101
H	-5.325799	1.123600	0.465897
H	-3.352101	-5.417098	6.393199
H	1.839001	1.274603	6.019600
H	-7.029002	-2.820797	3.066701
O	0.404348	-0.121043	-2.036765
O	1.549626	-1.943205	0.263659

Lactone

Fe	-0.971384	0.427809	-1.046564
O	-2.612608	1.273283	-0.170027
N	-2.405557	-1.014596	-1.829521
N	-1.097497	2.128516	-2.397061
O	-0.680528	-1.264805	0.298737
O	0.421218	1.095026	0.399891
C	1.063613	0.122216	0.973760
C	0.459154	-1.173920	0.818505
C	1.671570	-2.666260	2.307102
C	2.466708	-1.861084	3.044124

C	2.832287	-0.497252	2.677396
C	2.241918	0.347906	1.772814
C	-1.784553	3.247179	-2.203086
N	-1.526892	4.128904	-3.191947
C	-0.631847	3.553240	-4.076791
C	-0.374525	2.303928	-3.566472
C	-2.231232	-2.327948	-1.762465
N	-3.311586	-2.966764	-2.248674
C	-4.235956	-2.024765	-2.648583
C	-3.657277	-0.806235	-2.378387
C	-3.187049	1.421746	0.971408
O	-2.632751	1.272100	2.077792
C	3.059924	-2.456831	4.328932
C	1.998923	-3.195879	5.167756
O	1.404878	-2.516859	6.081435
C	-4.652007	1.869390	0.925547
O	1.733432	-4.386867	4.899387
N	2.612365	1.541111	-2.402927
C	3.357904	1.822946	-3.529453
C	3.699234	3.157208	-3.544867
N	3.139474	3.684133	-2.397973
C	2.496096	2.679856	-1.745847
O	-1.828467	-2.426668	2.444576
C	-3.187342	-2.491566	2.567776
C	-4.056569	-2.117027	1.530815
C	-5.438068	-2.236515	1.717473
C	-5.955977	-2.717049	2.927256
C	-5.080170	-3.066601	3.963362
C	-3.699227	-2.953634	3.788069
N	0.566676	-0.203935	5.130112
C	1.058666	1.071798	5.289566
C	0.386902	1.864829	4.390086
N	-0.485508	1.039628	3.709212
C	-0.357999	-0.206580	4.168782
N	-0.969564	-4.987702	5.482346
C	-1.531658	-4.439158	6.558747
N	-0.811286	-3.614981	7.320704
N	-2.818638	-4.694933	6.866320
C	-0.770250	-2.180317	-4.613835
C	-0.069845	-3.277802	-3.828458
N	0.806157	-2.856319	-2.889549
O	-0.286996	-4.472826	-4.062529
H	0.275228	1.521502	-3.934330
H	-1.934172	5.055575	-3.272966
H	-2.459089	3.427853	-1.375176
H	-0.611774	-1.184344	-4.184402
H	-1.845110	-2.398112	-4.659690
H	1.255001	-3.563946	-2.312800
H	0.797478	-1.869383	-2.562282

H	3.602576	1.053372	-4.255360
H	3.202934	4.649703	-2.092069
H	1.944512	2.813706	-0.819482
H	-4.045382	0.195141	-2.519682
H	-3.412176	-3.974643	-2.322618
H	-1.356763	-2.827253	-1.371665
H	-3.243517	-4.282046	7.689490
H	0.038757	-4.829108	5.271144
H	-1.507887	-5.575630	4.855569
H	-1.227804	-3.175049	8.134139
H	0.091314	-3.235652	6.953729
H	0.455695	2.924348	4.177100
H	0.926873	-1.079154	5.610728
H	-1.178798	1.283062	2.961341
H	-0.902632	-1.070342	3.793714
H	-6.111998	-1.950173	0.909105
H	-5.474890	-3.430511	4.913431
H	-3.652045	-1.731174	0.593812
H	-3.002614	-3.218435	4.580925
H	-1.575784	-2.109246	1.545232
H	-5.013242	2.083540	1.937909
H	-4.728748	2.780201	0.313705
H	1.474333	-3.700097	2.582078
H	2.646687	1.357605	1.690320
H	3.677968	-0.085724	3.230388
H	3.499138	-1.656127	4.935253
H	3.862146	-3.165212	4.078574
H	1.285720	0.320447	-2.130988
H	4.275095	3.761152	-4.240895
H	-0.270200	4.082700	-4.958800
H	-0.389400	-2.199102	-5.642801
H	-5.190900	-2.322200	-3.064101
H	-5.325799	1.123600	0.465897
H	-3.352100	-5.417098	6.393199
H	1.839002	1.274603	6.019600
H	-7.029002	-2.820797	3.066701
O	0.463970	-0.236156	-2.054343
O	1.051640	-2.369475	1.109444

