Model 1
Optimized reactant, Fe(IV)Fe(III)
Reactant groundstate: 5a4b

C1	3.211694	-1.367832	-1.236036
C2	2.294472	-0.533711	-0.587154
N3	2.705951	0.591953	0.045958
C4	4.018633	0.920557	0.081388
C5	4.981556	0.126549	-0.537682
C6	4.568392	-1.031324	-1.213499
C7	0.811885	-0.776959	-0.572191
N8	0.210159	-0.212544	0.691424
C9	0.546538	-1.050935	1.905134
C10	1.382005	-0.330885	2.938570
C11	1.795434	-0.962213	4.116835
C12	2.563601	-0.249686	5.041737
C13	2.906585	1.082715	4.770765
C14	2.469784	1.658111	3.580999
N15	1.723299	0.957314	2.692894
Fe16	1.050460	1.746421	0.908604
N17	-0.869664	1.910246	1.976247
C18	-1.764179	0.970459	1.579809
C19	-3.064321	0.954501	2.097549
C20	-3.432644	1.919247	3.040227
C21	-2.492826	2.875588	3.451407
C22	-1.215519	2.842796	2.894442
C23	-1.275133	-0.005185	0.543412
H24	2.890496	-0.725757	5.959129
H25	3.500937	1.659814	5.468156
H26	1.519429	-1.993932	4.304399
H27	2.696975	2.677798	3.296724
H28	4.270651	1.827383	0.615571
H29	2.866358	-2.258973	-1.747068
H30	6.028044	0.401854	-0.489635
H31	5.294982	-1.666979	-1.706818
H32	-0.447140	3.553943	3.170077
H33	-3.769069	0.199736	1.768068
H34	-2.745261	3.624467	4.192109
H35	-4.433871	1.919381	3.456212
H36	-0.387017	-1.391277	2.368358
H37	1.075553	-1.952689	1.575160
H38	-1.801099	-0.964984	0.623810
H39	-1.457721	0.372663	-0.472441
H40	0.576168	-1.844487	-0.661108
H41	0.345128	-0.267584	-1.422070
O42	1.829148	3.313425	1.081548
O43	0.351899	2.345152	-0.615265
C44	5.263580	4.539121	-1.942766
C45	4.025182	4.559158	-1.301191
N46	3.013716	3.750045	-1.718221
C47	3.178745	2.913816	-2.771997
C48	4.400023	2.851044	-3.447966
C49	5.453444	3.670672	-3.028049
C50	3.700134	5.445563	-0.116942
N51	2.289052	5.935613	-0.233653
C52	2.118414	6.956407	-1.323365
C53	1.277674	6.491437	-2.497901
C54	1.093194	7.324543	-3.603937
C55	0.294592	6.887438	-4.666957
C56	-0.302399	5.624476	-4.596603
C57	-0.079321	4.830538	-3.471917

N58	0.699316	5.264517	-2.445069
Fe59	1.148468	4.062845	-0.736251
N60	-0.322708	5.255536	0.255940
C61	0.171006	6.306023	0.963237
C62	-0.688942	7.228702	1.561717
C63	-2.073459	7.055166	1.427689
C64	-2.565444	5.965215	0.698902
C65	-1.657978	5.076969	0.118930
C66	1.681044	6.370599	1.063220
H67	0.142465	7.523991	-5.531294
H68	-0.931493	5.248059	-5.393463
H69	1.565505	8.300732	-3.632551
H70	-0.534179	3.847930	-3.379181
H71	2.314441	2.322783	-3.068438
H72	6.060169	5.195955	-1.611884
H73	4.509866	2.183623	-4.293729
H74	6.406106	3.649133	-3.545534
H75	-1.975432	4.224237	-0.470050
H76	-0.286325	8.070612	2.113425
H77	-3.629730	5.812224	0.569343
H78	-2.756194	7.767790	1.876583
H79	1.660195	7.855916	-0.894078
H80	3.107496	7.260848	-1.686715
H81	2.013116	7.377081	1.349022
H82	2.017513	5.663514	1.828529
H83	4.411613	6.278317	-0.043486
H84	3.758574	4.856657	0.804323
Cl85	-1.012176	0.974730	-3.637064
O86	-1.589045	-0.167357	-2.456903
O87	0.672632	1.287210	-3.261602
O88	-1.143927	0.361711	-5.222934
O89	-1.900318	2.452367	-3.420584

Model 1
Optimized transition state for H-atom transfer
(from reactant state 5a4b)

C1	2.841364	-1.004301	-1.548025
C2	1.959666	-0.239865	-0.776034
N3	2.424382	0.667764	0.124006
C4	3.758533	0.817302	0.317927
C5	4.683747	0.059773	-0.394769
C6	4.216326	-0.855137	-1.350880
C7	0.464011	-0.328612	-0.900121
N8	-0.169211	-0.001227	0.423084
C9	0.042216	-1.084281	1.438341
C10	0.643830	-0.619597	2.748798
C11	0.689009	-1.482902	3.851433
C12	1.297625	-1.058494	5.034326
C13	1.846351	0.229347	5.093518
C14	1.760861	1.042582	3.967230
N15	1.174881	0.626486	2.815863
Fe16	0.871761	1.872283	1.026434
N17	-1.115160	2.077749	1.943285
C18	-2.051690	1.235145	1.432954
C19	-3.347526	1.203380	1.958635
C20	-3.675280	2.052566	3.021675
C21	-2.699622	2.916029	3.537310
C22	-1.425014	2.901121	2.971539
C23	-1.606216	0.388619	0.265693

H24	1.342241	-1.717415	5.893900
H25	2.325550	0.593881	5.993809
H26	0.255878	-2.474512	3.778826
H27	2.157056	2.048471	3.961698
H28	4.059336	1.556228	1.049806
H29	2.443698	-1.671018	-2.303378
H30	5.744060	0.185795	-0.212381
H31	4.915392	-1.444836	-1.932977
H32	-0.627825	3.543112	3.325295
H33	-4.082299	0.521744	1.545580
H34	-2.919749	3.578891	4.365248
H35	-4.672591	2.034043	3.446469
H36	-0.906445	-1.599866	1.633486
H37	0.713997	-1.833201	1.001965
H38	-2.245414	-0.496755	0.155955
H39	-1.679948	0.967042	-0.662317
H40	0.150087	-1.312089	-1.266207
H41	0.102851	0.413383	-1.619637
O42	1.774079	3.529218	1.414963
O43	0.359837	2.783155	-0.497256
C44	5.074894	5.391796	-2.185756
C45	3.904752	5.350340	-1.429439
N46	3.093868	4.256579	-1.445446
C47	3.406064	3.192396	-2.224784
C48	4.562718	3.179276	-3.008051
C49	5.411910	4.288401	-2.983292
C50	3.452914	6.486299	-0.542557
N51	1.961936	6.596092	-0.562465
C52	1.446282	7.232910	-1.830054
C53	0.903423	6.261612	-2.860287
C54	0.731899	6.639116	-4.192818
C55	0.153910	5.731773	-5.092326
C56	-0.243503	4.471032	-4.637595
C57	-0.043531	4.145981	-3.294819
N58	0.523406	5.030162	-2.433494
Fe59	1.168184	4.425403	-0.493981
N60	-0.399798	5.650879	0.358549
C61	-0.072192	6.905117	0.766761
C62	-1.046826	7.786610	1.238777
C63	-2.382347	7.366101	1.280449
C64	-2.710054	6.078436	0.840060
C65	-1.690717	5.242141	0.383722
C66	1.393138	7.259699	0.651421
H67	0.024916	6.006956	-6.132982
H68	-0.667801	3.728080	-5.302070
H69	1.045298	7.622731	-4.525738
H70	-0.308826	3.170964	-2.904694
H71	2.692855	2.376511	-2.254659
H72	5.704106	6.274556	-2.166401
H73	4.762512	2.323363	-3.639724
H74	6.310568	4.309350	-3.589374
H75	-1.876144	4.240848	0.018273
H76	-0.770496	8.786930	1.552312
H77	-3.736292	5.732640	0.836798
H78	-3.154703	8.040096	1.633252
H79	0.638595	7.920175	-1.550647
H80	2.236552	7.847914	-2.277944
H81	1.527519	8.349584	0.623071
H82	1.936186	6.883356	1.524910
H83	3.928081	7.428476	-0.847206
H84	3.757295	6.286188	0.490354

