

Electronic Supplementary Material (ESI) for RSC Advances.

**Do the dual oxidants (ferric-peroxo and ferryl-oxo species) act in the
biosynthesis of estrogens? A DFT calculation**

**Xiang-Yun Wang,^a Hui-Min Yan,^a Yan-Li Han,^a Zhu-Xia Zhang,^a Xiao-Yun Zhang,^a Wen-Jing
Yang,^a Zhen Guo^{*a} and Yan-Rong Li^{*b}**

^a *College of Material Science & Engineering, Taiyuan University of Technology, Shanxi,
030024, P. R. China. E-mail: guozhen@tyut.edu.cn.*

^b *Department of Earth Sciences and Engineering, Taiyuan University of Technology, Shanxi
030024, P. R. China. E-mail: li.dennis@hotmail.com*

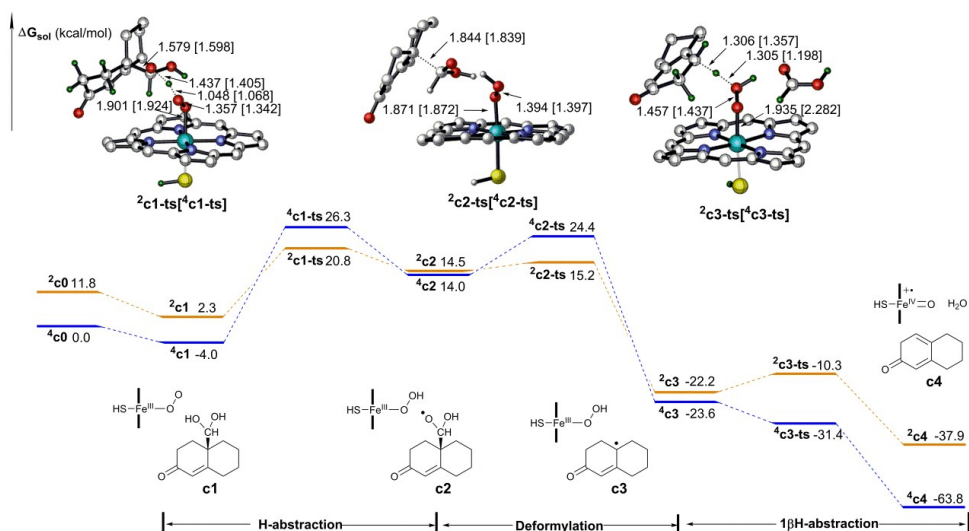


Fig. S1 DFT calculated energy diagram for the the aromatized reaction by ferric-peroxo species in doublet and quartet states (in square brackets), followed by the computed key structures of transition states and intermediates with selected bond distances.

