

Supporting Information

Oxoiron(IV) as oxidative active intermediate of p-chlorophenol in the Fenton reaction: a DFT study

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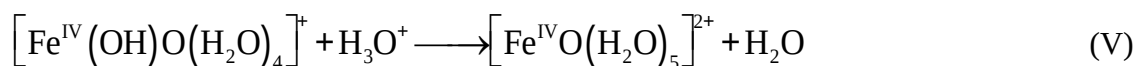
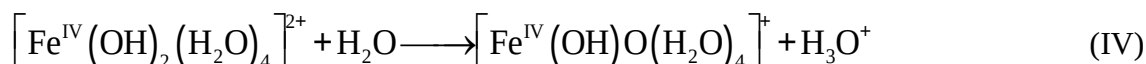
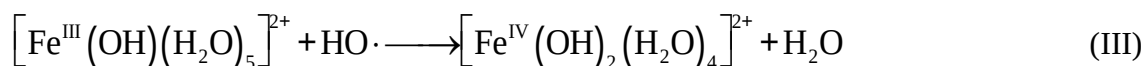
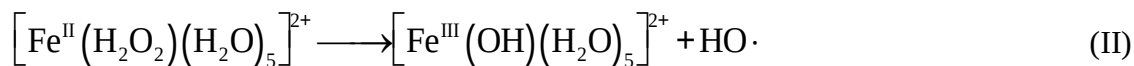
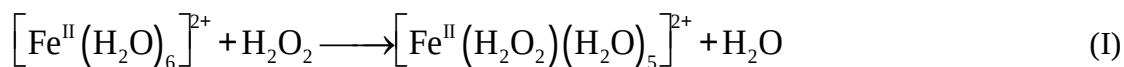
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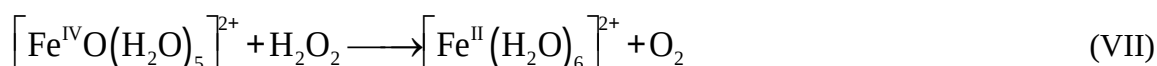
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LIST OF ESTABLISHED REACTIONS INVOLVING FERRYL CATIONS

1. Generation of ferry cations:



2. Removal of ferry cations:



3. Regeneration of Fe^{2+} cations

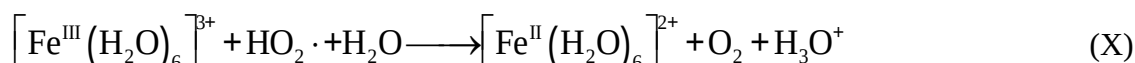
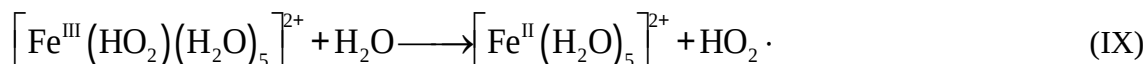
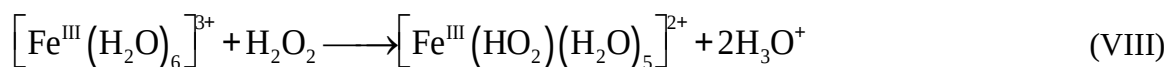


Table 1. Electronic energy, enthalpy and free energy changes computed in kcal/mol for the gas-phase and micro-solvated models, relative to the reactants. The internal energy and entropy terms were computed from a frequency calculation at 1 Atm, 298.15 K.

		ΔE	ΔH	ΔG	ΔE_{Solv}
Gas Phase	I1gp	-36.5	-36.5	-26.8	2.0
	TS1gp	-31.7	-32.6	-21.0	7.7
	I2gp	-63.1	-63.2	-52.1	-28.4
	TS2gp	-61.3	-65.3	-51.3	-25.9
	I3gp	-61.6	-63.5	-52.5	-21.3
	TS3gp	-50.6	-54.3	-40.4	-8.3
	TS2'gp	-53.7	-54.1	-41.8	-15.8
	I3'gp	-56.7	-57.5	-45.3	-19.6
	TS3'gp	-52.5	-53.3	-42.9	-15.1
	I4gp	-57.6	-60.6	-47.7	-13.3
	TS4gp	-55.0	-58.5	-43.3	-11.3
	I5gp	-57.6	-62.1	-47.6	-11.2
	I5gp+H ₂ O	-76.9	-79.8	-56.3	-19.1
	TS5gp+H ₂ O	-68.3	-70.7	-47.0	-14.7
	I6gp+H ₂ O	-71.9	-72.9	-51.0	-1.9
	I5'gp+H ₂ O	5.3	1.8	1.9	8.8
	TS5'gp+H ₂ O	14.2	10.8	13.1	17.3
	I6'gp+H ₂ O	5.6	3.3	4.8	6.9
	I7gp+2H ₂ O	-22.0	-23.7	-13.3	-2.9
	TS7gp+2H ₂ O	-19.4	-20.6	-8.3	-2.5
	I8gp+2H ₂ O	-28.0	-27.1	-15.7	-10.3
Micro Solvated	I1ms	-57.2	-55.2	-33.5	-8.8
	TS1ms	-51.8	-50.9	-29.2	-2.0
	I2ms	-83.6	-82.0	-60.7	-37.5
	TS2ms	-69.6	-68.8	-45.3	-22.6
	I3ms	-72.7	-70.7	-51.3	-23.1
	TS3ms	-66.7	-65.7	-45.3	-16.2
	I4ms	-75.6	-74.5	-53.5	-26.8
	I4ms+H ₂ O	-93.0	-91.0	-60.0	-33.8
	TS4ms+H ₂ O	-90.2	-90.9	-58.4	-31.7
	I5ms+H ₂ O	-100.5	-99.6	-65.2	-35.1
	I6ms+H ₂ O	-37.4	-36.6	-17.1	-11.9
	TS2'ms	-74.9	-73.6	-51.3	-25.6
	I3'ms	-77.1	-76.2	-54.3	-28.6
	TS3'ms	-75.7	-75.8	-52.6	-27.4
	I4'ms	-79.3	-81.1	-55.7	-25.1
	TS4'ms	-76.2	-78.4	-54.9	-21.3
	I5'ms	-76.9	-79.8	-56.3	-19.1

STRUCTURES:

REACTANTS

C1-Phenol

1.C	0.063796	0.022949	0.000000
2.C	0.062972	1.418926	0.000000
3.C	1.272416	-0.668170	0.000000
4.C	2.480090	0.036505	0.000000
5.C	2.472079	1.435670	0.000000
6.C	1.261948	2.129864	0.000000
7.Cl	-1.458654	2.285642	0.000000
8.H	-0.880114	-0.519716	0.000000
9.H	1.293874	-1.757418	0.000000
10.O	3.641070	-0.698558	0.000000
11.H	3.414016	1.989359	0.000000
12.H	1.249869	3.218631	0.000000
13.H	4.395951	-0.087057	0.000000

FeO2

1.O	-3.025116	-0.198347	-1.816769
2.Fe	-2.234351	1.199006	-1.709698
3.O	-0.414361	0.242057	-1.630385
4.O	-4.010747	2.249497	-1.584348
5.O	-2.134748	1.501193	-3.780079
6.O	-1.199502	3.018059	-1.560353
7.O	-2.159655	1.345929	0.409493
8.H	-0.958104	3.401095	-0.694333
9.H	-1.020591	3.692415	-2.243663
10.H	0.475383	0.621600	-1.486672
11.H	-0.330985	-0.728086	-1.726647
12.H	-4.143864	3.190957	-1.814847
13.H	-4.863455	1.784474	-1.707263
14.H	-2.989794	1.607527	0.859542
15.H	-1.827681	0.568192	0.904117
16.H	-1.281466	1.487482	-4.260209
17.H	-2.754989	0.972945	-4.324359

H2O

1.O	0.000000	0.000000	-0.005390
2.H	-0.765758	0.000000	0.591256
3.H	0.765758	0.000000	0.591256

HCl

1.Cl	0.000000	0.000000	-0.007974
2.H	0.000000	0.000000	1.284671

HQ

1.C	0.060596	0.011538	0.000000
2.C	0.037249	1.410320	0.000000
3.C	1.274635	-0.674134	0.000000
4.C	2.476343	0.037137	0.000000
5.C	2.452754	1.436011	0.000000
6.C	1.238617	2.121804	0.000000
7.O	-1.135459	2.137758	0.000000
8.H	-0.876694	-0.550201	0.000000
9.H	1.302206	-1.763333	0.000000