C85	3.504913	5.735090	5.350901
C86	4.729899	4.849647	5.645000
C87	2.565955	5.067355	4.302351
C88	3.357508	4.711917	3.049980
C89	5.503113	4.501055	4.359704
C90	4.572133	3.828985	3.305933
H91	2.575607	4.095167	2.250482
H92	3.631297	5.609807	2.478722
H93	5.128348	3.645935	2.378175
H94	4.256846	2.850709	3.696224
H95	5.934915	5.415055	3.928351
H96	6.340485	3.828246	4.579539
H97	5.395051	5.359159	6.352348
H98	4.402011	3.922486	6.138628
H99	3.838111	6.709520	4.966581
H100	2.938128	5.932728	6.268532
H101	1.728815	5.736930	4.066208
H102	2.135061	4.159743	4.750380
Cl103	0.320027	0.584857	-4.291449
O104	0.522490	-1.114241	-4.039189
O105	1.731414	1.404871	-3.670907
O106	0.038731	1.035760	-5.920345
O107	-1.019932	1.135273	-3.292712

Model 1
Optimized intermediate, Fe(III)Fe(III)
Ground state: 5a5b

C1	5.312299	2.188349	3.822963
C2	3.982051	2.361997	3.428113
N3	3.545391	3.562251	2.962207
C4	4.393965	4.613194	2.878988
C5	5.731075	4.502788	3.260134
C6	6.196828	3.269451	3.735737
C7	2.947239	1.264482	3.474122
N8	1.603158	1.861926	3.780869
C9	1.511206	2.386945	5.185421
C10	1.106728	3.845724	5.308827
C11	0.787577	4.379757	6.564270
C12	0.478787	5.736970	6.676639
C13	0.491517	6.538162	5.526397
C14	0.805099	5.945451	4.307279
N15	1.106124	4.625896	4.200027
Fe16	1.448395	3.523725	2.336711
N17	-0.603609	2.920904	2.587598
C18	-0.772399	1.690117	3.133932
C19	-2.053427	1.168964	3.347433
C20	-3.167069	1.935735	2.998384
C21	-2.979936	3.211958	2.445932
C22	-1.681897	3.671924	2.250193
C23	0.486901	0.923389	3.425180
H24	0.232287	6.163383	7.642284
H25	0.259986	7.594937	5.576484
H26	0.784600	3.739258	7.439499
H27	0.823935	6.518360	3.388994
H28	3.977709	5.540023	2.504617
H29	5.644148	1.227126	4.198579
H30	6.387835	5.361724	3.195757
H31	7.229260	3.154625	4.046249
H32	-1.472925	4.640058	1.814018

H33	-2.166554	0.173707	3.758016
H34	-3.824337	3.832825	2.172647
H35	-4.166638	1.546464	3.154422
H36	0.808442	1.768096	5.756177
H37	2.489454	2.264075	5.666894
H38	0.328690	0.185859	4.222003
H39	0.781636	0.378515	2.519482
H40	3.217387	0.498074	4.212038
H41	2.862132	0.776515	2.495293
O42	1.215875	5.027472	0.985343
O43	1.889910	2.603878	0.809849
C44	4.895174	6.276090	-2.037579
C45	3.675645	5.687506	-1.696337
N46	3.627499	4.562322	-0.936950
C47	4.772917	3.980121	-0.511125
C48	6.022842	4.517305	-0.821487
C49	6.084300	5.685191	-1.591229
C50	2.333049	6.226489	-2.137352
N51	1.409986	5.081848	-2.411917
C52	1.804821	4.326416	-3.657687
C53	2.113729	2.852587	-3.451041
C54	2.366159	2.019848	-4.541842
C55	2.665466	0.669352	-4.316017
C56	2.697068	0.181483	-3.006674
C57	2.434296	1.056750	-1.952521
N58	2.158463	2.366307	-2.185296
Fe59	1.655453	3.687173	-0.626271
N60	-0.376680	3.377137	-1.218508
C61	-0.886486	4.242205	-2.138857
C62	-2.110828	3.995565	-2.755465
C63	-2.819674	2.829716	-2.421326
C64	-2.284820	1.949146	-1.477926
C65	-1.054734	2.252024	-0.887668
C66	-0.038252	5.463854	-2.410082
H67	2.855418	0.008366	-5.154019
H68	2.881383	-0.863058	-2.794773
H69	2.323953	2.414713	-5.551303
H70	2.404940	0.722516	-0.922312
H71	4.659561	3.073646	0.069343
H72	4.916077	7.169899	-2.650744
H73	6.924687	4.024693	-0.479380
H74	7.041483	6.121074	-1.854166
H75	-0.614586	1.584377	-0.158899
H76	-2.500795	4.690202	-3.491077
H77	-2.779337	1.026075	-1.203977
H78	-3.766011	2.613403	-2.904171
H79	1.005170	4.424007	-4.401984
H80	2.687546	4.813250	-4.089814
H81	-0.329893	5.944380	-3.353321
H82	-0.182790	6.199655	-1.609527
H83	2.443790	6.881296	-3.012215
H84	1.891206	6.825475	-1.332504
H85	0.859735	5.931492	1.042604
Cl86	0.251606	-1.223355	0.245004
O87	0.226700	-0.829045	-1.440238
O88	-0.985583	-0.245929	1.022611
O89	0.020870	-2.884363	0.555754
O90	1.784698	-0.671697	0.908195

Model 1

Optimized transition state for OH group transfer (from intermediate state 5a4b)