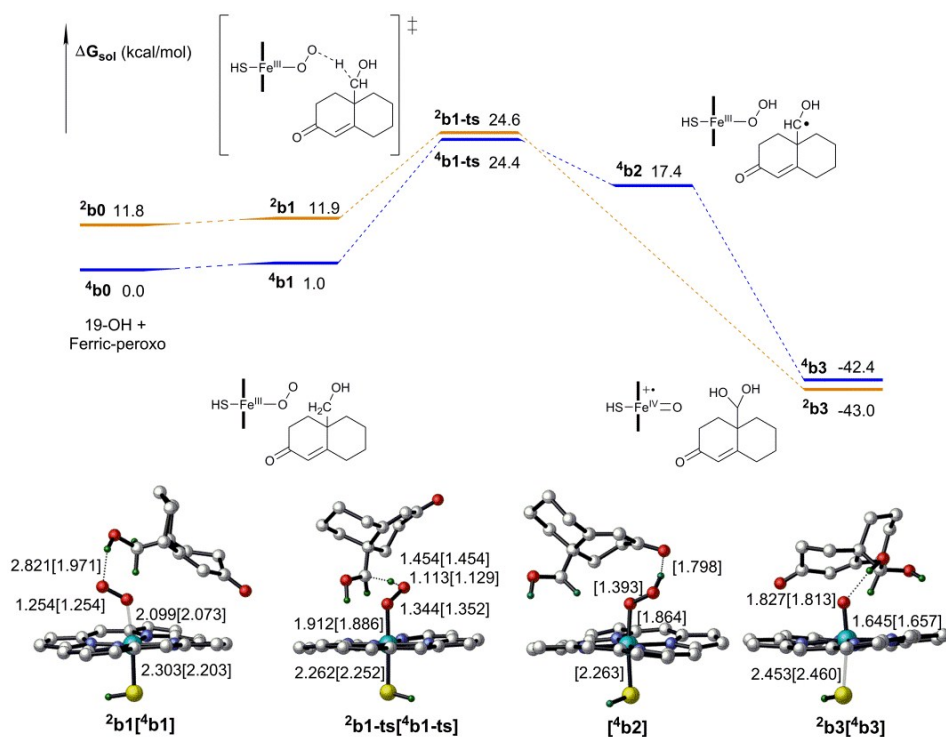


Fig. S2 DFT calculated energy diagram for the oxidation of 19-OH androgen by ferric-peroxo species in doublet and quartet states without a free energy correction of -2.6 kcal/mol.

Cartesian Coordinates of optimized Structures

$$\Delta G_{\text{solv}} = \Delta E_{\text{solv}}(\text{SMD}) + \Delta G_{\text{correction}}$$

ΔE_{solv} refers to the solvation single point energy by M06/6-311+G(d,p): Sdd level of theory.

$\Delta G_{\text{correction}}$ refers to the thermal correction to the free energy of the solute in the gas phase by M06L/6-311G(d) level of theory.

1. Coordinates of all stationary points in Fig. 2

RC₁

Charge = 0 Multiplicity = 1

H	-0.441	-1.89293	-1.21416
C	-0.25747	-1.55933	-0.18085
C	0.27918	-0.11061	-0.20982
C	-1.55848	-1.68208	0.59352
H	0.52754	-2.21236	0.2157
C	-0.82314	0.89783	-0.43736
C	1.03245	0.28506	1.07415
C	1.20833	-0.119	-1.41333
C	-2.62089	-0.73408	0.07988
H	-1.94935	-2.7029	0.56554
C	-0.33136	2.30073	-0.599
C	-2.12737	0.58111	-0.35266
C	1.53071	1.72486	1.00935
H	1.85517	-0.41352	1.2513
H	0.34531	0.16629	1.92311
O	2.93066	-2.33373	0.62658
O	-3.80682	-1.00591	0.09436
C	0.416	2.70929	0.67933
H	0.36331	2.37012	-1.45203
H	-1.15807	2.98686	-0.80984
H	-2.89128	1.33908	-0.52765
H	2.00564	1.99626	1.95876
H	2.3222	1.79906	0.25103
H	-0.30497	2.74751	1.50764
H	0.81307	3.72485	0.56983
H	3.59206	-3.00008	0.42691
O	2.39103	-0.36079	-1.38628
H	3.01049	-1.65881	-0.06179
H	0.69712	0.03907	-2.39614
H	-1.3938	-1.44783	1.65522