La-OH

Fe	-1.506943	0.845114	-0.845035
O	-2.849551	1.798289	0.222230
N	-2.665323	-0.722507	-1.633906
N	-1.296919	2.374184	-2.305664
O	-0.501877	-0.534611	0.538619
O	0.948863	2.057666	0.706330
C	1.337486	0.909967	0.943519

C	0.698375	-0.219086	0.087505
C	1.950179	-2.221283	0.890062
C	2.412729	-1.909045	2.133500
C	2.645274	-0.552632	2.568439
C	2.250017	0.642892	2.038744
C	-1.631622	3.630499	-2.046256
N	-1.263600	4.433852	-3.068856
C	-0.660308	3.657854	-4.038947
C	-0.689159	2.375894	-3.546908
C	-2.395814	-2.009527	-1.453193
N	-3.359973	-2.770277	-2.008502
C	-4.306926	-1.937888	-2.568936
C	-3.859357	-0.661011	-2.329837
C	-3.456160	1.755186	1.357073
O	-2.893030	1.731481	2.468071
C	2.832420	-3.048784	3.051633
C	1.709685	-3.489543	4.004743
O	1.440451	-2.726698	4.998608
C	-4.975588	1.780033	1.275793
O	1.118554	-4.564618	3.760531
N	2.267482	2.045716	-2.216239
C	3.123764	2.051882	-3.300879
C	3.586784	3.330799	-3.517284
N	2.986301	4.100009	-2.540377
C	2.205364	3.292959	-1.782499
O	-1.846631	-2.199392	2.176202
C	-3.197699	-2.318058	2.338745
C	-4.156072	-1.631214	1.575621
C	-5.523516	-1.815295	1.838577
C	-5.960454	-2.678829	2.854178
C	-4.994344	-3.367929	3.604478
C	-3.631302	-3.193325	3.350074
N	0.672965	-0.178454	4.917447
C	1.033627	1.095243	5.309124
C	0.201041	1.954896	4.635400
N	-0.628911	1.178535	3.850346
C	-0.323424	-0.105373	4.032186
N	-1.112399	-5.272672	5.179086
C	-1.584796	-4.418406	6.081521
N	-0.907757	-3.303546	6.350120
N	-2.737131	-4.685560	6.732014
C	-0.673569	-1.858710	-4.635297
C	-0.223381	-2.907150	-3.633460
N	0.620537	-2.489798	-2.657896
O	-0.594535	-4.079483	-3.726941
H	-0.303206	1.464849	-3.986844
H	-1.422634	5.435306	-3.118263
H	-2.133671	3.968122	-1.146438
H	-0.238098	-0.868508	-4.453445

H	-1.768980	-1.778331	-4.602750
H	0.869704	-3.159323	-1.935127
H	0.710955	-1.510762	-2.385808
H	3.352897	1.143635	-3.849009
H	3.123822	5.095474	-2.397291
H	1.618975	3.633315	-0.936692
H	-4.305221	0.290141	-2.596945
H	-3.362901	-3.785605	-2.034355
H	-1.530099	-2.395554	-0.931164
H	-3.159380	-3.987659	7.335034
H	-0.243391	-5.043659	4.633895
H	-1.598417	-6.141357	4.985408
H	-1.273912	-2.627953	7.010936
H	0.006680	-3.108408	5.878798
H	0.129857	3.035391	4.647688
H	1.156766	-1.090763	5.100490
H	-1.403789	1.495914	3.213408
H	-0.790421	-0.948627	3.528853
H	-6.251314	-1.268618	1.237454
H	-5.306644	-4.050486	4.396916
H	-3.833242	-0.956508	0.783806
H	-2.874877	-3.732060	3.916560
H	-1.536684	-1.572362	1.470977
H	-5.427252	1.478000	2.226995
H	-5.301650	2.802864	1.033052
H	1.946240	-3.262203	0.557011
H	2.577965	1.551816	2.544050
H	3.255161	-0.474999	3.471448
H	3.694648	-2.734310	3.656635
H	3.135263	-3.922293	2.462875
H	1.269442	0.916983	-1.586063
H	4.275095	3.761152	-4.240895
H	-0.270200	4.082700	-4.958800
H	-0.389400	-2.199102	-5.642801
H	-5.190900	-2.322200	-3.064101
H	-5.325799	1.123600	0.465897
H	-3.352101	-5.417098	6.393199
H	1.839001	1.274603	6.019600
H	-7.029002	-2.820797	3.066701
O	0.549100	0.245249	-1.263239
O	1.590761	-1.382587	-0.094523

Product

Fe	-1.334646	0.831019	-0.944364
O	-2.539175	0.847343	0.651291
N	-2.557194	-0.712695	-1.828574
N	-1.248479	2.474616	-2.233570