10.O	3.648555	-0.690702	0.000000
11.H	3.390202	1.997630	0.000000
12.H	1.211160	3.211004	0.000000
13.H	4.394634	-0.069227	0.000000
14.H	-1.880924	1.515696	0.000000

Gas Phase

I1gp

1.C	-3.576551	-3.048012	-3.306758
2.C	-4.939004	-3.268537	-3.356891
3.C	-5.674523	-3.381274	-2.151855
4.C	-5.027295	-3.265977	-0.897505
5.C	-3.666990	-3.049727	-0.848136
6.C	-2.942851	-2.938079	-2.052578
7.O	-6.992162	-3.602883	-2.119145
8.Cl	-1.206370	-2.860172	-1.994887
9.O	-3.034302	-0.082142	-1.919570
10.Fe	-2.167625	1.334427	-1.709408
11.O	-0.405081	0.225882	-1.430235
12.O	-3.945442	2.503810	-1.548608
13.O	-1.992491	1.690058	-3.821025
14.O	-1.017154	3.182128	-1.471850
15.O	-2.137126	1.567325	0.479604
16.H	-2.987139	-2.997633	-4.220853
17.H	-5.444095	-3.375935	-4.318413
18.H	-5.620444	-3.378091	0.009280
19.H	-3.146078	-3.002684	0.106547
20.H	-7.365058	-3.717336	-3.014944
21.H	-0.830400	3.484150	-0.563951
22.H	-0.715166	3.885694	-2.073219
23.H	0.537382	0.452473	-1.534243
24.H	-0.535653	-0.731966	-1.638709
25.H	-4.050880	3.434136	-1.823052
26.H	-4.757414	2.029960	-1.808921
27.H	-2.996034	1.744665	0.907763
28.H	-1.721291	0.849463	0.992866
29.H	-1.219101	1.976605	-4.341119
30.H	-2.434588	0.992913	-4.340340

I2gp

1.C	0.788506	0.159365	1.060576
2.C	1.503314	0.188064	-0.101603
3.C	1.659527	1.425016	-0.794005
4.C	1.062528	2.635109	-0.309301
5.C	0.357001	2.616656	0.852617
6.C	0.226613	1.385138	1.617514
7.O	2.345640	1.542317	-1.910954
8.Cl	-2.125668	0.569899	0.428463
9.O	-0.215607	1.407052	2.818798
10.Fe	-1.765282	1.554431	3.933844
11.O	-2.739806	2.604644	2.427542
12.O	-0.765318	0.705570	5.615457
13.O	-2.638026	-0.219308	3.222026
14.O	-3.540838	1.538874	5.195291

15.O	-1.392225	3.491075	4.831684
16.H	0.666214	-0.762291	1.627505
17.H	1.947843	-0.721978	-0.509061
18.H	1.201341	3.545381	-0.892815
19.H	-0.087990	3.523969	1.258862
20.H	2.734769	0.695914	-2.215841
21.H	-3.874627	2.249922	5.772269
22.H	-4.295442	0.960952	4.977354
23.H	-3.677901	2.866820	2.481086
24.H	-2.635749	2.034145	1.573945
25.H	-1.196482	0.459601	6.454612
26.H	0.131120	0.323120	5.621228
27.H	-0.705741	3.643602	5.507104
28.H	-1.456048	4.310583	4.307795
29.H	-2.531418	-0.190402	2.204273
30.H	-2.457148	-1.129236	3.519318

I3gp			
1.fe	-0.002800	0.002287	-0.002944
2.o	2.169539	-0.004761	-0.016089
3.o	0.294967	2.223834	0.010543
4.o	0.211113	0.451206	2.111634
5.o	-2.028960	0.640044	0.050026
6.o	-0.014737	-0.128334	-1.876218
7.cl	-2.779901	-0.235099	-2.726642
8.o	-0.258991	-1.832408	0.463891
9.c	-0.741644	-2.994065	0.183597
10.c	-0.200312	-4.157948	0.852695
11.c	-0.715994	-5.397275	0.604609
12.c	-1.799239	-5.530863	-0.321917
13.c	-2.341341	-4.393780	-1.000609
14.c	-1.821816	-3.156814	-0.760865
15.o	-2.361366	-6.686962	-0.607059
16.h	2.732311	-0.120640	0.771210
17.h	2.620350	-0.449841	-0.757385
18.h	0.243879	1.368037	2.441001
19.h	0.060063	-0.136099	2.873221
20.h	1.097482	2.686822	-0.292771
21.h	-0.464757	2.783459	-0.237140
22.h	-2.655545	0.506133	0.784109
23.h	-2.517777	0.445348	-0.808602
24.h	-1.429289	-0.283318	-2.505527
25.h	0.375963	0.560051	-2.446491
26.h	0.623340	-4.015113	1.551870
27.h	-0.316175	-6.282534	1.103277
28.h	-1.961044	-7.441056	-0.124855
29.h	-3.163806	-4.552862	-1.698561
30.h	-2.220536	-2.278853	-1.271821

I3PRIMgp			
1.C	1.835317	-0.394378	0.356315
2.C	2.379604	-0.085206	-0.846851
3.C	2.546384	1.295877	-1.208420
4.C	2.093854	2.362130	-0.369991
5.C	1.526071	2.067571	0.828230
6.C	1.490900	0.672654	1.326575
7.O	3.098753	1.661225	-2.339446
8.Cl	-0.973894	0.736433	0.394206

9.O	1.395609	0.392190	2.538760
10.Fe	-1.844081	1.738548	4.101573
11.O	-2.196560	2.680444	2.297349
12.O	0.161546	1.803373	4.267171
13.O	-1.826681	-0.118260	3.123443
14.O	-3.629883	1.036863	4.914051
15.O	-2.078587	3.578837	5.182505
16.H	1.716650	-1.424483	0.692142
17.H	2.695243	-0.864324	-1.544826
18.H	2.207324	3.383612	-0.732889
19.H	1.191229	2.853335	1.504960
20.H	3.391361	0.903207	-2.889220
21.H	-4.284917	1.491059	5.474604
22.H	-4.061763	0.248511	4.534946
23.H	-2.959386	3.214632	2.012807
24.H	-1.866323	2.151383	1.497920
25.H	0.693067	2.057903	5.041288
26.H	0.747700	1.265483	3.604897
27.H	-2.170565	3.738788	6.139648
28.H	-1.921462	4.450279	4.774033
29.H	-1.541811	-0.052111	2.155331
30.H	-1.492065	-0.962572	3.475200

I4gp

1.C	3.131695	0.906357	0.849263
2.C	3.905484	0.790344	-0.266771
3.C	3.311823	0.330030	-1.487898
4.C	1.923586	-0.017762	-1.558300
5.C	1.150194	0.090186	-0.444186
6.C	1.715108	0.561528	0.812792
7.O	3.991546	0.193127	-2.607722
8.Cl	-2.915972	2.956255	0.796216
9.O	0.994799	0.658070	1.854796
10.Fe	-1.617287	1.869429	4.287262
11.O	-2.421257	3.433152	3.843611
12.O	0.445054	1.865428	4.142966
13.O	-1.592234	0.852051	2.479156
14.O	-2.705590	0.212825	4.950704
15.O	-1.379430	2.270916	6.408154
16.H	3.552459	1.245873	1.795132
17.H	4.968494	1.039720	-0.245305
18.H	1.530509	-0.364832	-2.514955
19.H	0.093539	-0.175346	-0.466311
20.H	4.937385	0.434587	-2.517520
21.H	-3.286260	0.163165	5.732216
22.H	-3.019732	-0.443302	4.300366
23.H	-3.204927	3.875108	4.217248
24.H	-2.748419	3.515178	1.980001
25.H	1.013524	2.546913	4.541645
26.H	0.888221	1.503616	3.318530
27.H	-0.924916	1.746129	7.092871
28.H	-1.594178	3.134945	6.804550
29.H	-2.089403	1.395586	1.793678
30.H	-0.687416	0.667542	2.086682