C1	2.873070	-1.065273	-1.417323
C2	2.002569	-0.263570	-0.668962
N3	2.476273	0.665325	0.205189
C4	3.814649	0.794349	0.385195
C5	4.731130	0.008796	-0.307931
C6	4.250241	-0.928686	-1.233836
C7	0.506307	-0.347839	-0.812863
N8	-0.163265	0.009615	0.482246
C9	0.009907	-1.049000	1.525983
C10	0.590776	-0.565882	2.841974
C11	0.598339	-1.410998	3.960885
C12	1.182661	-0.974823	5.151022
C13	1.748743	0.306487	5.202624
C14	1.702711	1.099009	4.059875
N15	1.137473	0.673441	2.901725
Fe16	0.885144	1.884768	1.070357
N17	-1.192393	2.110643	1.974369
C18	-2.086358	1.242430	1.428730
C19	-3.398869	1.159587	1.908804
C20	-3.795857	1.981838	2.968426
C21	-2.867472	2.868398	3.528901
C22	-1.575951	2.901484	3.003786
C23	-1.587469	0.407552	0.272872
H24	1.196667	-1.619315	6.022543
H25	2.210422	0.678628	6.109083
H26	0.153932	-2.398083	3.894348
H27	2.119304	2.098183	4.043730
H28	4.127458	1.543664	1.098827
H29	2.465366	-1.749546	-2.150956
H30	5.793620	0.128177	-0.132600
H31	4.938608	-1.543685	-1.802299
H32	-0.820508	3.564216	3.408596
H33	-4.093086	0.456538	1.462532
H34	-3.135740	3.510572	4.359137
H35	-4.806317	1.923593	3.357041
H36	-0.949422	-1.547906	1.715473
H37	0.679920	-1.819186	1.124434
H38	-2.229425	-0.471604	0.127024
H39	-1.619142	0.996777	-0.650617
H40	0.202364	-1.341746	-1.161605
H41	0.164089	0.372889	-1.563595
O42	1.705988	3.727892	1.589609
O43	0.447302	2.823009	-0.505137
C44	4.952407	5.661821	-2.132502
C45	3.769797	5.576300	-1.399138
N46	3.041671	4.425983	-1.367740
C47	3.451659	3.344931	-2.076818
C48	4.626395	3.373352	-2.832947
C49	5.389871	4.542980	-2.856776
C50	3.222834	6.730372	-0.589065
N51	1.731529	6.742336	-0.619663
C52	1.181291	7.325237	-1.895870
C53	0.785607	6.301256	-2.939952
C54	0.676339	6.638539	-4.289097
C55	0.217029	5.675604	-5.200014
C56	-0.127033	4.401760	-4.739225
C57	0.008770	4.118697	-3.378375
N58	0.461067	5.055863	-2.505840

Fe59	1.053083	4.497138	-0.545025
N60	-0.579094	5.648998	0.314813
C61	-0.332808	6.933323	0.688401
C62	-1.364980	7.771131	1.115536
C63	-2.675777	7.276934	1.145544
C64	-2.920907	5.960276	0.739559
C65	-1.846142	5.170156	0.329303
C66	1.110578	7.374120	0.582760
H67	0.137914	5.919307	-6.253458
H68	-0.458625	3.617409	-5.408910
H69	0.945679	7.633725	-4.626056
H70	-0.217250	3.136551	-2.980223
H71	2.798792	2.480061	-2.076011
H72	5.513228	6.589615	-2.154401
H73	4.904104	2.500543	-3.409678
H74	6.298598	4.597284	-3.445607
H75	-1.967794	4.149342	-0.007236
H76	-1.152139	8.795021	1.401608
H77	-3.925493	5.556067	0.727737
H78	-3.491914	7.916301	1.462430
H79	0.287873	7.905572	-1.635298
H80	1.901928	8.036010	-2.320030
H81	1.176516	8.470838	0.556267
H82	1.670553	7.033952	1.461935
H83	3.639899	7.681098	-0.949198
H84	3.528960	6.623970	0.457935
C85	4.443005	5.711748	4.899837
C86	5.442363	4.584872	5.213560
C87	3.301578	5.195903	3.945010
C88	3.916294	4.557234	2.746481
C89	6.029454	3.968220	3.932363
C90	4.888980	3.455857	2.973290
H91	1.426911	4.206592	2.392983
H92	3.966868	5.106551	1.814397
H93	5.327810	3.101763	2.036715
H94	4.405228	2.600662	3.469014
H95	6.634018	4.713844	3.400457
H96	6.689828	3.125789	4.166009
H97	6.253761	4.978228	5.837428
H98	4.944407	3.803553	5.806227
H99	4.961193	6.549796	4.416386
H100	3.983080	6.100665	5.815066
H101	2.634048	6.024349	3.681293
H102	2.716605	4.460598	4.521496
Cl103	0.576521	0.584012	-4.253335
O104	0.795263	-1.112371	-4.009229
O105	1.939748	1.434273	-3.571356
O106	0.360121	1.039255	-5.893323
O107	-0.825156	1.093585	-3.321686

Model 1
Optimized product, Fe(III)Fe(II)
Ground state: 5a4b

C1	3.473281	-2.201109	-0.975008
C2	2.745409	-1.280575	-0.219999
N3	2.512335	-0.021365	-0.686690
C4	2.988372	0.352766	-1.902777
C5	3.717920	-0.524876	-2.701437
C6	3.965670	-1.819951	-2.229763

C7	2.180572	-1.594235	1.148716
N8	0.902084	-0.849296	1.351235
C9	0.566696	-0.640275	2.788844
C10	1.368151	0.502812	3.374270
C11	1.681564	0.587346	4.732909
C12	2.366721	1.711877	5.208526
C13	2.726939	2.729558	4.313732
C14	2.395287	2.589137	2.968720
N15	1.732877	1.492615	2.512158
Fe16	1.253954	1.221702	0.477330
N17	-0.752977	0.907239	0.049097
C18	-1.218692	-0.373199	0.133203
C19	-2.515392	-0.694155	-0.267550
C20	-3.337564	0.304827	-0.799992
C21	-2.862163	1.621655	-0.863632
C22	-1.571895	1.889217	-0.426217
C23	-0.231619	-1.435616	0.567219
H24	2.617198	1.791720	6.260244
H25	3.256353	3.611501	4.653896
H26	1.392372	-0.211400	5.406609
H27	2.638456	3.337211	2.225415
H28	2.758064	1.362079	-2.214605
H29	3.641879	-3.201960	-0.594821
H30	4.071836	-0.206823	-3.674238
H31	4.522573	-2.527021	-2.833734
H32	-1.140076	2.878122	-0.491894
H33	-2.860694	-1.720062	-0.210058
H34	-3.451113	2.393475	-1.346576
H35	-4.313335	0.062982	-1.205591
H36	-0.500326	-0.392061	2.841961
H37	0.712888	-1.557511	3.375451
H38	-0.735291	-2.228687	1.136026
H39	0.193865	-1.908897	-0.325991
H40	2.885374	-1.267243	1.923722
H41	2.041351	-2.676739	1.272893
O42	1.598916	2.821012	-0.199888
C43	5.867253	5.684267	-2.252486
C44	4.483911	5.519316	-2.132440
N45	3.956289	4.515326	-1.381793
C46	4.784821	3.648397	-0.746184
C47	6.171950	3.754972	-0.832675
C48	6.722196	4.792049	-1.597813
C49	3.493510	6.403912	-2.855469
N50	2.225481	6.531415	-2.085189
C51	1.062162	6.871268	-2.955426
C52	0.555969	5.649402	-3.686971
C53	-0.096802	5.741150	-4.916474
C54	-0.637048	4.585539	-5.493586
C55	-0.505897	3.361934	-4.828433
C56	0.165509	3.333524	-3.606691
N57	0.698012	4.454033	-3.042348
Fe58	1.795986	4.446764	-1.209626
N59	0.981155	5.801009	0.275056
C60	1.319684	7.111971	0.144858
C61	0.762701	8.089439	0.974361
C62	-0.154758	7.710419	1.960557
C63	-0.498749	6.359166	2.089503
C64	0.088556	5.433288	1.228833
C65	2.350534	7.441232	-0.913244
H66	-1.171291	4.635459	-6.433888
H67	-0.943462	2.454559	-5.224035