$$\Delta E_{\text{solv}} = -654.247142659$$

$$\Delta G_{\text{correction}} = 0.213196$$

RC₂

Charge = 0 Multiplicity = 1

H	-0.26206	-2.18909	-0.2504
C	-0.51606	-1.50732	0.57392
C	-0.03974	-0.09197	0.21103
C	-2.00629	-1.61473	0.84055
H	0.06272	-1.85713	1.43357
C	-1.07045	0.66886	-0.61141
C	0.29245	0.73415	1.47733
C	1.18829	-0.22792	-0.68581
C	-2.81889	-1.07655	-0.31435
H	-2.30959	-2.64504	1.04618
C	-0.70835	2.08033	-0.94748
C	-2.28355	0.1574	-0.90032
C	0.55601	2.21448	1.22636
H	1.14705	0.25848	1.9711
H	-0.56502	0.62694	2.1582
O	2.54787	-1.68813	0.98784
O	-3.87457	-1.5663	-0.67112
C	-0.52006	2.85666	0.3635
H	0.22575	2.12879	-1.5213
H	-1.49197	2.5342	-1.56275
H	-2.97838	0.72688	-1.51831
H	0.62715	2.73371	2.18973
H	1.52931	2.33394	0.74194
H	-1.47837	2.87543	0.90229
H	-0.26958	3.90093	0.14464
H	2.52897	-2.63107	1.16572
O	2.03616	0.61836	-0.85743
H	3.73016	-0.20255	-1.17741
H	1.22477	-1.18271	-1.26113
H	-2.28082	-1.03017	1.73132
O	4.33647	-0.93611	-0.98443
H	3.31945	-1.53532	0.40968
H	4.43288	-1.42922	-1.80192

 $\Delta E_{\text{solv}} = -730.680550499$ $\Delta G_{\text{correction}} = 0.23521$

RC₃

Charge = 0 Multiplicity = 1

H	-0.62531	-2.15894	-0.46547
C	-0.92201	-1.57597	0.41894
C	-0.44214	-0.12728	0.23878
C	-2.42174	-1.72101	0.60081
H	-0.38037	-2.0155	1.26077
C	-1.44454	0.71753	-0.53855
C	-0.1845	0.55413	1.6044
C	0.82184	-0.15068	-0.61918
C	-3.18635	-1.06071	-0.52235
H	-2.72261	-2.76968	0.67547
C	-1.08883	2.16209	-0.69498
C	-2.63807	0.23511	-0.93835
C	0.08434	2.05258	1.53184
H	0.63997	0.02341	2.0915
H	-1.07946	0.37549	2.21901
O	1.98184	-1.75412	0.9712
O	-4.21934	-1.5122	-0.98158
C	-0.95863	2.78595	0.70162
H	-0.13615	2.28464	-1.22483
H	-1.85607	2.67624	-1.28302
H	-3.31166	0.8684	-1.51657
H	0.1123	2.46122	2.54923
H	1.07673	2.22522	1.10521
H	-1.93797	2.74157	1.19962
H	-0.70737	3.84911	0.61211
H	1.94373	-2.67115	0.68946
O	1.63745	0.74375	-0.6912
H	3.19479	0.49129	-1.57543
H	0.89418	-1.03019	-1.29763
H	-2.74277	-1.2424	1.5381
O	4.1145	0.27105	-1.81634
H	4.56452	1.11034	-1.93399
H	4.53601	-0.58111	-0.36077
O	4.57051	-1.07366	0.48718
H	2.92649	-1.49364	0.8944
H	5.21521	-1.77349	0.37095

 $\Delta E_{\text{solv}} = -807.118983917$ $\Delta G_{\text{correction}} = 0.259378$

TS₁Charge = 0 Multiplicity = 1 **TS₁ = -1920.10i cm⁻¹**

H	-0.90907	-2.13823	-0.40074
C	-0.75914	-1.50201	0.48481
C	0.25742	-0.40443	0.13328
C	-2.1142	-0.97834	0.92061
H	-0.32105	-2.15515	1.24764
C	-0.39818	0.76912	-0.57379
C	0.97565	0.13004	1.39301
C	1.24602	-1.02608	-0.8591
C	-2.70446	-0.04827	-0.11642
H	-2.82102	-1.78816	1.12154
C	0.51636	1.89978	-0.92082
C	-1.73294	0.85607	-0.74057
C	1.8337	1.37122	1.16287
H	1.57433	-0.68078	1.82536
H	0.1958	0.35832	2.13422
O	1.93447	-2.3639	-0.06632
O	-3.89791	0.01001	-0.34883
C	1.09618	2.45423	0.38927
H	1.34378	1.5614	-1.55559
H	-0.0297	2.67693	-1.46552
H	-2.15763	1.7051	-1.27691
H	2.16694	1.76131	2.13239
H	2.73449	1.08923	0.61226
H	0.27307	2.86151	0.99425
H	1.76503	3.2952	0.17359
H	1.79518	-3.17576	-0.57306
O	2.41938	-0.5131	-1.1109
H	2.76107	-1.6344	-0.5587
H	0.70795	-1.5193	-1.69888
H	-2.025	-0.40916	1.85764