I5gp

1.C	2.783119	0.784176	1.029620
2.C	3.839225	0.575543	0.180459

3.C	3.589839	0.120503	-1.149367
4.C	2.257878	-0.124457	-1.603776
5.C	1.206334	0.091564	-0.755981
6.C	1.447395	0.555473	0.572489
7.O	4.552855	-0.098674	-2.031101
8.Cl	-3.763061	4.086683	1.540162
9.O	0.394079	0.762532	1.349235
10.Fe	-1.351247	1.864440	4.331967
11.O	-1.883338	3.541363	4.619937
12.O	0.423379	1.732872	3.687109
13.O	-2.227350	1.533893	2.407193
14.O	-2.362015	0.070031	4.667245
15.O	-0.903517	1.517065	6.442233
16.H	2.952128	1.123037	2.052221
17.H	4.864506	0.752540	0.511558
18.H	2.115955	-0.477071	-2.625117
19.H	0.178820	-0.078966	-1.074736
20.H	5.444264	0.091518	-1.672452
21.H	-2.527549	-0.289928	5.558595
22.H	-3.040319	-0.274821	4.056941
23.H	-2.703710	4.046351	4.768766
24.H	-2.907619	4.825799	0.900043
25.H	0.955884	2.540848	3.807450
26.H	0.595443	1.148406	2.298716
27.H	-0.045150	1.153855	6.730883
28.H	-1.087834	2.282709	7.019669
29.H	-2.686224	2.341589	2.040869
30.H	-1.602507	1.229209	1.716212

I5gp+H2O

1.C	2.750921	0.659435	1.054182
2.C	3.670940	0.158255	0.169178
3.C	3.239037	-0.298371	-1.111541
4.C	1.863826	-0.237397	-1.485080
5.C	0.950092	0.271502	-0.604503
6.C	1.371402	0.728223	0.682994
7.O	4.066541	-0.797460	-2.018800
8.Cl	-4.459579	1.004855	1.752691
9.O	0.447729	1.206172	1.491159
10.Fe	-1.215299	2.434262	4.406991
11.O	-1.841139	4.056398	4.840563
12.O	0.519011	1.868755	3.848381
13.O	-1.744168	2.636895	2.316488
14.O	-2.669128	0.964891	4.332952
15.O	-0.895579	1.774508	6.393627
16.H	3.062555	1.024157	2.033084
17.H	4.729223	0.110868	0.432501
18.H	1.576813	-0.603932	-2.470253
19.H	-0.108474	0.326172	-0.855958
20.H	4.996264	-0.813017	-1.712993
21.H	-3.074950	0.583196	5.131744
22.H	-3.322982	0.913921	3.583862
23.H	-1.482472	4.950068	4.984622
24.H	-5.451788	0.178985	1.907952
25.H	1.160667	1.587711	4.530843
26.H	0.695856	1.446116	2.519627
27.H	0.041595	1.488611	6.613306
28.H	-1.196098	2.381835	7.095039

29.H	-1.989462	3.532673	2.020895
30.H	-1.115935	2.253417	1.663611
31.O	1.675603	1.072163	6.544343
32.H	1.884379	0.164615	6.833445
33.H	2.291308	1.642326	7.041211

I5PRIMgp+H2O			
1.Fe	-4.561041	-0.836318	-1.629590
2.O	-5.065300	-0.405887	-3.206255
3.O	-4.205823	-1.372901	0.031441
4.O	-2.614897	-0.736484	-2.046777
5.O	-5.384262	-2.656943	-1.792269
6.O	-5.275769	0.883497	-0.915858
7.H	-6.151581	-2.866572	-2.362073
8.H	-5.456030	-3.159646	-0.951908
9.H	-4.855992	-0.420930	-4.349924
10.H	-3.672945	-0.852072	0.669516
11.H	-5.628065	0.960042	-0.004851
12.H	-5.803914	1.455029	-1.511534
13.H	-2.259023	-0.570261	-2.942565
14.H	-1.958051	-1.250239	-1.533285
15.O	-4.603185	-0.372386	-5.589521
16.H	-4.860856	0.463985	-6.028550
17.H	-4.958665	-1.106273	-6.130399

I6gp+H2O			
1.fe	0.143044	-0.115837	-0.006427
2.o	1.977022	-0.266992	-0.220174
3.o	0.200723	2.064044	0.233388
4.o	-2.046398	0.420667	-0.347724
5.o	-0.038780	0.570246	-2.127972
6.o	-0.325937	-1.992393	-0.922533
7.o	-0.245955	-0.595536	1.783914
8.o	1.288850	-0.077900	3.835041
9.c	1.132972	-0.631629	5.023169
10.c	1.926004	-0.103453	6.088220
11.c	1.811741	-0.622574	7.348108
12.c	0.901077	-1.693894	7.586875
13.c	0.110031	-2.232914	6.528431
14.c	0.225014	-1.709578	5.266017
15.o	0.842965	-2.142901	8.832515
16.cl	2.027299	-1.653779	-2.936312
17.h	-0.561604	2.543009	0.608074
18.h	1.006549	2.493552	0.574844
19.h	2.624621	-0.496042	0.471226
20.h	0.292606	1.478056	-2.266450
21.h	0.481336	-0.001253	-2.746370
22.h	2.336093	-1.052217	-1.780196
23.h	-2.126725	0.532686	-1.315767
24.h	-2.833891	-0.086937	-0.079650
25.h	-0.408214	-2.783776	-0.359219
26.h	0.331261	-2.217615	-1.633323
27.h	-1.172363	-0.503256	2.070257
28.h	0.657431	-0.412531	3.104259
29.h	2.607656	0.717145	5.867973
30.h	2.394671	-0.241273	8.186018
31.h	0.203031	-2.875799	8.940236
32.h	-0.575269	-3.058197	6.730334

33.h	-0.361219	-2.116755	4.441564

I6PRIMgp+H2O			
1.Fe	0.072500	-0.064020	-0.059778
2.O	1.798748	-0.263685	-0.045508
3.O	0.263491	2.115540	0.179360
4.O	-1.937817	0.253591	-0.203019
5.O	0.061319	0.515966	-2.018537
6.O	-0.231075	-2.007864	-1.045093
7.O	-0.253184	-0.514818	1.582440
8.H	-0.440206	2.641765	0.609321
9.H	1.110479	2.483366	0.502669
10.H	2.329786	-0.590978	0.714717
11.H	0.466603	1.374940	-2.260188
12.H	0.283821	-0.138983	-2.712548
13.H	-2.439981	0.487165	-1.008867
14.H	-2.557389	0.071819	0.532552
15.H	-1.040932	-2.536905	-0.899200
16.H	0.508472	-2.648538	-1.050518
17.H	0.402328	-0.741727	2.279298

I7gp+2H2O			
1.Fe	-4.449311	-0.760069	-1.631085
2.O	-4.861575	0.827297	-2.309325
3.O	-3.303402	-0.105201	-0.598337
4.O	-3.171389	-1.300178	-3.382607
5.O	-5.798248	-1.784630	-2.816208
6.O	-6.238671	-0.818228	-0.308453
7.H	-6.749210	-1.877991	-2.613751
8.H	-5.628674	-2.057114	-3.738621
9.H	-5.562304	0.760361	-2.995580
10.H	-2.881421	0.994788	-0.637586
11.H	-6.215632	-1.337307	0.519206
12.H	-6.638097	0.040784	-0.068785
13.H	-2.843165	-0.551912	-3.918914
14.H	-2.411345	-1.906626	-3.287384
15.O	-4.013565	-2.623481	-0.861709
16.H	-4.343746	-3.491158	-1.163372
17.H	-3.303085	-2.759806	-0.205804
18.O	-2.345490	2.122099	-0.716291
19.H	-1.666873	2.294917	-0.032692
20.H	-2.963925	2.879200	-0.727273

I8gp+2H2O			
1.Fe	-4.246786	-0.948956	-1.190222
2.O	-3.689472	1.015530	-1.634656
3.O	-2.916691	-1.147299	-0.301571
4.O	-3.436965	-1.334369	-3.121949
5.O	-6.004463	-0.680418	-2.242565
6.O	-5.413871	-0.527255	0.401891
7.H	-6.880939	-0.465570	-1.817076
8.H	-6.105746	-0.777831	-3.206869
9.H	-4.291948	1.727119	-1.926829
10.H	-8.661974	-0.746322	-0.253562
11.H	-5.097737	-0.496830	1.324134
12.H	-6.394220	-0.339490	0.344290
13.H	-2.760921	-0.708583	-3.451610
14.H	-3.079128	-2.230674	-3.282224