O	0.382098	-0.175334	-1.466011
O	0.239525	1.833562	0.282120
C	1.054315	0.872980	0.564866
C	1.373553	0.010812	-0.665763
C	0.885268	-2.190899	1.124395
C	1.953851	-1.840787	2.042085
C	2.235323	-0.518673	2.334546
C	1.668839	0.676802	1.797005
C	-0.852126	3.663712	-1.800511
N	-0.443141	4.424923	-2.836015
C	-0.569198	3.687412	-3.996961
C	-1.079811	2.474518	-3.606595
C	-2.341192	-1.990714	-1.540133
N	-3.353487	-2.753602	-2.004158
C	-4.279000	-1.933314	-2.616500
C	-3.767906	-0.661064	-2.497194
C	-3.373420	1.563073	1.348146
O	-3.171767	1.858917	2.535053
C	2.614138	-2.976936	2.798966
C	1.687043	-3.488457	3.920453
O	1.388407	-2.663876	4.861397
C	-4.649882	1.987633	0.627685
O	1.251808	-4.659696	3.867749
N	3.453574	0.808808	-3.075134
C	3.420248	2.176458	-2.905228
C	4.057952	2.730943	-3.982883
N	4.456299	1.672160	-4.776851
C	4.082781	0.518226	-4.207736
O	-2.091911	-1.430399	1.949873
C	-3.375452	-1.837406	2.191630
C	-4.411115	-1.580746	1.277457
C	-5.721224	-1.942389	1.599171
C	-6.002202	-2.578800	2.813299
C	-4.957532	-2.882756	3.696554
C	-3.644456	-2.515285	3.388843
N	0.618387	-0.119573	4.888894
C	0.968836	1.124956	5.376480
C	0.039268	2.009061	4.881098
N	-0.838629	1.275110	4.104014
C	-0.460801	-0.004110	4.116656
N	-1.192552	-5.203052	5.013058
C	-1.659125	-4.342024	5.911380
N	-0.934139	-3.269916	6.232822
N	-2.879174	-4.521601	6.464400
C	-0.623032	-1.961431	-4.594449
C	-0.194192	-3.129802	-3.717304
N	0.597488	-2.824367	-2.662139
O	-0.553232	-4.281714	-3.977049
H	-1.321066	1.601064	-4.202146

H	-0.104112	5.379665	-2.768141
H	-0.815292	3.971745	-0.762350
H	-0.152494	-1.011333	-4.311537
H	-1.713482	-1.845999	-4.514711
H	0.778154	-3.546648	-1.966477
H	0.676546	-1.857529	-2.334060
H	2.957147	2.627870	-2.035765
H	4.960837	1.746018	-5.656849
H	4.269621	-0.474466	-4.601371
H	-4.182722	0.280544	-2.839328
H	-3.408403	-3.764567	-1.923270
H	-1.486891	-2.387765	-1.000791
H	-3.187928	-3.916916	7.218103
H	-0.250227	-5.052246	4.575491
H	-1.777190	-5.956118	4.666933
H	-1.225702	-2.666459	6.993403
H	-0.012587	-3.081625	5.766472
H	-0.070313	3.078165	5.014672
H	1.126873	-1.043497	4.953598
H	-1.649747	1.611391	3.539626
H	-0.932890	-0.798491	3.544021
H	-6.527235	-1.719804	0.898616
H	-5.164952	-3.391430	4.639086
H	-4.185826	-1.085146	0.335827
H	-2.822545	-2.718429	4.073691
H	-2.133624	-0.596447	1.406767
H	-5.188309	2.746145	1.207108
H	-4.395812	2.387847	-0.364078
H	0.138320	-1.390360	0.956490
H	1.613923	1.529396	2.479975
H	2.925280	-0.359660	3.169998
H	3.552663	-2.637339	3.258647
H	2.834971	-3.814386	2.126609
H	3.074454	0.132887	-2.345818
H	4.275095	3.761152	-4.240894
H	-0.270200	4.082700	-4.958800
H	-0.389399	-2.199103	-5.642801
H	-5.190900	-2.322200	-3.064101
H	-5.325799	1.123600	0.465897
H	-3.352100	-5.417098	6.393198
H	1.839002	1.274603	6.019600
H	-7.029002	-2.820797	3.066701
O	2.538485	-0.360440	-0.916811
O	0.711459	-3.282427	0.574125

Gem-diol (larger model)