H68	-0.195068	6.703709	-5.405717
H69	0.247337	2.410213	-3.049774
H70	4.299710	2.873593	-0.166695
H71	6.265747	6.498402	-2.847796
H72	6.806296	3.049653	-0.311172
H73	7.797218	4.907782	-1.675947
H74	-0.144322	4.377578	1.279108
H75	1.039254	9.129735	0.845918
H76	-1.215202	6.032714	2.833459
H77	-0.600587	8.457155	2.608043
H78	0.266062	7.250986	-2.303755
H79	1.308537	7.676781	-3.661823
H80	2.265565	8.495353	-1.213611
H81	3.353672	7.306838	-0.491418
H82	3.242043	5.946617	-3.820022
H83	3.937548	7.386819	-3.071276
Cl84	-3.424573	1.415226	-4.321087
O85	-3.206490	1.741531	-5.999833
O86	-3.771858	2.908061	-3.484703
O87	-4.617407	0.225967	-3.961978
O88	-1.888406	0.840441	-3.680782

Model 2
Optimized reactant, Fe(IV)Fe(III)
Isomer with oxo-group trans to amine-N of TPA ligand
Reactant groundstate: 5a4b

C1	4.2124550029	0.7386748401	0.2295422490
N2	2.9246046748	0.9038552860	-0.1738198163
C3	2.5876467442	0.7048585026	-1.4707763093
C4	3.5357735959	0.3345148707	-2.4238486929
C5	4.8656113014	0.1631319172	-2.0212845749
C6	5.2071030174	0.3677570328	-0.6787028745
Fe7	1.4298685974	1.1817581755	1.3895221502
O8	2.1281626033	3.1792746626	1.5090669586
C9	4.5023078271	1.0180665040	1.6910203015
N10	3.3528474123	0.6219318225	2.5557900205
C11	3.2356714306	1.4280504168	3.8141612356
C12	1.8362432855	1.2867219586	4.3705965622
C13	1.5545614666	1.2634121899	5.7377611473
C14	0.2260010395	1.1245344597	6.1592888769
C15	-0.7878242119	0.9976398231	5.2024651059
C16	-0.4459424185	1.0299211507	3.8507731309
N17	0.8398298976	1.1820666531	3.4504276621
O18	-0.1004742289	1.7381507491	0.5726157509
Fe19	-1.0001275727	3.2503316618	0.0002277599
O20	0.2047364636	4.3565167851	0.4205514927
N21	-2.2646301857	3.4701996679	1.7395263149
C22	-2.1219866468	4.3954718801	2.7178027057
C23	-3.0385749812	4.4867316935	3.7648445548
C24	-4.1256843354	3.6008435385	3.7915366720
C25	-4.2680213287	2.6526616321	2.7727816990
C26	-3.3157788027	2.6080003861	1.7480519559
C27	-3.3415961378	1.5978759881	0.6401629926

N28	-2.7441642362	2.1874287861	-0.6152873836
C29	-3.7439981132	3.0888247228	-1.3158822583
C30	-3.3370480021	4.5371034939	-1.3227399863
N31	-2.1321909763	4.8420074780	-0.7854883834
C32	-1.6913634264	6.1236572876	-0.7623783395
C33	-2.4555681829	7.1594337353	-1.2931286293
C34	-3.7040725540	6.8600991303	-1.8566432170
C35	-4.1503293737	5.5358229476	-1.8692087070
N36	-0.5758479940	2.8023627768	-2.1060346905
C37	-1.3246436501	1.7662560755	-2.5714786674
C38	-1.2172563065	1.3468278304	-3.9020827738
C39	-0.3260846146	2.0102982677	-4.7546064482
C40	0.4337835143	3.0804593795	-4.2616751912
C41	0.2814148344	3.4533505275	-2.9256226284
C42	-2.2371835203	1.1247568534	-1.5623429376
N43	1.3656420450	-0.9446108535	1.3452263282
C44	2.3776408800	-1.6304952916	1.9395317723
C45	2.4715648569	-3.0170550108	1.8104625676
C46	1.4846081339	-3.7121328347	1.0957913565
C47	0.4262287661	-3.0005413853	0.5233229572
C48	0.4122379177	-1.6119374302	0.6502019670
C49	3.3220683122	-0.8549823873	2.8322592206
H50	-4.3201699078	7.6462737951	-2.2779804628
H51	-2.0831872018	8.1758741463	-1.2655286470
H52	-5.1128981855	5.2778974111	-2.2965860793
H53	-0.7196814792	6.2703117666	-0.3081991370
H54	-1.2668498560	5.0538397544	2.6321306892
H55	-5.1033704264	1.9617656831	2.7632551701
H56	-2.9111430421	5.2382453171	4.5343235253
H57	-4.8594687182	3.6568681678	4.5879202436
H58	0.8308544073	4.2777372871	-2.4880934492
H59	-1.8281937743	0.5265547843	-4.2615876835
H60	1.1194271982	3.6220665871	-4.9019468721
H61	-0.2377703980	1.7067887480	-5.7918415514
H62	-3.8706046351	2.7368526161	-2.3457519698
H63	-4.7199104483	2.9733032755	-0.8322249958
H64	-3.0772154906	0.5893054367	-2.0171004025
H65	-1.7036174837	0.3887048868	-0.9561823883
H66	-4.3482770796	1.2211918588	0.4315898329
H67	-2.7597843138	0.7026232893	0.9015799736
H68	1.5376479044	-4.7912210753	1.0055828165
H69	-0.3912349387	-3.4856389931	0.0024110975
H70	3.2910837681	-3.5505767910	2.2795439634
H71	-0.4023838879	-1.0336019366	0.2403214079
H72	-1.1823002490	0.9197514152	3.0665171632
H73	2.3595344845	1.3414353286	6.4594992931
H74	-1.8215663561	0.8630102252	5.4951898206
H75	-0.0097433206	1.0983861337	7.2171122967
H76	1.5435454454	0.8420977841	-1.7186483840
H77	6.2287685720	0.2346763079	-0.3413185447
H78	3.2375186802	0.1744683261	-3.4524262567
H79	5.6237120623	-0.1327771963	-2.7373134968
H80	4.3353139207	-1.2711749320	2.7678464379
H81	2.9957527652	-0.9939797196	3.8700663159
H82	5.4271615803	0.5109342199	1.9974789883
H83	4.6767039264	2.0913945778	1.8329146293
H84	3.9820499837	1.1277481963	4.5615219038
H85	3.4127387285	2.4759979186	3.5541982509
H86	2.9731583531	3.4867388223	1.1371786382
H87	1.3436073978	3.7639448882	1.1377121001
Cl88	-3.7373825544	-2.0124359324	-0.0011773773