15.O	-4.556094	-3.016683	-1.207373
16.H	-5.413586	-3.461466	-1.350807
17.H	-4.034329	-3.563433	-0.586771
18.O	-7.940798	-0.118613	-0.460285
19.H	-8.357048	0.764619	-0.404232
20.H	-2.972651	1.424568	-1.109930

TS1gp

1.C	0.264163	-0.040729	0.336573
2.C	1.587145	0.240696	0.113719
3.C	2.007409	1.592729	-0.006698
4.C	1.070629	2.658510	0.083066
5.C	-0.251365	2.381646	0.303204
6.C	-0.676352	1.028260	0.521140
7.O	3.269516	1.942559	-0.229498
8.Cl	-2.355389	0.652758	0.151672
9.O	-0.721254	1.014390	2.463803
10.Fe	-1.714778	1.485859	3.798626
11.O	-3.330498	2.296686	2.668752
12.O	-0.076954	1.117073	5.123109
13.O	-2.576277	-0.463709	4.086932
14.O	-2.909560	1.971139	5.666220
15.O	-1.210411	3.594283	4.160709
16.H	-0.088869	-1.069631	0.389383
17.H	2.311811	-0.567487	-0.001573
18.H	1.426162	3.676980	-0.070777
19.H	-0.994526	3.178261	0.312000
20.H	3.858184	1.167615	-0.322736
21.H	-2.846119	2.883230	6.003686
22.H	-3.319410	1.446421	6.377056
23.H	-4.245315	2.470243	2.958532
24.H	-3.360107	1.903122	1.765903
25.H	-0.141996	0.845081	6.057145
26.H	0.671191	0.632467	4.728125
27.H	-0.289827	3.801776	4.407785
28.H	-1.480736	4.269838	3.512023
29.H	-3.492547	-0.689063	4.331900
30.H	-2.282085	-1.145450	3.455616

TS2gp

1.C	0.032848	0.028373	0.256862
2.C	1.476066	0.010761	0.393804
3.C	2.195483	1.159352	0.245189
4.C	1.510407	2.381782	-0.049215
5.C	0.088088	2.421396	-0.204298
6.C	-0.632144	1.273962	-0.066458
7.O	2.132132	3.531344	-0.195780
8.O	-0.634660	-1.047555	0.473643
9.Fe	-1.998154	-2.202693	-0.196579
10.O	-3.709246	-1.614554	1.016440
11.O	-2.512645	-0.959690	-1.605636
12.O	-1.639132	-3.613012	1.400839
13.O	-0.696621	-3.214303	-1.531415
14.O	-3.327635	-3.798108	-0.885031
15.Cl	-0.089606	-0.672022	-2.910842
16.H	1.961649	-0.936421	0.625971
17.H	3.282621	1.160164	0.347820
18.H	-0.378240	3.379461	-0.433757

19.H	-1.714530	1.268572	-0.181472
20.H	3.104116	3.462845	-0.084227
21.H	-4.294431	-3.856832	-0.775293
22.H	-3.094273	-4.283641	-1.698562
23.H	-3.226672	-1.160059	-2.240153
24.H	-1.494069	-0.717097	-2.269684
25.H	-1.994444	-4.520938	1.409178
26.H	-0.948184	-3.560901	2.085925
27.H	-3.779157	-1.802941	1.970419
28.H	-4.214013	-0.797108	0.853470
29.H	-0.297536	-2.493322	-2.132066
30.H	0.035691	-3.797392	-1.259795

TS2PRIMgp

1.C	1.076554	0.107360	1.030693
2.C	1.747706	0.166758	-0.146438
3.C	1.705836	1.375801	-0.926444
4.C	0.934397	2.505032	-0.524511
5.C	0.238132	2.449484	0.642933
6.C	0.354669	1.287914	1.549351
7.O	2.354437	1.497215	-2.060775
8.Cl	-1.880052	0.629716	0.468218
9.O	0.073593	1.391542	2.771106
10.Fe	-2.070541	1.604910	4.127726
11.O	-2.694244	2.672648	2.466862
12.O	-0.489177	0.734945	5.177703
13.O	-2.798446	-0.128837	3.202586
14.O	-3.783282	1.603130	5.323046
15.O	-1.459735	3.412955	5.163085
16.H	1.103856	-0.784475	1.656277
17.H	2.321362	-0.686305	-0.515939
18.H	0.918364	3.380385	-1.173544
19.H	-0.336403	3.301819	1.002638
20.H	2.867945	0.697036	-2.301006
21.H	-3.960579	2.241226	6.038997
22.H	-4.563645	1.024147	5.242781
23.H	-3.591551	3.047578	2.387200
24.H	-2.538065	2.090465	1.643935
25.H	-0.483683	-0.092112	5.693419
26.H	0.155495	0.647539	4.430551
27.H	-0.747600	3.347218	5.826499
28.H	-1.324024	4.262255	4.703901
29.H	-2.556211	-0.142556	2.223515
30.H	-2.927418	-1.044681	3.505331

TS3gp

1.C	0.138277	0.048672	-0.092510
2.C	1.481234	-0.021910	-0.668844
3.C	2.242917	1.098994	-0.797151
4.C	1.713736	2.359508	-0.362295
5.C	0.404662	2.464638	0.213009
6.C	-0.356602	1.346277	0.352992
7.O	2.384281	3.485501	-0.466774
8.O	-0.577487	-0.990749	0.007357
9.Fe	-2.751323	-2.402885	0.548011
10.O	-2.005623	-3.851814	2.028259
11.O	-3.300259	-1.204315	1.814715
12.O	-1.247108	-3.330162	-0.594669

13.O	-3.741151	-1.361683	-1.019771
14.O	-4.246464	-3.839392	0.196194
15.Cl	-4.181081	1.313085	0.374511
16.H	1.855372	-0.996614	-0.982610
17.H	3.247767	1.055998	-1.223704
18.H	0.056115	3.452521	0.515489
19.H	-1.362798	1.391669	0.769069
20.H	3.271992	3.371258	-0.867974
21.H	-4.409537	-4.617532	0.760732
22.H	-5.084001	-3.608094	-0.246878
23.H	-3.700924	-1.359272	2.688049
24.H	-3.824554	0.362723	1.241119
25.H	-1.328590	-3.689789	-1.496595
26.H	-0.605311	-2.560520	-0.601293
27.H	-1.276800	-4.443780	1.763658
28.H	-1.885243	-3.669502	2.978045
29.H	-3.964426	-0.417050	-0.768719
30.H	-3.522404	-1.357356	-1.969026

TS3PRIMgp

1.C	2.522915	-0.500176	0.375205
2.C	2.962060	-0.270435	-0.888038
3.C	2.762276	1.029245	-1.473388
4.C	2.111724	2.091710	-0.763214
5.C	1.657398	1.870063	0.497089
6.C	1.843134	0.559715	1.137505
7.O	3.166487	1.322525	-2.686258
8.Cl	-1.641145	1.428750	0.610691
9.O	1.448935	0.316239	2.300071
10.Fe	-1.741726	1.812055	4.262070
11.O	-2.428135	2.864282	2.839656
12.O	0.271349	1.716892	4.122024
13.O	-1.903849	-0.020924	3.186874
14.O	-3.148941	0.838797	5.454914
15.O	-1.483096	3.332037	5.771245
16.H	2.655154	-1.462382	0.869879
17.H	3.467497	-1.047259	-1.466639
18.H	1.998953	3.050420	-1.269730
19.H	1.163466	2.653099	1.068931
20.H	3.609941	0.572951	-3.138510
21.H	-3.729654	1.157233	6.170143
22.H	-3.559907	0.038221	5.075523
23.H	-3.298371	3.300351	2.779458
24.H	-2.125618	2.334789	1.742147
25.H	0.901858	2.035515	4.791187
26.H	0.777314	1.209065	3.388347
27.H	-1.574906	3.295825	6.741043
28.H	-1.337512	4.268157	5.539683
29.H	-1.838097	0.228568	2.202683
30.H	-1.304962	-0.778734	3.320573

TS4gp

1.C	2.770203	1.146330	0.876330
2.C	3.797299	0.977366	-0.009596
3.C	3.587873	0.192760	-1.186912
4.C	2.318845	-0.407330	-1.457187
5.C	1.290191	-0.226505	-0.579015
6.C	1.483534	0.546843	0.620946