 $\Delta E_{\text{solv}} = -654.180103384$ $\Delta G_{\text{correction}} = 0.214035$

TS₂Charge = 0 Multiplicity = 1 **TS₂ = -1524.16i cm⁻¹**

H	-0.56802	-2.22961	-0.08848
C	-0.72396	-1.47438	0.69888
C	-0.00983	-0.17642	0.2819
C	-2.21918	-1.33534	0.91126
H	-0.2443	-1.86893	1.60211
C	-0.88042	0.67371	-0.62692
C	0.36673	0.66764	1.52134
C	1.24748	-0.58833	-0.51424
C	-2.89429	-0.75534	-0.31144
H	-2.6871	-2.29072	1.16491
C	-0.31563	2.00101	-1.02161
C	-2.14661	0.33263	-0.94525
C	0.85784	2.07757	1.20944
H	1.11574	0.11369	2.09847
H	-0.53006	0.72852	2.15632
O	2.05843	-1.66082	0.54811
O	-4.00428	-1.0972	-0.67799
C	-0.07192	2.81531	0.25734
H	0.63573	1.88262	-1.54998
H	-1.01174	2.52279	-1.687
H	-2.71925	0.95917	-1.62978
H	0.95868	2.63814	2.14713
H	1.85624	2.0214	0.76867
H	-1.03934	3.00554	0.74516
H	0.33993	3.79784	-0.00088
H	1.64432	-2.52805	0.47492
O	2.11783	0.29876	-0.83512
H	3.29455	-0.32473	-0.95891
H	0.97549	-1.33816	-1.29467
H	-2.42512	-0.65745	1.75256
O	4.03544	-1.11531	-0.66539
H	3.21312	-1.60214	-0.0015
H	4.27058	-1.6616	-1.42014

 $\Delta E_{\text{solv}} = -730.639154226$ $\Delta G_{\text{correction}} = 0.237471$

TS₃Charge = 0 Multiplicity = 1 **TS₃ = -1025.97i cm⁻¹**

H	-0.64434	-2.22273	0.00975
C	-0.99943	-1.48423	0.74735
C	-0.38978	-0.11377	0.40012
C	-2.51542	-1.53086	0.74745
H	-0.61593	-1.80953	1.72271
C	-1.2307	0.62237	-0.62397
C	-0.27968	0.76886	1.66382
C	1.01844	-0.37534	-0.22215
C	-3.07859	-1.04274	-0.5689
H	-2.89484	-2.53576	0.95393
C	-0.78907	2.01066	-0.9621
C	-2.38826	0.12656	-1.11218
C	0.08476	2.22435	1.39241
H	0.44915	0.30752	2.33964
H	-1.25164	0.72899	2.17974
O	1.76881	-1.2906	0.92391
O	-4.07849	-1.52082	-1.07558
C	-0.8018	2.84784	0.32469
H	0.22838	2.00393	-1.36483
H	-1.45579	2.44498	-1.71516
H	-2.93161	0.67751	-1.88062
H	0.00996	2.79614	2.32615
H	1.12815	2.27494	1.07102
H	-1.83712	2.92175	0.68973
H	-0.48107	3.87308	0.10442
H	1.32812	-2.14763	0.96192
O	1.77914	0.62384	-0.46767
H	2.96007	0.37836	-1.26
H	0.91301	-1.14164	-1.03016
H	-2.91777	-0.87974	1.53741
O	3.91046	0.07373	-1.6074
H	4.48078	0.8459	-1.61459
H	4.16815	-0.73594	-0.63614
O	4.13546	-1.43284	0.26123
H	3.0925	-1.40158	0.61201
H	4.36597	-2.32719	-0.00205

 $\Delta E_{\text{solv}} = -807.083488215$ $\Delta G_{\text{correction}} = 0.258768$