O89	-2.3189146921	-1.2323107751	0.7193193253
O90	-3.1156017775	-3.2198926147	-1.0542467959
O91	-4.7348544933	-2.6102669345	1.2490741901
O92	-4.5616893521	-0.7605101222	-0.8988326410

Model 2
Optimized reactant, Fe(IV)Fe(III)
Isomer with oxo-group trans to pyrine-N of TPA ligand
Reactant groundstate: 5a4b

C1	3.9397612795	0.3059562639	-0.1865592759
N2	2.5911523425	0.3532787340	-0.3219870665
C3	1.9834800397	-0.2123654251	-1.3908476692
C4	2.7300152597	-0.8263735519	-2.3989798984
C5	4.1248552299	-0.8608740323	-2.2864755939
C6	4.7381455057	-0.2968307802	-1.1603144193
Fe7	1.5687879617	1.2643045104	1.3539154571
O8	2.2038985690	2.8278543891	1.1384175856
C9	4.4873194920	0.9479329263	1.0678532664
N10	3.5417824140	0.7203458215	2.2086358780
C11	3.7302869295	1.6967865271	3.3271419359
C12	2.4762671620	1.7415215289	4.1699324690
C13	2.4771125716	1.9435815481	5.5524430327
C14	1.2546445557	1.9884570449	6.2335149414
C15	0.0630029890	1.8208056811	5.5171668327
C16	0.1289757244	1.6188940800	4.1380294719
N17	1.3138853765	1.5873592500	3.4896814817
O18	-0.0655302780	1.6382226650	0.6629254647
Fe19	-1.0294791914	3.0656674662	-0.0102258175
O20	0.3540895927	4.3712067763	0.7178054256
N21	-2.6094875524	2.8182174560	1.4414914783
C22	-2.7058007524	3.4646983050	2.6290787758
C23	-3.7717414133	3.2343332849	3.4964072725
C24	-4.7604834222	2.3124948541	3.1210016145
C25	-4.6573223488	1.6559886140	1.8908857520
C26	-3.5646459970	1.9301841978	1.0602427555
C27	-3.3386739188	1.2322250599	-0.2544438456
N28	-2.6145261158	2.1322298568	-1.2185183296
C29	-3.5220240558	3.1559275158	-1.8440714959
C30	-3.3612050317	4.5667281689	-1.3248942100
N31	-2.2991419908	4.8543885269	-0.5348626157
C32	-2.1438172888	6.1243380188	-0.0761795872
C33	-3.0174696791	7.1535959893	-0.4100913717
C34	-4.1082930937	6.8634973734	-1.2412959803
C35	-4.2838068528	5.5554861215	-1.6939615284
N36	-0.2112950689	3.0874512999	-2.0233618310
C37	-0.7969434343	2.1977291250	-2.8700600765
C38	-0.3552329470	2.0647064704	-4.1910519053
C39	0.7002460728	2.8637623191	-4.6409951338
C40	1.2937550390	3.7795713463	-3.7603813277
C41	0.8136345295	3.8633902254	-2.4555764431
C42	-1.8838894303	1.3495573119	-2.2770406493
N43	1.2225257580	-0.7134323016	1.8334487468
C44	2.2448280683	-1.4309487382	2.3729562391
C45	2.1043344003	-2.7976611900	2.6173722213
C46	0.9071331046	-3.4398317513	2.2763428841
C47	-0.1275501506	-2.6939144008	1.7061895948
C48	0.0585045099	-1.3253473186	1.5106082799
C49	3.5299386612	-0.7046788863	2.6945138663
H50	-4.8098414442	7.6402284257	-1.5228729369

H51	-2.8529405909	8.1530328123	-0.0266729985
H52	-5.1252535134	5.2979779413	-2.3279326538
H53	-1.3095774186	6.3008586090	0.5896530038
H54	-1.9154720560	4.1681999473	2.8619846381
H55	-5.4067518495	0.9400094234	1.5740011174
H56	-3.8331069430	3.7684211418	4.4368617005
H57	-5.6029386534	2.1154703376	3.7742988541
H58	1.2431853053	4.5412632043	-1.7310454976
H59	-0.8361068248	1.3483101130	-4.8473118293
H60	2.1089912915	4.4167215949	-4.0803600648
H61	1.0508658685	2.7796244930	-5.6635467847
H62	-3.3303835359	3.1636680703	-2.9235429849
H63	-4.5638573677	2.8355731320	-1.7212584653
H64	-2.5757748524	0.9718758753	-3.0380496716
H65	-1.4546148687	0.4568017337	-1.7993295453
H66	-4.2771738093	0.8689268923	-0.6858672260
H67	-2.7195519785	0.3409225339	-0.1052618132
H68	0.7950793636	-4.5058335623	2.4381483477
H69	-1.0472939871	-3.1558588795	1.3718034075
H70	2.9273428579	-3.3561935283	3.0497355240
H71	-0.6960546224	-0.7137331490	1.0402888302
H72	-0.7535610098	1.4708254129	3.5301535400
H73	3.4144382998	2.0583945578	6.0849571323
H74	-0.8965563663	1.8327686114	6.0191609267
H75	1.2342878132	2.1394887916	7.3067364899
H76	0.9004736630	-0.2087947238	-1.4027778406
H77	5.8145805472	-0.3339078451	-1.0361375378
H78	2.2233447987	-1.2866128588	-3.2382827686
H79	4.7263091002	-1.3390020571	-3.0513341447
H80	4.3792033729	-1.2442372332	2.2584332889
H81	3.6866967333	-0.7071438113	3.7798441811
H82	5.4881390660	0.5632182717	1.3018871587
H83	4.5552836162	2.0303688562	0.9220955726
H84	4.6061641023	1.4391180629	3.9362470106
H85	3.8958988711	2.6787748239	2.8742799927
H86	0.5161149284	5.3169870548	0.5753625906
H87	1.2360657286	3.7893406068	0.9457805480
O88	-1.2802931482	-1.2970314117	-0.8886775871
Cl89	-2.6308066967	-2.1886166953	-1.6343370633
O90	-2.7653429621	-1.5915090338	-3.2490653917
O91	-2.2749012542	-3.8573098976	-1.5259225098
O92	-4.0207666055	-1.7607976300	-0.6982876727

Model 2
Optimized transition state for H-atom transfer
(from reactant state 5a4b)

C1	3.5601290000	-0.1331310000	0.1343240000
N2	2.2361000000	0.0747530000	-0.1166750000
C3	1.6783070000	-0.4067020000	-1.2574740000
C4	2.4365430000	-1.1004590000	-2.2032100000
C5	3.7990910000	-1.2990300000	-1.9652950000
C6	4.3661360000	-0.8131670000	-0.7777150000
Fe7	1.0312980000	0.8169290000	1.5208160000
O8	1.9475780000	2.7648110000	1.2726980000
C9	4.0852630000	0.4351170000	1.4325030000
N10	3.0668950000	0.3165050000	2.5202430000
C11	3.2346260000	1.3512440000	3.5862270000
C12	1.9432790000	1.4941010000	4.3540080000
C13	1.8885960000	1.7759520000	5.7217850000