7.O	4.533315	-0.023957	-2.082794
8.Cl	-3.559262	3.690515	1.342502
9.O	0.490344	0.669210	1.447071
10.Fe	-1.513622	1.877961	4.223265
11.O	-2.346544	3.480982	4.310918
12.O	0.300208	1.908762	3.499623
13.O	-2.201977	1.151481	2.360575
14.O	-2.509693	0.158255	4.858137
15.O	-0.864347	1.893121	6.302600
16.H	2.914442	1.733810	1.782948
17.H	4.774079	1.430188	0.171350
18.H	2.210787	-0.998231	-2.366665
19.H	0.311864	-0.672161	-0.754482
20.H	5.382865	0.407482	-1.854635
21.H	-2.750718	-0.089492	5.770647
22.H	-3.085664	-0.330153	4.239937
23.H	-3.139712	3.722359	4.826188
24.H	-3.014192	4.095859	2.463280
25.H	0.825013	2.717807	3.631668
26.H	0.551653	1.339913	2.449127
27.H	-0.075762	1.438043	6.653804
28.H	-0.954066	2.723389	6.807035
29.H	-2.708262	1.873108	1.874114
30.H	-1.499165	0.836338	1.747543

TS5gp+H2O

1.C	0.301473	1.329626	-0.179673
2.C	1.413362	1.893820	0.393356
3.C	2.448087	1.053342	0.902665
4.C	2.343282	-0.366589	0.821291
5.C	1.235919	-0.926276	0.247819
6.C	0.190938	-0.094326	-0.263331
7.O	3.549157	1.523629	1.471357
8.Cl	-5.124266	3.090476	-2.243755
9.O	-0.842172	-0.713499	-0.800818
10.Fe	-4.497583	-0.586542	-2.452823
11.O	-5.994140	0.201213	-1.747305
12.O	-3.052155	0.301581	-1.622116
13.O	-4.590092	0.677043	-4.187265
14.O	-5.351937	-2.134626	-3.672043
15.O	-4.283511	-2.300305	-1.122161
16.H	-0.494004	1.960362	-0.577371
17.H	1.515729	2.978568	0.461732
18.H	3.154967	-0.971552	1.224324
19.H	1.118671	-2.006443	0.171515
20.H	3.570695	2.501810	1.503848
21.H	-6.031675	-1.946240	-4.345931
22.H	-4.600055	-2.579149	-4.120634
23.H	-6.925863	-0.086548	-1.727414
24.H	-5.775392	2.022303	-1.803699
25.H	-3.320250	1.204954	-1.355104
26.H	-1.634889	-0.135081	-1.115207
27.H	-5.002561	-2.961390	-1.126674
28.H	-4.126055	-2.075220	-0.185574
29.H	-4.810890	1.589210	-3.854799
30.H	-3.840517	0.794036	-4.799570
31.O	-2.698079	-2.092923	-3.600822
32.H	-2.012346	-1.890282	-4.262839

33.H	-2.269611	-2.701408	-2.971194

TS5PRIMgp+H2O			
1.Fe	-4.637838	-0.590166	-2.424019
2.O	-6.215279	0.024238	-2.038152
3.O	-3.614782	0.397491	-1.452497
4.O	-4.045648	0.486859	-4.160046
5.O	-5.326875	-1.998438	-3.622174
6.O	-4.233598	-2.231849	-1.157385
7.H	-6.142672	-2.017977	-4.162594
8.H	-4.513451	-2.366572	-4.088341
9.H	-6.541281	0.480869	-1.228883
10.H	-3.896410	1.135622	-0.863580
11.H	-4.893348	-2.943358	-1.026234
12.H	-3.765267	-2.103541	-0.307457
13.H	-4.695508	0.727069	-4.852563
14.H	-3.493034	1.282905	-4.013440
15.O	-2.827574	-2.166148	-3.820671
16.H	-2.250674	-1.814021	-4.526928
17.H	-2.314082	-2.889578	-3.409304

TS7gp+2H2O			
1.Fe	-4.366374	-0.749739	-1.568137
2.O	-4.488682	1.047716	-1.887917
3.O	-3.221855	-0.498708	-0.408276
4.O	-3.041078	-1.123738	-3.316305
5.O	-5.772809	-1.204502	-3.009132
6.O	-6.195975	-0.812219	-0.316324
7.H	-6.735849	-1.259225	-2.860355
8.H	-5.574071	-1.380920	-3.948264
9.H	-5.128905	1.274102	-2.593662
10.H	-2.675967	0.871246	-0.223150
11.H	-6.268515	-1.481515	0.391986
12.H	-6.504961	0.024413	0.082466
13.H	-2.553975	-0.364587	-3.692174
14.H	-2.390901	-1.851913	-3.271660
15.O	-4.230947	-2.776505	-1.209953
16.H	-4.698317	-3.517271	-1.640829
17.H	-3.615633	-3.130924	-0.539295
18.O	-2.542365	1.897084	-0.449618
19.H	-2.519077	2.484215	0.336388
20.H	-3.345881	2.061689	-1.038348

Mirco Solvated			

I1ms			
1.C	-3.582847	-2.949899	-3.540644
2.C	-4.928692	-3.249032	-3.447858
3.C	-5.479945	-3.616994	-2.198644
4.C	-4.667801	-3.681872	-1.042768
5.C	-3.323211	-3.391232	-1.135560
6.C	-2.784783	-3.019593	-2.383244
7.O	-6.774021	-3.922774	-2.032807
8.Cl	-1.058866	-2.833030	-2.542061
9.O	-3.154935	-0.384379	-1.739156

10.Fe	-2.404070	1.059781	-1.392831
11.O	-0.527244	0.126200	-1.569488
12.O	-4.098854	2.312614	-1.532020
13.O	-2.008618	1.873813	-3.421001
14.O	-1.301597	2.962493	-0.968603
15.O	-2.509701	1.147353	0.732240
16.H	-3.133551	-2.693436	-4.498574
17.H	-5.560084	-3.215703	-4.337378
18.H	-5.120250	-3.989384	-0.100814
19.H	-2.673004	-3.477411	-0.266501
20.H	-7.256030	-3.915919	-2.881785
21.H	-0.637234	3.104794	-0.270662
22.H	-0.980503	3.435129	-1.759188
23.H	0.332246	0.302636	-1.145030
24.H	-0.599974	-0.843866	-1.760105
25.H	-4.245755	2.871571	-0.722127
26.H	-4.932507	1.839972	-1.712335
27.H	-3.037743	1.919571	1.063764
28.H	-2.820149	0.355331	1.207662
29.H	-1.485150	1.321613	-4.031791
30.H	-2.762562	2.213590	-3.937918
31.O	-4.063193	3.452610	0.971026
32.H	-3.630774	4.320457	1.080071
33.H	-4.862878	3.500007	1.528437

I2ms			
1.C	0.859712	0.167574	0.912533
2.C	1.513772	0.226089	-0.284407
3.C	1.577718	1.466479	-0.982303
4.C	0.952773	2.648279	-0.467951
5.C	0.307117	2.600487	0.728277
6.C	0.273827	1.367197	1.498903
7.O	2.198828	1.610510	-2.136190
8.Cl	-2.111692	0.463774	0.431464
9.O	-0.101387	1.365915	2.722548
10.Fe	-1.601320	1.515734	3.919154
11.O	-2.587322	2.577546	2.410264
12.O	-0.574165	0.621087	5.549446
13.O	-2.477268	-0.253757	3.243855
14.O	-3.431533	1.624870	5.099157
15.O	-1.179525	3.373338	4.904943
16.H	0.804732	-0.757163	1.484741
17.H	1.977898	-0.663342	-0.714738
18.H	1.018776	3.562017	-1.058411
19.H	-0.162306	3.486073	1.153944
20.H	2.613015	0.780401	-2.451854
21.H	-3.718083	2.338930	5.694409
22.H	-4.181340	1.013031	4.989029
23.H	-3.507162	2.881287	2.518534
24.H	-2.559839	1.979966	1.576591
25.H	-0.273311	1.201744	6.295721
26.H	0.117298	-0.050249	5.413936
27.H	-0.671653	3.371583	5.757468
28.H	-0.999798	4.212045	4.446065
29.H	-2.416608	-0.266993	2.222490
30.H	-2.466359	-1.164151	3.587012
31.O	0.098466	2.704451	7.231954
32.H	1.039208	2.915956	7.382085