Fe	-1.009696	0.326127	-0.992680
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C	-0.651085	3.617730	-4.046438
N	-1.182276	4.346073	-2.996892
C	-0.679589	2.311688	-3.620880
C	-1.505346	3.484306	-2.002068
N	-1.207315	2.240414	-2.342979
C	-0.589000	-2.338500	-4.600900
C	0.438467	-3.286543	-4.006881
O	0.640226	-4.409941	-4.487058
N	1.086066	-2.819244	-2.922535
C	6.202947	0.163348	-1.911731
C	5.005613	0.301604	-1.116490
C	6.368265	-1.240000	-2.100011
N	4.443524	-0.853483	-0.821751
C	5.266561	-1.843836	-1.413457
C	7.314204	-2.042360	-2.762700
C	5.105953	-3.217651	-1.382152
C	7.150289	-3.438732	-2.730506
C	6.067747	-4.015601	-2.054025
C	3.629063	3.213925	-3.596539
N	3.146980	3.780262	-2.437639
C	3.100357	1.945475	-3.631095
C	2.357868	2.857573	-1.826161
N	2.312081	1.739366	-2.522704
C	-4.248930	-2.064298	-2.599441
N	-3.348705	-3.022051	-2.181745
C	-3.673000	-0.857654	-2.290107
C	-2.278604	-2.399081	-1.647744
N	-2.447100	-1.085781	-1.698282
N	-2.723882	-4.864896	6.966068
C	-1.504384	-4.527894	6.497322
N	-1.023089	-5.111457	5.404204
N	-0.760372	-3.631724	7.149557
C	0.974489	1.193605	5.364932
N	0.421316	-0.037602	5.091784
C	0.260296	2.115766	4.638792
C	-0.574998	0.110944	4.220092
N	-0.695167	1.409053	3.932635
C	-5.961306	-2.665719	2.915239
C	-5.477987	-2.125014	1.717477
C	-5.050899	-3.001797	3.926304
C	-4.105956	-1.919143	1.521614
C	-3.680803	-2.805214	3.740319
C	-3.196347	-2.264269	2.535376
O	-1.849165	-2.097262	2.435558
C	-4.698497	1.999517	0.727265
C	-3.220716	1.667485	1.003164
O	-2.544267	1.223791	0.007845
O	-2.756227	1.894808	2.142170
C	2.251534	-1.520682	2.800527

C	1.287539	-1.897012	1.925726
C	0.879177	-1.032518	0.747797
C	1.269138	0.456201	0.920474
C	2.340702	0.785814	1.830864
C	2.784283	-0.162164	2.708611
C	2.846223	-2.478141	3.831017
C	1.783394	-3.176835	4.693422
O	1.467909	-4.356440	4.429653
O	1.262833	-2.488394	5.646061
O	-0.449151	-1.076596	0.416103
O	0.633537	1.296913	0.262667
H	-0.335818	1.418527	-4.125521
H	-1.322728	5.351282	-2.974278
H	-1.942967	3.796180	-1.059782
H	-0.606341	-1.368073	-4.093449
H	-1.581858	-2.805342	-4.527487
H	1.754654	-3.419565	-2.450030
H	0.884335	-1.892757	-2.516961
H	4.565036	1.238635	-0.783432
H	2.622323	-1.238038	-0.335335
H	8.157906	-1.596254	-3.290134
H	7.872177	-4.079072	-3.237033
H	4.268905	-3.677150	-0.856467
H	5.957997	-5.100093	-2.042072
H	3.237439	1.174906	-4.383586
H	3.345511	4.717162	-2.101544
H	1.836452	3.041522	-0.892829
H	-4.050033	0.146758	-2.441466
H	-3.467716	-4.027785	-2.257302
H	-1.413425	-2.904578	-1.235494
H	-3.148423	-4.332904	7.718264
H	-0.069733	-4.872913	5.042617
H	-1.561450	-5.820644	4.918452
H	-1.165374	-3.111834	7.920862
H	0.079820	-3.231286	6.671495
H	0.354402	3.191662	4.558211
H	0.802024	-0.983062	5.394727
H	-1.396537	1.751737	3.233626
H	-1.155712	-0.693306	3.771070
H	-6.173982	-1.852680	0.922753
H	-5.413204	-3.417525	4.868328
H	-3.741954	-1.481933	0.592929
H	-2.962128	-3.061815	4.517748
H	-1.506628	-1.708857	1.571579
H	-5.143187	2.485785	1.603585
H	-4.753757	2.687539	-0.129151
H	0.877249	-2.907541	1.923678
H	2.727551	1.803976	1.848203
H	3.576739	0.112457	3.408219

H	3.523388	-1.927729	4.497167
H	3.438942	-3.249025	3.320097
H	1.031792	0.453129	-2.359737
H	6.828600	0.969800	-2.296700
H	4.275699	3.752001	-4.269998
H	-0.270200	4.082700	-4.958800
H	-0.389400	-2.199100	-5.642800
H	-5.190900	-2.322200	-3.064100
H	-5.325802	1.123599	0.465899
H	-3.352105	-5.417103	6.393199
H	1.838997	1.274597	6.019603
H	-7.029004	-2.820803	3.066700
O	0.230010	-0.131834	-2.277334
O	1.687821	-1.585916	-0.319102