PC₁

Charge = 0 Multiplicity = 1

H	-1.02337	-2.11559	-0.33703
C	-0.82894	-1.46304	0.5296
C	0.26477	-0.44497	0.14669
C	-2.15196	-0.84707	0.93909
H	-0.44359	-2.11614	1.32158
C	-0.32198	0.75	-0.5781
C	0.99779	0.05904	1.41107
C	1.2214	-1.24744	-0.77463
C	-2.6784	0.07101	-0.14194
H	-2.90376	-1.60775	1.16703
C	0.62686	1.86016	-0.9055
C	-1.64879	0.90106	-0.77191
C	1.90359	1.26821	1.19365
H	1.56426	-0.77798	1.83626
H	0.22742	0.31587	2.15317
O	1.70415	-2.41323	-0.12869
O	-3.86408	0.18126	-0.39559
C	1.21427	2.3799	0.41524
H	1.44212	1.51559	-1.54819
H	0.09857	2.66131	-1.43321
H	-2.01914	1.76327	-1.32731
H	2.23641	1.64522	2.16856
H	2.80435	0.95602	0.65946
H	0.39967	2.81035	1.01589
H	1.91308	3.20031	0.21452
H	1.02515	-3.09385	-0.18189
O	2.34748	-0.51167	-1.11896
H	2.96721	-1.13401	-1.51696
H	0.65153	-1.54795	-1.67819
H	-2.03204	-0.24676	1.85263

 $\Delta E_{\text{solv}} = -654.245872112$ $\Delta G_{\text{correction}} = 0.221166$

PC₂

Charge = 0 Multiplicity = 1

H	-0.51951	-2.23857	0.18071
C	-0.74985	-1.40701	0.86686
C	-0.02603	-0.13799	0.37004
C	-2.2593	-1.29044	0.94458
H	-0.34172	-1.69138	1.84507
C	-0.83851	0.58198	-0.68978
C	0.21717	0.83547	1.54711
C	1.31486	-0.64775	-0.22013
C	-2.83752	-0.87367	-0.3898
H	-2.72486	-2.22584	1.267
C	-0.2993	1.89443	-1.16515
C	-2.06289	0.16362	-1.07382
C	0.67013	2.23539	1.14282
H	0.94338	0.37633	2.22826
H	-0.72643	0.90962	2.10814
O	2.03391	-1.4254	0.76387
O	-3.90233	-1.29126	-0.80709
C	-0.20168	2.83217	0.0474
H	0.69436	1.78101	-1.60707
H	-0.96337	2.31732	-1.92653
H	-2.59143	0.69627	-1.86492
H	0.6566	2.88419	2.02725
H	1.70739	2.1963	0.80175
H	-1.2156	3.01702	0.43189
H	0.18878	3.80667	-0.26788
H	1.53295	-2.23205	0.93183
O	2.14478	0.37434	-0.59639
H	2.96296	-0.02833	-0.95194
H	1.08402	-1.32384	-1.07054
H	-2.54854	-0.5287	1.68287
O	4.25036	-1.30328	-0.91324
H	3.78038	-1.63994	-0.13408
H	4.30434	-2.02854	-1.53964

 $\Delta E_{\text{solv}} = -730.68340503$ $\Delta G_{\text{correction}} = 0.243373$