33.H	-0.328959	2.826985	8.100872

I3ms			
1.C	0.994313	0.265568	0.469547
2.C	1.207316	0.266154	-0.882097
3.C	1.312206	1.509189	-1.555046
4.C	1.183784	2.775649	-0.867006
5.C	1.022093	2.795446	0.473692
6.C	1.051630	1.535073	1.250329
7.O	1.515230	1.613147	-2.848775
8.Cl	-1.599047	0.715129	0.861915
9.O	1.256569	1.554861	2.470426
10.Fe	-2.482274	1.600333	4.556415
11.O	-3.452498	2.089642	2.766951
12.O	-1.012612	1.445711	6.076429
13.O	-1.722753	-0.080253	3.736694
14.O	-4.160156	1.029871	5.667262
15.O	-2.121810	3.651699	4.691218
16.H	0.957989	-0.663980	1.034812
17.H	1.262457	-0.667322	-1.445729
18.H	1.242927	3.682785	-1.469675
19.H	0.969012	3.726553	1.036854
20.H	1.597938	0.743033	-3.293830
21.H	-5.015142	0.756028	5.287301
22.H	-4.128813	0.650635	6.564539
23.H	-4.390227	2.140692	2.509030
24.H	-2.933334	1.748949	1.969209
25.H	-1.013862	1.462758	7.049000
26.H	-0.181992	0.981654	5.764718
27.H	-1.525994	4.094809	5.320957
28.H	-2.530646	4.328034	4.121915
29.H	-1.668464	-0.022143	2.726697
30.H	-0.819747	-0.334927	4.063438
31.O	0.804781	0.061126	4.698187
32.H	1.180788	0.544526	3.914885
33.H	1.495604	-0.533441	5.039220

I3PRIMms			
1.C	1.772950	-0.514419	0.212463
2.C	2.324400	-0.155097	-0.973647
3.C	2.588762	1.234170	-1.238689
4.C	2.227415	2.261178	-0.317837
5.C	1.652104	1.917148	0.865753
6.C	1.521270	0.497059	1.261673
7.O	3.156215	1.640196	-2.352191
8.Cl	-1.004520	0.989057	0.365215
9.O	1.389262	0.138811	2.449349
10.Fe	-1.707443	1.672318	4.140391
11.O	-2.011707	2.817890	2.469461
12.O	0.287610	1.558004	4.302015
13.O	-1.878044	-0.046806	2.989437
14.O	-3.310320	0.909942	5.230515
15.O	-1.701437	3.216656	5.633630
16.H	1.584513	-1.556345	0.471422
17.H	2.576582	-0.901258	-1.730980
18.H	2.410183	3.296682	-0.604771
19.H	1.383119	2.670776	1.604883
20.H	3.382779	0.903727	-2.958632

21.H	-3.647016	1.254586	6.077706
22.H	-3.934081	0.235521	4.904393
23.H	-2.612079	3.557387	2.273712
24.H	-1.757556	2.354711	1.600935
25.H	0.826643	2.080339	4.939388
26.H	0.851814	1.043304	3.621147
27.H	-0.818960	3.375307	6.063928
28.H	-2.158188	4.075464	5.594021
29.H	-1.627987	0.111347	2.015739
30.H	-1.493721	-0.903957	3.249154
31.O	0.930770	3.265374	6.414780
32.H	1.192935	2.874338	7.269550
33.H	1.456997	4.083776	6.344088

I4ms

1.C	0.862286	0.546002	0.597607
2.C	1.213161	0.139973	-0.667554
3.C	1.363516	1.113447	-1.677507
4.C	1.161409	2.527713	-1.425708
5.C	0.879916	2.956011	-0.176192
6.C	0.808665	1.996594	0.940505
7.O	1.699348	0.828434	-2.918443
8.Cl	-1.719119	0.735041	0.762794
9.O	0.799751	2.403578	2.112356
10.Fe	-2.021715	1.433575	4.708469
11.O	-2.436076	2.587965	3.005329
12.O	-1.589862	0.289950	6.532837
13.O	-2.116120	-0.271892	3.520637
14.O	-4.138336	1.118743	5.145049
15.O	-2.210946	3.204006	5.957823
16.H	0.842843	-0.155035	1.428873
17.H	1.353691	-0.916897	-0.901090
18.H	1.270631	3.208134	-2.271068
19.H	0.762361	4.011894	0.065413
20.H	1.828215	-0.131997	-3.065687
21.H	-4.708957	0.588112	4.559377
22.H	-4.720773	1.750867	5.603704
23.H	-3.235287	3.121978	2.851588
24.H	-2.230812	2.111109	2.136505
25.H	-2.275505	-0.076551	7.119874
26.H	-0.808844	-0.284264	6.629693
27.H	-2.108233	3.220580	6.926583
28.H	-2.049643	4.113770	5.647642
29.H	-1.996621	-0.140632	2.522955
30.H	-2.227503	-1.218373	3.712163
31.O	0.036218	1.644675	4.494040
32.H	0.394588	1.860524	3.572263
33.H	0.597241	2.119339	5.132064

I4ms+H2O

1.C	0.827910	0.306513	1.250235
2.C	0.993289	-0.193333	2.512790
3.C	2.303956	-0.485223	2.968009
4.C	3.470943	-0.292785	2.138459
5.C	3.334176	0.250056	0.907989
6.C	2.007139	0.672210	0.420570
7.O	2.560561	-0.949665	4.173737
8.Cl	0.701077	-1.815795	-0.488978

9.O	1.909632	1.384051	-0.588726
10.Fe	0.018739	-1.602631	-4.452865
11.O	1.592121	-2.277022	-3.263792
12.O	-1.610204	-0.965476	-5.867668
13.O	-1.177864	-1.622777	-2.755143
14.O	-0.806005	-3.570986	-4.803817
15.O	1.147647	-1.853112	-6.285063
16.H	-0.150567	0.606076	0.880353
17.H	0.137184	-0.383540	3.163302
18.H	4.438087	-0.573247	2.556944
19.H	4.188599	0.456789	0.264577
20.H	1.750345	-1.064234	4.713296
21.H	-1.232764	-4.051759	-4.071257
22.H	-0.527639	-4.231418	-5.463041
23.H	2.092033	-3.105476	-3.363807
24.H	1.450771	-2.137038	-2.261886
25.H	-2.410858	-1.470142	-6.096305
26.H	-1.840317	-0.022760	-5.948993
27.H	0.777456	-1.579770	-7.144184
28.H	2.100270	-2.003582	-6.419541
29.H	-0.675439	-1.627601	-1.866143
30.H	-2.011716	-1.138573	-2.626580
31.O	0.446960	0.390054	-4.382066
32.H	0.248932	0.984382	-3.533675
33.H	1.261007	0.729529	-4.792285
34.O	-0.092817	1.747016	-2.327510
35.H	-0.275331	2.693620	-2.458710
36.H	0.612412	1.686955	-1.620638

I4PRIMms

1.C	3.158343	1.073149	0.690612
2.C	3.921900	0.847283	-0.416925
3.C	3.348888	0.167581	-1.539156
4.C	1.986732	-0.274150	-1.524779
5.C	1.218540	-0.041984	-0.425082
6.C	1.768498	0.635938	0.741114
7.O	4.025411	-0.095326	-2.641225
8.Cl	-3.311802	3.215288	1.276953
9.O	1.060047	0.828734	1.777881
10.Fe	-1.610474	1.743639	4.306371
11.O	-2.511380	3.325607	4.167982
12.O	0.440327	1.703369	4.267832
13.O	-1.513020	1.102837	2.354085
14.O	-2.941680	0.135448	4.482556
15.O	-1.448519	1.639320	6.422827
16.H	3.564226	1.590185	1.559523
17.H	4.962075	1.177716	-0.463248
18.H	1.607342	-0.792610	-2.405698
19.H	0.181704	-0.375325	-0.383435
20.H	4.951155	0.224757	-2.605688
21.H	-3.478387	-0.121563	5.253438
22.H	-3.333317	-0.271369	3.687707
23.H	-2.236291	4.214857	4.455338
24.H	-3.143757	3.480567	2.573378
25.H	1.000190	1.653155	5.080492
26.H	0.940096	1.430329	3.454132
27.H	-0.536817	1.674640	6.817954
28.H	-2.032959	2.194205	6.970324