C14	0.6410710000	1.9006840000	6.3439940000
C15	-0.5226230000	1.7355870000	5.5831580000
C16	-0.4029210000	1.4581430000	4.2218370000
N17	0.8064570000	1.3431490000	3.6243880000
O18	-0.5047670000	1.5226890000	0.8711470000
Fe19	-1.3664020000	3.1465710000	0.4973640000
O20	-0.1755830000	4.1639080000	1.4436050000
N21	-3.0618400000	2.7011920000	1.7985580000
C22	-3.2828980000	3.2451630000	3.0197380000
C23	-4.3633020000	2.8542060000	3.8094400000
C24	-5.2359010000	1.8728950000	3.3190710000
C25	-5.0124840000	1.3278640000	2.0506010000
C26	-3.9140130000	1.7634630000	1.3005100000
C27	-3.5978340000	1.2542350000	-0.0824180000
N28	-2.9901220000	2.3728780000	-0.8817140000
C29	-4.0126770000	3.4276190000	-1.1920550000
C30	-3.5381350000	4.8363950000	-0.9332610000
N31	-2.4880180000	4.9945850000	-0.0922840000
C32	-2.0652450000	6.2437290000	0.2215670000
C33	-2.6855020000	7.3835110000	-0.2853440000
C34	-3.7689580000	7.2286220000	-1.1594120000
C35	-4.1959420000	5.9399080000	-1.4897480000
N36	-0.5185240000	3.4567310000	-1.4740190000
C37	-1.1614910000	2.8270570000	-2.4922900000
C38	-0.7478320000	3.0112190000	-3.8179290000
C39	0.3348450000	3.8521200000	-4.0885200000
C40	0.9784290000	4.5071990000	-3.0286100000
C41	0.5195180000	4.2901480000	-1.7319870000
C42	-2.2722960000	1.8901680000	-2.1063150000
N43	0.7693580000	-1.2529670000	2.0178280000
C44	1.8237960000	-1.8949470000	2.5884410000
C45	1.8157470000	-3.2813980000	2.7560530000
C46	0.7045850000	-4.0204090000	2.3329040000
C47	-0.3756100000	-3.3525490000	1.7489560000
C48	-0.3130610000	-1.9669270000	1.6074320000
C49	2.9818840000	-1.0651950000	3.1006640000
H50	-4.2680480000	8.0947300000	-1.5788950000
H51	-2.3249100000	8.3669490000	-0.0094650000
H52	-5.0291640000	5.7891470000	-2.1672390000
H53	-1.2096510000	6.2922200000	0.8793760000
H54	-2.5776700000	4.0016540000	3.3410490000
H55	-5.6848220000	0.5840770000	1.6386000000
H56	-4.5257700000	3.3147650000	4.7764050000
H57	-6.0871640000	1.5510300000	3.9082890000
H58	0.9470940000	4.7920460000	-0.8726760000
H59	-1.2709040000	2.5020530000	-4.6191770000
H60	1.8078290000	5.1806230000	-3.2074810000
H61	0.6643830000	4.0056180000	-5.1098880000
H62	-4.3477620000	3.3245950000	-2.2315230000
H63	-4.8931190000	3.2446430000	-0.5643960000
H64	-2.9700470000	1.7354760000	-2.9376640000
H65	-1.8450830000	0.9103120000	-1.8577300000
H66	-4.4961870000	0.8585730000	-0.5734730000
H67	-2.8624470000	0.4408710000	-0.0489210000
H68	0.6917840000	-5.0985810000	2.4452070000
H69	-1.2381690000	-3.8811970000	1.3644230000
H70	2.6697810000	-3.7765520000	3.2052420000
H71	-1.0905750000	-1.4184720000	1.0951680000
H72	-1.2625010000	1.3213710000	3.5804840000
H73	2.8055440000	1.8847560000	6.2896960000
H74	-1.5030560000	1.8099810000	6.0370540000

H75	0.5795730000	2.1097080000	7.4060060000
H76	0.6061560000	-0.2854570000	-1.3649340000
H77	5.4158130000	-0.9743400000	-0.5589300000
H78	1.9422270000	-1.4978950000	-3.0807130000
H79	4.4103980000	-1.8416340000	-2.6775530000
H80	3.9243510000	-1.6014720000	2.9319140000
H81	2.8745210000	-0.9667400000	4.1878040000
H82	5.0271610000	-0.0561320000	1.7117440000
H83	4.3005030000	1.5015830000	1.3063350000
H84	4.0659760000	1.1087030000	4.2618270000
H85	3.4536020000	2.2987570000	3.0867720000
H86	2.3706700000	2.9104050000	0.4066540000
H87	1.1313600000	3.4111910000	1.3942950000
H88	0.2561550000	5.1279870000	2.3722050000
Cl89	-1.9401560000	-2.0002960000	-1.9420150000
O90	-1.3369460000	-0.7083530000	-0.8652770000
O91	-0.6367830000	-2.3835060000	-2.9984610000
O92	-2.3994320000	-3.3106610000	-0.9286300000
O93	-3.2811380000	-1.2898120000	-2.7597140000
C94	2.8089330000	7.3481260000	3.5023100000
C95	1.8653630000	8.4840630000	3.9383470000
C96	0.5656700000	7.9386110000	4.5576390000
C97	-0.1533500000	6.9588030000	3.5832080000
C98	0.8064470000	5.8472530000	3.1685520000
C99	2.0939510000	6.3640120000	2.5320430000
H100	1.6216280000	9.1119000000	3.0687340000
H101	0.7936990000	7.4111620000	5.4946820000
H102	-0.1178300000	8.7576350000	4.8116290000
H103	-1.0540450000	6.5507850000	4.0589440000
H104	-0.4774900000	7.5276950000	2.6997630000
H105	1.0150180000	5.1639010000	4.0049610000
H106	2.7627870000	5.5327440000	2.2757560000
H107	1.8599670000	6.8978270000	1.5990450000
H108	3.1521010000	6.7941670000	4.3879060000
H109	3.7032870000	7.7529960000	3.0135170000
H110	2.3753630000	9.1352790000	4.6587690000

Model 2
Optimized intermediate, Fe(III)Fe(III)
Ground state: 5a5b

C1	3.5370640996	-0.2868117889	-0.0608258656
N2	2.2062779394	-0.0542268519	-0.2437306572
C3	1.5698739667	-0.5503357722	-1.3359609332
C4	2.2550885705	-1.2908400710	-2.3016580126
C5	3.6239428627	-1.5204384708	-2.1337985111
C6	4.2714893818	-1.0148801172	-0.9964012449
Fe7	1.1254186699	0.7558605526	1.4309221671
O8	2.0686349922	2.6595121253	1.1119343222
C9	4.1484340510	0.3050237575	1.1906762922
N10	3.1930898274	0.2266909487	2.3380187826
C11	3.4231689696	1.2828078468	3.3717437526
C12	2.1659806862	1.4660374707	4.1896132012
C13	2.1736625895	1.7883435789	5.5495493138
C14	0.9558938163	1.9512974357	6.2200030849
C15	-0.2427393758	1.7810214235	5.5157817050
C16	-0.1860453516	1.4622439621	4.1597925639
N17	0.9956731843	1.3139174977	3.5162258760
O18	-0.4278059838	1.4563511506	0.8168885802
Fe19	-1.2751213984	3.0623250094	0.4152951041