PC₃

Charge = 0 Multiplicity = 1

H	-0.74162	-2.24456	-0.00085
C	-1.02141	-1.49288	0.75507
C	-0.3968	-0.13906	0.36016
C	-2.53407	-1.48924	0.85343
H	-0.57467	-1.82861	1.6984
C	-1.26506	0.59727	-0.64246
C	-0.23059	0.76033	1.60721
C	0.97881	-0.49863	-0.2594
C	-3.15896	-1.00807	-0.43747
H	-2.9302	-2.47769	1.10241
C	-0.82143	1.9749	-1.02289
C	-2.46311	0.12633	-1.04826
C	0.12818	2.2131	1.30779
H	0.51808	0.30347	2.26521
H	-1.1816	0.73117	2.15988
O	1.73626	-1.29687	0.68865
O	-4.20237	-1.4591	-0.87436
C	-0.78228	2.8277	0.25407
H	0.17543	1.96191	-1.47182
H	-1.51751	2.40456	-1.7513
H	-3.03553	0.67826	-1.79442
H	0.0706	2.79449	2.23638
H	1.1659	2.26916	0.97001
H	-1.80545	2.91695	0.64806
H	-0.45798	3.84628	0.01084
H	1.43536	-2.20939	0.62624
O	1.73829	0.59672	-0.55168
H	2.48862	0.2998	-1.12056
H	0.80951	-1.13088	-1.15237
H	-2.86661	-0.812	1.65348
O	3.82439	-0.47816	-1.85621
H	4.3917	0.09879	-2.37141
H	4.29988	-0.67416	-1.02061
O	4.49135	-0.82179	0.71039
H	3.53945	-0.90121	0.90194
H	4.91354	-1.58317	1.11277

 $\Delta E_{\text{solv}} = -807.125974366$ $\Delta G_{\text{correction}} = 0.265497$

2. Coordinates of all stationary points in Fig. 3

²Cpd I

Charge = 0 Multiplicity = 2

C	-1.62086	-2.58198	-0.09655
N	-0.40135	-1.96569	-0.10574
C	0.5285	-2.96923	-0.13579
C	-0.12416	-4.24781	-0.13429
C	-1.45925	-4.00778	-0.10599
Fe	-0.04823	0.02513	-0.22213
O	0.08043	-0.02789	-1.84052
C	1.9028	-2.79117	-0.158
C	2.56694	-1.57741	-0.13895
N	1.95979	-0.34974	-0.09856
C	2.97074	0.57364	-0.12467
C	4.24441	-0.08752	-0.15042
C	3.99343	-1.42108	-0.16125
C	2.7824	1.94497	-0.12855
C	1.55897	2.59948	-0.11485
N	0.33254	1.99166	-0.09842
C	-0.58704	3.00363	-0.08479
C	0.07199	4.27721	-0.08047
C	1.40575	4.02589	-0.10099
C	-1.96119	2.82444	-0.07603
C	-2.61587	1.60406	-0.08775
N	-2.00207	0.38051	-0.11619
C	-3.01073	-0.5446	-0.09164
C	-4.28581	0.11107	-0.05446
C	-4.04059	1.44561	-0.05234
C	-2.83751	-1.91984	-0.08394
S	0.23445	-0.21212	2.20342
H	1.04546	0.84473	2.41587
H	-4.75094	2.26314	-0.0224
H	-5.24056	-0.40039	-0.02685
H	-3.73653	-2.53128	-0.06852
H	-2.27391	-4.72197	-0.09354
H	0.38985	-5.2015	-0.14806
H	2.51531	-3.68902	-0.19021
H	4.70265	-2.23994	-0.18264
H	5.20247	0.41843	-0.16268
H	3.67369	2.56773	-0.14725
H	2.22623	4.73359	-0.10463
H	-0.43493	5.2346	-0.06394
H	-2.57912	3.71891	-0.05754