29.H	-2.038521	1.725649	1.761168
30.H	-0.606747	0.943586	1.950381
31.O	1.242733	1.678343	6.896143
32.H	1.649044	0.914237	7.346975
33.H	1.678363	2.462641	7.279880

I5ms+H2O

1.fe	0.077659	-0.016152	-0.109247
2.o	1.829242	-0.144242	0.050472
3.o	-0.181580	2.119622	0.231302
4.o	-0.220729	-0.391251	1.963550
5.o	-2.184345	0.139851	-0.126233
6.o	-0.397149	-2.000767	-0.718962
7.o	-0.083861	0.506494	-2.131091
8.o	3.461006	-1.809908	-0.960788
9.cl	1.214058	-1.922008	-3.258881
10.c	1.307223	-3.667024	-6.622206
11.c	2.087697	-2.487860	-6.833012
12.c	2.680521	-2.278884	-8.048552
13.c	2.513566	-3.240515	-9.088917
14.c	1.739646	-4.419313	-8.883683
15.c	1.145500	-4.629442	-7.667733
16.o	0.707236	-3.930413	-5.479018
17.o	3.119507	-2.962227	-10.237933
18.h	2.580975	-0.761332	-0.310277
19.h	0.156893	2.651570	-0.514393
20.h	0.221138	2.504932	1.032489
21.h	0.542263	-0.580599	2.539963
22.h	-1.035372	-0.473606	2.492027
23.h	-2.797035	-0.598915	-0.291671
24.h	-2.720978	0.922454	0.091805
25.h	-0.133324	-2.724490	-0.119710
26.h	0.096650	-2.171405	-1.589618
27.h	-0.987828	0.548830	-2.496264
28.h	0.415113	-0.174463	-2.696918
29.h	3.070732	-1.951750	-1.853253
30.h	4.402200	-1.597613	-1.087567
31.h	0.873056	-3.223589	-4.775855
32.h	2.197918	-1.770493	-6.019565
33.h	3.282326	-1.393734	-8.254621
34.h	2.967176	-3.655343	-10.911867
35.h	1.627002	-5.143814	-9.692530
36.h	0.546467	-5.517023	-7.465656

I5PRIMms

1.C	2.750921	0.659435	1.054182
2.C	3.670940	0.158255	0.169178
3.C	3.239037	-0.298371	-1.111541
4.C	1.863826	-0.237397	-1.485080
5.C	0.950092	0.271502	-0.604503
6.C	1.371402	0.728223	0.682994
7.O	4.066541	-0.797460	-2.018800
8.Cl	-4.459579	1.004855	1.752691
9.O	0.447729	1.206172	1.491159
10.Fe	-1.215299	2.434262	4.406991
11.O	-1.841139	4.056398	4.840563
12.O	0.519011	1.868755	3.848381
13.O	-1.744168	2.636895	2.316488

14.O	-2.669128	0.964891	4.332952
15.O	-0.895579	1.774508	6.393627
16.H	3.062555	1.024157	2.033084
17.H	4.729223	0.110868	0.432501
18.H	1.576813	-0.603932	-2.470253
19.H	-0.108474	0.326172	-0.855958
20.H	4.996264	-0.813017	-1.712993
21.H	-3.074950	0.583196	5.131744
22.H	-3.322982	0.913921	3.583862
23.H	-1.482472	4.950068	4.984622
24.H	-5.451788	0.178985	1.907952
25.H	1.160667	1.587711	4.530843
26.H	0.695856	1.446116	2.519627
27.H	0.041595	1.488611	6.613306
28.H	-1.196098	2.381835	7.095039
29.H	-1.989462	3.532673	2.020895
30.H	-1.115935	2.253417	1.663611
31.O	1.675603	1.072163	6.544343
32.H	1.884379	0.164615	6.833445
33.H	2.291308	1.642326	7.041211

I6ms+H2O

1.Cl	0.439013	-0.583790	-1.364459
2.Fe	-0.420598	-1.731407	-5.067019
3.O	1.270311	-1.707469	-3.943662
4.O	-2.072548	-1.934224	-6.309685
5.O	-1.574541	-1.714677	-3.320183
6.O	-0.539182	-3.815284	-4.801020
7.O	0.826043	-2.280808	-6.719207
8.H	-0.968241	-4.237039	-4.033062
9.H	-0.068896	-4.499826	-5.312758
10.H	1.620132	-2.570401	-3.643397
11.H	1.181944	-1.141380	-3.093130
12.H	-2.622464	-2.729078	-6.450202
13.H	-2.524564	-1.164393	-6.705762
14.H	0.461789	-2.151850	-7.618001
15.H	1.695638	-1.830803	-6.723574
16.H	-1.066230	-1.258024	-2.573537
17.H	-2.437507	-1.257644	-3.367937
18.O	-0.403798	-0.137225	-5.292567
19.H	1.790603	1.939454	0.201629
20.H	0.467167	2.593269	-0.398002
21.O	1.212722	1.986463	-0.589502
22.H	0.856370	0.939842	-0.925235

TS1ms

1.C	0.044920	-0.894977	0.143085
2.C	0.001864	0.132094	1.051866
3.C	1.212472	0.682103	1.549004
4.C	2.470471	0.167824	1.133698
5.C	2.518640	-0.859678	0.229975
6.C	1.307151	-1.354312	-0.357710
7.O	1.250029	1.674109	2.434531
8.Cl	1.346924	-3.009354	-0.971336
9.O	1.328372	-0.362116	-2.013796
10.Fe	1.813762	-0.572448	-3.657135
11.O	3.341903	-2.028344	-3.238988
12.O	0.433253	0.801738	-4.584051

13.O	0.511509	-2.135940	-4.342587
14.O	2.666774	-0.567795	-5.784457
15.O	3.173024	1.074690	-3.502519
16.H	-0.870295	-1.357428	-0.223058
17.H	-0.956418	0.505673	1.417195
18.H	3.374461	0.577663	1.583454
19.H	3.470610	-1.307153	-0.053416
20.H	0.355898	1.954662	2.711434
21.H	2.465517	0.175473	-6.381366
22.H	2.852524	-1.330655	-6.360308
23.H	3.923604	-2.527083	-3.840620
24.H	3.055304	-2.640209	-2.526587
25.H	0.102311	1.528479	-4.026230
26.H	-0.345775	0.412540	-5.055605
27.H	3.347197	1.389808	-2.597357
28.H	3.997708	1.173272	-4.012389
29.H	0.168839	-2.712783	-3.634845
30.H	-0.259340	-1.878323	-4.911059
31.O	-1.419525	-0.834405	-5.864870
32.H	-2.363499	-0.856379	-5.620050
33.H	-1.415464	-0.891690	-6.838791

TS2ms

1.C	0.959848	0.369111	0.760816
2.C	1.429923	0.514524	-0.513696
3.C	1.235226	1.754385	-1.178170
4.C	0.521395	2.846955	-0.563125
5.C	0.065262	2.722222	0.704649
6.C	0.376239	1.517636	1.500885
7.O	1.661248	1.991918	-2.397652
8.Cl	-1.735730	0.134824	0.737369
9.O	0.325479	1.542867	2.748826
10.Fe	-2.089765	1.694268	4.306708
11.O	-3.029940	2.156289	2.497416
12.O	-0.796029	1.407445	5.928549
13.O	-1.867954	-0.259994	3.735309
14.O	-3.951146	1.529411	5.312195
15.O	-1.587795	3.732552	4.502997
16.H	1.113841	-0.556207	1.314529
17.H	1.922878	-0.310639	-1.031291
18.H	0.381149	3.753587	-1.152530
19.H	-0.444489	3.540502	1.212111
20.H	2.134469	1.230031	-2.794442
21.H	-4.727225	1.105143	4.901037
22.H	-4.057907	1.400850	6.272452
23.H	-3.954901	2.397794	2.312236
24.H	-2.709115	1.564420	1.739591
25.H	-0.940074	1.398078	6.890413
26.H	-0.059093	0.755060	5.703405
27.H	-0.930802	4.033526	5.156842
28.H	-2.122644	4.503785	4.242969
29.H	-1.847833	-0.358471	2.732006
30.H	-1.072180	-0.718360	4.088167
31.O	0.787661	-0.271688	4.730001
32.H	0.974341	0.308364	3.949634
33.H	1.614997	-0.704609	5.003761