O20	0.0811370912	4.1141905916	1.3406114028
N21	-2.9059264569	2.7550718789	1.8170847837
C22	-3.0321497810	3.3401103251	3.0332106247
C23	-4.0799737471	3.0170096799	3.8935864263
C24	-5.0183466146	2.0589922485	3.4831317054
C25	-4.8892902018	1.4677860291	2.2224600210
C26	-3.8199276846	1.8369884688	1.3986113869
C27	-3.5962330954	1.2630958099	0.0236604035
N28	-2.9762774867	2.3237035284	-0.8449356801
C29	-3.9683226553	3.4047716921	-1.1578365697
C30	-3.4290164347	4.8076107414	-1.0130336507
N31	-2.3560890652	4.9935015629	-0.2051701175
C32	-1.8986070430	6.2547775684	-0.0022590421
C33	-2.4965751856	7.3716574878	-0.5804375570
C34	-3.6006243040	7.1818492077	-1.4214354592
C35	-4.0660565012	5.8840456534	-1.6430409418
N36	-0.5127124169	3.3066360235	-1.6020189705
C37	-1.2245478381	2.6631634250	-2.5630501635
C38	-0.8809549804	2.7916268957	-3.9141795101
C39	0.2061100338	3.5952527691	-4.2694411799
C40	0.9242913288	4.2645442238	-3.2673211394
C41	0.5329326790	4.1000423676	-1.9406170425
C42	-2.3249376490	1.7627945848	-2.0754093123
N43	0.8438178615	-1.3009243283	1.9940855380
C44	1.9159182980	-1.9551826812	2.5150828335
C45	1.8915635306	-3.3388696764	2.7039912281
C46	0.7448932160	-4.0624716099	2.3551395982
C47	-0.3551583026	-3.3809561307	1.8259168198
C48	-0.2745733771	-1.9986985193	1.6613197017
C49	3.1161376992	-1.1410428078	2.9494782040
H50	-4.0846168987	8.0269023534	-1.8975335859
H51	-2.1033238701	8.3617878033	-0.3853707588
H52	-4.9150009253	5.7037496836	-2.2933299831
H53	-1.0242705699	6.3554537632	0.6253599473
H54	-2.2778774854	4.0709416195	3.2965007140
H55	-5.6104801691	0.7378752377	1.8728619017
H56	-4.1673143298	3.5097789061	4.8542782811
H57	-5.8459604727	1.7890348907	4.1293761847
H58	1.0261264165	4.6107266924	-1.1229354544
H59	-1.4571859841	2.2674643335	-4.6678788976
H60	1.7609833131	4.9069881923	-3.5134031355
H61	0.4839261069	3.7071205228	-5.3114454064
H62	-4.3687682966	3.2558744765	-2.1682645270
H63	-4.8164976103	3.2961935383	-0.4711968520
H64	-3.0640199822	1.5600845289	-2.8582574178
H65	-1.8861154910	0.8019051405	-1.7811554470
H66	-4.5305096197	0.8892546184	-0.4127627061
H67	-2.8976836133	0.4177257506	0.0544881025
H68	0.7191964750	-5.1388395187	2.4832006965
H69	-1.2490119958	-3.8990458481	1.5025469052
H70	2.7606498012	-3.8438141113	3.1115392693
H71	-1.0701073519	-1.4431009272	1.1860603132
H72	-1.0742119675	1.3166202095	3.5605987025
H73	3.1153157784	1.9012341788	6.0744398235
H74	-1.2010452394	1.8833088139	6.0098844672
H75	0.9434714106	2.1945905264	7.2764042682
H76	0.4966592604	-0.4055778402	-1.3878576929
H77	5.3278096076	-1.1974296548	-0.8335992384
H78	1.7025233523	-1.6976376619	-3.1395802244
H79	4.1793861220	-2.1003000210	-2.8624153422
H80	4.0378841396	-1.6984594891	2.7393945967

H81	3.0704594232	-1.0216998728	4.0389727757
H82	5.0977217573	-0.1949146580	1.4258642817
H83	4.3718555575	1.3644671164	1.0266653456
H84	4.2768652595	1.0405993197	4.0189322491
H85	3.6383067683	2.2150547044	2.8428654574
H86	2.4651948732	2.7849781225	0.2308640127
H87	1.2957447325	3.3737359924	1.2854706238
H88	0.0570825163	4.9971353663	1.7433990510
Cl89	-2.1916421337	-1.9846866447	-1.8394050988
O90	-1.4318403345	-0.8068457551	-0.7316147387
O91	-1.1020410080	-2.1155243412	-3.1665849589
O92	-2.3985462210	-3.4468727079	-0.9653289291
O93	-3.6878320588	-1.2421016604	-2.2873743150

Model 2
Optimized transition state for OH group transfer
(from intermediate state 5a5a)

C1	3.803893	-0.014124	0.145968
N2	2.513870	0.324085	-0.140490
C3	1.991760	0.025788	-1.354492
C4	2.744303	-0.618007	-2.339279
C5	4.068625	-0.959219	-2.058313
C6	4.604970	-0.653852	-0.797594
Fe7	1.244947	0.882785	1.525565
O8	2.128167	2.848538	1.420029
C9	4.303868	0.385147	1.516517
N10	3.239234	0.224886	2.552759
C11	3.392912	1.164033	3.703754
C12	2.080026	1.278935	4.441805
C13	1.992064	1.441745	5.827453
C14	0.730273	1.547190	6.423880
C15	-0.414250	1.482292	5.619912
C16	-0.260983	1.318926	4.242773
N17	0.962515	1.222667	3.670534
O18	-0.320205	1.520882	0.870624
Fe19	-1.281036	3.148358	0.341789
O20	0.108520	4.338535	1.150670
N21	-2.877237	2.780102	1.819238
C22	-3.045075	3.388531	3.017818
C23	-4.043563	3.000255	3.910653
C24	-4.895233	1.947707	3.549488
C25	-4.729321	1.329999	2.305621
C26	-3.709702	1.767229	1.452154
C27	-3.466708	1.161802	0.089972
N28	-2.957665	2.216495	-0.847360
C29	-4.025818	3.214680	-1.167197
C30	-3.553578	4.647998	-1.173894
N31	-2.506616	4.966519	-0.370610
C32	-2.143468	6.268364	-0.259933
C33	-2.788355	7.293141	-0.948234
C34	-3.849343	6.963107	-1.800050
C35	-4.234624	5.625242	-1.910440
N36	-0.520066	3.229882	-1.711512
C37	-1.207613	2.474989	-2.606247
C38	-0.825241	2.424893	-3.953875
C39	0.273973	3.171956	-4.380367
C40	0.972332	3.957858	-3.451494
C41	0.546990	3.959181	-2.126904
C42	-2.330289	1.628539	-2.070561