$\Delta E_{\text{solv}} = -1585.81551347$

$\Delta G_{\text{correction}} = 0.235793$

⁴Cpd I

Charge = 0 Multiplicity = 4

C	2.76412	1.24559	-0.26378
N	1.41429	1.40952	-0.11067
C	1.20779	2.75499	0.02802
C	2.46084	3.45289	-0.01797
C	3.42506	2.51812	-0.21455
Fe	0.0142	-0.01769	-0.24121
O	0.02949	-0.01984	-1.87954
C	-0.03455	3.364	0.11264
C	-1.25834	2.7232	0.02991
N	-1.43019	1.36869	-0.11541
C	-2.77514	1.17381	-0.29097
C	-3.46666	2.42916	-0.23923
C	-2.52841	3.38659	-0.0249
C	-3.37849	-0.06644	-0.41636
C	-2.73348	-1.28999	-0.30135
N	-1.38834	-1.44777	-0.11713
C	-1.18859	-2.78654	0.07678
C	-2.43959	-3.48725	0.02751
C	-3.39737	-2.56	-0.22971
C	0.05092	-3.39191	0.21602
C	1.27674	-2.75614	0.09203
N	1.4441	-1.41501	-0.10333
C	2.78617	-1.2199	-0.25833
C	3.48355	-2.47171	-0.17216
C	2.54675	-3.42428	0.06714
C	3.40124	0.01993	-0.36508
S	-0.05389	0.23658	2.2526
H	-1.3616	-0.03509	2.44136
H	2.68692	-4.48981	0.20407
H	4.55706	-2.58809	-0.2609
H	4.48348	0.02952	-0.47045
H	4.49531	2.66166	-0.30275
H	2.57215	4.52625	0.07826
H	-0.04924	4.44764	0.2001
H	-2.66845	4.45631	0.07444
H	-4.53876	2.54742	-0.34174
H	-4.45809	-0.08379	-0.54506
H	-4.46525	-2.70577	-0.34045
H	-2.55386	-4.55648	0.15981
H	0.06296	-4.46953	0.36134

 $\Delta E_{\text{solv}} = -1585.81457027$ $\Delta G_{\text{correction}} = 0.235193$

²a1

Charge = 0 Multiplicity = 2

C	2.44647	-2.79732	-0.38018
N	2.68521	-1.45488	-0.52015
C	3.68049	-1.34222	-1.45524
C	4.10107	-2.6445	-1.88807
C	3.33122	-3.54551	-1.22736
Fe	1.59786	0.06329	0.30092
O	0.55329	-0.05288	-0.95111
C	4.18373	-0.14293	-1.92806
C	3.74868	1.12394	-1.56351
N	2.76049	1.39207	-0.65636
C	2.62932	2.75272	-0.63457
C	3.56806	3.35857	-1.53399
C	4.26673	2.34624	-2.10817
C	1.72699	3.44881	0.15428
C	0.83373	2.8846	1.05096
N	0.67725	1.54097	1.27097
C	-0.25606	1.42815	2.26487
C	-0.70147	2.72618	2.6783
C	-0.03206	3.63195	1.917
C	-0.72332	0.23512	2.79652
C	-0.32104	-1.0301	2.40816
N	0.61222	-1.2879	1.43867
C	0.66838	-2.65087	1.32543
C	-0.24447	-3.26289	2.24865
C	-0.85214	-2.25697	2.92715
C	1.50304	-3.35065	0.46717
S	3.32372	-0.25507	2.0158
H	4.40057	0.10365	1.28613
H	-1.60365	-2.32288	3.70469
H	-0.38546	-4.33155	2.35792
H	1.42375	-4.435	0.47839
H	3.35216	-4.62667	-1.29406
H	4.88318	-2.83058	-2.61436
H	4.97639	-0.19666	-2.67052
H	5.06214	2.40586	-2.84139
H	3.6711	4.42524	-1.69308
H	1.73457	4.53349	0.07895
H	-0.09537	4.71338	1.94328
H	-1.44599	2.90562	3.44429
H	-1.48522	0.30218	3.5687
H	-4.82161	2.05071	-0.55616
C	-4.86442	1.33913	-1.38841
C	-3.54118	0.56081	-1.40536
C	-6.09545	0.46664	-1.22107
H	-4.93807	1.94168	-2.30396
C	-3.55027	-0.5802	-0.40901

C	-5.99257	-0.41931	0.00267
H	-7.01362	1.0578	-1.1551
C	-2.28425	-1.36569	-0.3438
C	-4.65781	-0.96111	0.25743
O	-6.96578	-0.7295	0.66923
C	-2.0081	-1.98484	-1.72145
H	-1.4353	-0.72393	-0.08404
H	-2.3511	-2.14477	0.42356
H	-4.60823	-1.77926	0.97724
H	-2.7779	-2.74209	-1.93138
H	-1.04559	-2.51006	-1.69808
H	-6.22435	-0.19933	-2.08792
C	-2.42072	1.55179	-1.06652
H	-2.4726	2.38448	-1.79149
H	-1.42533	1.09573	-1.16366
O	-2.62769	2.01314	0.25711
H	-1.91067	2.61487	0.48397
C	-2.00263	-0.92983	-2.8202
H	-1.91255	-1.41011	-3.80237
H	-1.10412	-0.31301	-2.70631
C	-3.25487	-0.05728	-2.79327
H	-3.17739	0.74956	-3.53563
H	-4.12862	-0.65539	-3.09018