TS2PRIMms

1.C	1.002071	0.052162	0.875239
2.C	1.596612	0.045506	-0.346542
3.C	1.671503	1.264331	-1.096805
4.C	1.090123	2.482858	-0.623707
5.C	0.488482	2.501663	0.593271
6.C	0.520962	1.316433	1.477503
7.O	2.254062	1.331623	-2.272367
8.Cl	-1.876246	0.737089	0.495924
9.O	0.346535	1.431534	2.708209
10.Fe	-2.074955	1.611426	4.266729
11.O	-2.585219	2.711120	2.586691
12.O	-0.404774	0.840017	5.166606
13.O	-2.498942	-0.139871	3.240550
14.O	-3.887282	1.334232	5.274776
15.O	-1.797812	3.414056	5.403413
16.H	0.945529	-0.848068	1.486521
17.H	2.010269	-0.871768	-0.771444
18.H	1.144941	3.361150	-1.266967
19.H	0.056132	3.413354	1.003757
20.H	2.630438	0.474367	-2.563257
21.H	-4.255163	1.927088	5.954981
22.H	-4.602320	0.741832	4.977426
23.H	-3.407331	3.222848	2.477862
24.H	-2.459820	2.148174	1.743643
25.H	-0.004858	1.347585	5.918990
26.H	0.251943	0.799225	4.426862
27.H	-1.135065	3.367340	6.140127
28.H	-1.700143	4.288459	4.985836
29.H	-2.322742	-0.086260	2.243406
30.H	-2.488506	-1.069992	3.525565
31.O	0.167250	2.649659	7.199953
32.H	1.018735	3.122443	7.256458
33.H	-0.045490	2.409147	8.121453

TS3ms			
1.C	0.953876	0.548852	0.474998
2.C	1.182262	0.209443	-0.841681
3.C	1.244958	1.233401	-1.802547
4.C	1.080997	2.638059	-1.458306
5.C	0.928595	3.003849	-0.169409
6.C	0.970102	1.986576	0.900183
7.O	1.464450	1.021665	-3.083288
8.Cl	-1.518809	0.617883	0.896855
9.O	1.100333	2.321087	2.081794
10.Fe	-2.278368	1.416650	4.790718
11.O	-2.414709	2.567274	2.993046
12.O	-2.036896	0.541485	6.749162
13.O	-1.658862	-0.258271	3.823930
14.O	-4.389086	1.186219	4.971572
15.O	-1.955228	3.296672	5.665473
16.H	1.047930	-0.192536	1.264811
17.H	1.293924	-0.833865	-1.141733
18.H	1.114714	3.359316	-2.275881
19.H	0.847240	4.046485	0.136329
20.H	1.573212	0.071154	-3.297047
21.H	-5.001502	1.012182	4.234150
22.H	-4.929716	1.193402	5.782140
23.H	-3.233509	3.011586	2.707504

24.H	-2.084834	2.049826	2.187679
25.H	-2.537189	-0.248085	7.027401
26.H	-1.190518	0.500242	7.230459
27.H	-1.951741	3.567365	6.600932
28.H	-1.637666	4.049470	5.134646
29.H	-1.710431	-0.182514	2.820536
30.H	-0.684473	-0.172788	4.015864
31.O	0.479309	1.129679	4.444309
32.H	0.805588	1.547208	3.599452
33.H	1.255444	1.086627	5.029581

TS3PRIMms

1.C	1.627912	-0.550935	0.374496
2.C	2.112217	-0.401343	-0.887302
3.C	2.675304	0.859013	-1.274651
4.C	2.743692	1.967254	-0.365727
5.C	2.264429	1.823602	0.896706
6.C	1.691452	0.552356	1.337734
7.O	3.158842	1.080692	-2.476433
8.Cl	-1.509120	1.507199	0.295821
9.O	1.286211	0.381309	2.519014
10.Fe	-1.809539	1.859679	4.052326
11.O	-2.356295	2.883578	2.546655
12.O	0.197866	1.972278	4.276889
13.O	-1.464025	0.146565	2.903820
14.O	-3.123131	0.603936	5.063785
15.O	-1.948992	3.123795	5.739896
16.H	1.202225	-1.494777	0.714824
17.H	2.080211	-1.220830	-1.608732
18.H	3.181926	2.897817	-0.726846
19.H	2.304629	2.643527	1.613014
20.H	3.092598	0.300622	-3.067301
21.H	-3.466429	0.665751	5.973607
22.H	-3.296429	-0.295802	4.729115
23.H	-3.188032	3.375895	2.419036
24.H	-2.006007	2.389402	1.466686
25.H	0.674528	2.516221	4.944997
26.H	0.815087	1.472671	3.654199
27.H	-1.097245	3.477845	6.119942
28.H	-2.664561	3.744145	5.965362
29.H	-1.585000	0.412225	1.921270
30.H	-0.537231	-0.190441	2.926742
31.O	0.612557	3.694570	6.433061
32.H	0.942364	3.369967	7.292354
33.H	0.973074	4.597173	6.348755

TS4ms+H2O

C	0.867384	0.462850	1.160592
C	0.948285	-0.002594	2.444360
C	2.213338	-0.381116	2.964886
C	3.416725	-0.288563	2.179506
C	3.358976	0.213358	0.921157
C	2.087550	0.665237	0.363199
O	2.382447	-0.844759	4.189546
Cl	0.632662	-1.775102	-0.552388
O	2.091334	1.281694	-0.736330
Fe	-0.043533	-1.532476	-4.431830
O	1.548816	-2.295570	-3.301597

O	-1.658582	-1.022166	-5.869201
O	-1.264227	-1.778274	-2.781000
O	-0.727812	-3.568858	-4.937043
O	1.151693	-1.742857	-6.256459
H	-0.078735	0.801045	0.742448
H	0.054663	-0.099401	3.063532
H	4.349971	-0.614684	2.639083
H	4.247118	0.332256	0.301805
H	1.542748	-0.897060	4.691264
H	-1.167445	-4.121988	-4.266177
H	-0.379811	-4.165645	-5.623275
H	1.871474	-3.210650	-3.384076
H	1.411562	-2.132898	-2.299730
H	-2.398676	-1.600427	-6.127001
H	-1.981684	-0.105026	-5.923720
H	0.817141	-1.487040	-7.134938
H	2.122071	-1.794306	-6.322080
H	-0.752795	-1.752342	-1.890140
H	-2.140638	-1.380605	-2.638691
O	0.303314	0.347199	-4.203170
H	0.217675	1.107664	-3.063607
H	0.964981	0.741841	-4.797282
O	0.117617	1.669358	-2.144492
H	0.000746	2.617480	-2.338579
H	0.978249	1.523508	-1.467363

TS4PRIMms

1.C	2.848288	0.861605	1.084821
2.C	3.868557	0.737973	0.179952
3.C	3.588895	0.254497	-1.134105
4.C	2.260600	-0.098520	-1.519421
5.C	1.243126	0.029245	-0.617188
6.C	1.506282	0.507359	0.711330
7.O	4.521822	0.106882	-2.062024
8.Cl	-4.331004	3.162869	1.714116
9.O	0.507079	0.593352	1.544543
10.Fe	-1.440897	1.969095	4.242827
11.O	-2.200161	3.615195	4.173881
12.O	0.373081	1.485842	3.775300
13.O	-2.042025	1.273484	2.359438
14.O	-2.819934	0.501127	4.860361
15.O	-0.960812	1.951786	6.301372
16.H	3.040878	1.235005	2.090579
17.H	4.891681	1.006118	0.450446
18.H	2.095403	-0.464957	-2.532395
19.H	0.219649	-0.237771	-0.877904
20.H	5.412869	0.362221	-1.746810
21.H	-3.236374	0.505495	5.742190
22.H	-3.456500	0.123241	4.224992
23.H	-1.771871	4.484483	4.066061
24.H	-3.813727	3.704537	2.788250
25.H	0.992259	1.229499	4.489290
26.H	0.621778	1.016114	2.638443
27.H	-0.078031	1.557464	6.570239
28.H	-1.131540	2.740598	6.847266
29.H	-2.725906	1.842320	1.899534
30.H	-1.347995	0.989642	1.721322
31.O	1.443320	0.826064	6.522589

32.H	1.493841	-0.090125	6.854229
33.H	2.157617	1.300187	6.987195