N43	0.958894	-1.220372	1.765292
C44	1.945750	-1.945499	2.353867
C45	1.882822	-3.339039	2.398812
C46	0.783559	-3.995912	1.831390
C47	-0.219229	-3.241448	1.217858
C48	-0.097908	-1.853020	1.195721
C49	3.080043	-1.194351	3.016859
O50	-2.106354	-1.413241	-1.195919
Cl51	-1.060795	-1.927089	-2.517545
O52	-0.457943	-0.455094	-3.263317
O53	0.290611	-2.758449	-1.833606
O54	-1.939685	-2.867883	-3.637126
H55	-4.366249	7.731795	-2.362989
H56	-2.465147	8.319613	-0.825316
H57	-5.058204	5.338720	-2.554941
H58	-1.320166	6.483379	0.407223
H59	-2.362181	4.198781	3.240445
H60	-5.387386	0.527299	1.992722
H61	-4.161236	3.516649	4.855792
H62	-5.685933	1.625703	4.217750
H63	1.047493	4.544228	-1.365800
H64	-1.368834	1.787725	-4.639965
H65	1.824662	4.555443	-3.751620
H66	0.582987	3.143574	-5.419024
H67	-4.496857	2.966053	-2.126477
H68	-4.809195	3.129815	-0.404005
H69	-3.083470	1.451987	-2.848902
H70	-1.928586	0.645051	-1.809355
H71	-4.382578	0.693863	-0.294221
H72	-2.702440	0.380265	0.143216
H73	0.726070	-5.078146	1.850863
H74	-1.060938	-3.705003	0.722054
H75	2.683054	-3.903318	2.865300
H76	-0.819587	-1.239791	0.674482
H77	-1.102817	1.257389	3.566665
H78	2.893961	1.472274	6.428292
H79	-1.405557	1.544260	6.051672
H80	0.642735	1.663094	7.498300
H81	0.955523	0.277837	-1.530403
H82	5.626588	-0.921237	-0.551301
H83	2.265823	-0.868783	-3.276081
H84	4.674207	-1.472464	-2.796542
H85	4.020920	-1.741856	2.875910
H86	2.892645	-1.174269	4.097244
H87	5.203817	-0.188557	1.777022
H88	4.591367	1.443097	1.507051
H89	4.194078	0.849002	4.386691
H90	3.655064	2.143362	3.293055
H91	2.735591	2.963449	0.666471
H92	1.327637	3.528747	1.355113
C93	-0.291659	6.704983	3.502195
C94	0.277464	7.907779	2.709893
H95	-0.418634	7.023331	4.557411
C96	1.767083	8.141727	3.021943
H97	0.167350	7.722926	1.629277
H98	-0.312686	8.802962	2.933535
C99	2.593909	6.878385	2.719718
H100	2.143984	8.988274	2.437171
H101	1.883502	8.416205	4.080260
C102	2.082042	5.657457	3.521448
H103	2.535041	6.656041	1.643037

H104	3.652444	7.045902	2.946018
C105	0.596802	5.503455	3.502044
H106	2.565471	4.731760	3.188204
H107	2.387802	5.789081	4.580176
H108	0.240428	5.277982	0.934846
H109	0.174217	4.544600	3.784944
H110	-1.302783	6.446569	3.160116

Model 2
Optimized product, Fe(III)Fe(II)
Ground state: 5a4b

C1	3.219296	-2.329424	-1.130865
C2	2.523289	-1.385991	-0.368275
N3	2.447845	-0.083089	-0.748876
C4	3.088229	0.311587	-1.879006
C5	3.815408	-0.574530	-2.671850
C6	3.875257	-1.921837	-2.296435
C7	1.878847	-1.740647	0.950987
N8	0.701645	-0.883458	1.235156
C9	0.463902	-0.722575	2.698390
C10	1.386156	0.319497	3.298467
C11	1.732682	0.304754	4.653306
C12	2.519428	1.337038	5.171517
C13	2.950942	2.360746	4.318560
C14	2.579628	2.315626	2.977872
N15	1.813408	1.314191	2.475118
Fe16	1.131760	1.244756	0.435023
N17	-1.011685	1.090050	0.567143
C18	-1.529108	-0.172095	0.501432
C19	-2.905129	-0.394488	0.515476
C20	-3.774641	0.701364	0.620794
C21	-3.241829	1.989205	0.745112
C22	-1.854570	2.147541	0.714108
C23	-0.516801	-1.295304	0.476016
H24	2.789169	1.344240	6.221209
H25	3.556640	3.178150	4.689183
H26	1.383654	-0.498446	5.292279
H27	2.873548	3.087203	2.277357
H28	2.992955	1.358906	-2.128042
H29	3.248397	-3.365225	-0.812345
H30	4.314761	-0.220888	-3.565900
H31	4.419685	-2.640420	-2.898535
H32	-1.421066	3.124945	0.886217
H33	-3.290881	-1.407234	0.467908
H34	-3.856822	2.872174	0.897828
H35	-4.846887	0.544860	0.640718
H36	-0.571590	-0.393913	2.838211
H37	0.568970	-1.679113	3.230023
H38	-0.958028	-2.218885	0.879919
H39	-0.200675	-1.510567	-0.552489
H40	2.609849	-1.570809	1.751248
H41	1.617512	-2.808727	0.979602
O42	1.715576	2.828095	-0.490336
C43	3.762993	4.776843	-5.216623
C44	3.532032	4.856589	-3.841433
N45	2.661524	4.012578	-3.225160
C46	1.987320	3.087977	-3.952776
C47	2.174366	2.959157	-5.328831
C48	3.080255	3.813620	-5.969570

C49	4.204341	5.874872	-2.947064
N50	3.239705	6.319609	-1.895104
C51	2.147308	7.180153	-2.477150
C52	0.746924	6.800152	-2.040678
C53	-0.299464	7.723492	-2.089988
C54	-1.584500	7.325093	-1.708348
C55	-1.803326	6.002268	-1.305320
C56	-0.722557	5.125029	-1.296356
N57	0.528484	5.519595	-1.646738
Fe58	2.271216	4.403573	-1.118280
N59	2.234618	5.738626	0.604186
C60	2.958160	6.887948	0.485438
C61	2.801393	7.935429	1.391998
C62	1.853043	7.816457	2.419471
C63	1.083059	6.653433	2.509676
C64	1.310282	5.625773	1.591296
C65	3.891035	6.952972	-0.704155
H66	-2.399289	8.039015	-1.703990
H67	-2.764276	5.677492	-0.928972
H68	-0.107939	8.744187	-2.401061
H69	-0.823974	4.097586	-0.979091
H70	1.287425	2.468159	-3.407144
H71	4.454216	5.463493	-5.691218
H72	1.614332	2.218379	-5.886225
H73	3.240281	3.743593	-7.039475
H74	0.697124	4.734944	1.612728
H75	3.386100	8.842113	1.281925
H76	0.281280	6.540956	3.226069
H77	1.696809	8.634213	3.113340
H78	2.338276	8.233317	-2.240112
H79	2.201909	7.091183	-3.568139
H80	4.177562	7.993068	-0.910736
H81	4.817496	6.402107	-0.500145
H82	4.583058	6.718330	-3.539669
H83	5.060850	5.415045	-2.443572
Cl84	-2.845081	5.671226	2.481300
O85	-3.701417	5.105825	1.063890
O86	-2.213876	7.250323	2.181212
O87	-3.814241	5.574368	3.883386
O88	-1.443166	4.599354	2.625498
O89	4.313308	3.679937	-0.582654
H90	4.138643	2.765239	-0.289863
H91	5.111360	4.046896	-0.164335