$$\Delta E_{\text{solv}} = -2164.85791806$$

$$\Delta G_{\text{correction}} = 0.47331$$

²a1-ts

Charge = 0 Multiplicity = 2

C	2.15805	-2.81921	-0.33755
N	2.37542	-1.50321	-0.62428
C	3.19746	-1.47617	-1.71231
C	3.51368	-2.81756	-2.12449
C	2.86289	-3.65079	-1.27581
Fe	1.54938	0.09097	0.33526
O	0.26611	-0.11859	-0.80289
C	3.65654	-0.32731	-2.33373
C	3.31774	0.96992	-1.98162
N	2.50343	1.32812	-0.94125
C	2.36802	2.68687	-1.01179
C	3.14011	3.20343	-2.10498
C	3.73486	2.13883	-2.70188
C	1.59126	3.45719	-0.16155
C	0.858	2.97843	0.91237
N	0.7507	1.6603	1.28134
C	0.01117	1.64341	2.43568
C	-0.38555	2.97481	2.78303
C	0.12843	3.8028	1.83245
C	-0.34365	0.50779	3.144
C	-0.01412	-0.78836	2.78794
N	0.7326	-1.13769	1.69369
C	0.75785	-2.50756	1.66825
C	0.01232	-3.02984	2.77586
C	-0.45818	-1.96463	3.47523
C	1.40175	-3.2893	0.7221
S	3.42465	0.07367	1.69889
H	4.30831	0.64146	0.8529
H	-1.06366	-1.96054	4.37377
H	-0.12038	-4.08502	2.98409
H	1.32116	-4.36748	0.83639
H	2.85834	-4.73425	-1.26394
H	4.15395	-3.07076	-2.9612
H	4.31463	-0.45197	-3.18995
H	4.39069	2.12816	-3.5644
H	3.20818	4.25171	-2.37074
H	1.57815	4.53057	-0.33302
H	0.0528	4.88191	1.76658
H	-0.9848	3.23255	3.64809
H	-0.94765	0.64447	4.03686
H	-4.15002	2.14437	-1.05348
C	-4.17018	1.30265	-1.75532
C	-3.09656	0.27961	-1.31272
C	-5.57776	0.73411	-1.77967
H	-3.89419	1.70957	-2.73683
C	-3.59381	-0.59277	-0.17817

C	-5.95809	0.12355	-0.44698
H	-6.31485	1.49747	-2.04582
C	-2.60454	-1.60066	0.30432
C	-4.87703	-0.59746	0.22862
O	-7.09751	0.15217	-0.01788
C	-2.35436	-2.57955	-0.85463
H	-1.65318	-1.13245	0.58595
H	-2.98164	-2.12759	1.18691
H	-5.18267	-1.24029	1.05442
H	-3.29329	-3.10921	-1.07158
H	-1.63108	-3.34319	-0.54497
H	-5.66938	-0.05584	-2.53925
C	-1.91696	1.12959	-0.85355
H	-1.54706	1.81626	-1.63389
H	-0.82796	0.43612	-0.72855
O	-2.20522	1.74112	0.33392
H	-1.5497	2.42703	0.52939
C	-1.8497	-1.855	-2.09651
H	-1.80816	-2.54934	-2.94449
H	-0.8214	-1.52686	-1.91827
C	-2.71066	-0.65281	-2.48439
H	-2.20936	-0.06215	-3.26402
H	-3.64993	-1.00295	-2.93485

$$\Delta E_{\text{solv}} = -2164.83686861$$

$$\Delta G_{\text{correction}} = 0.469486$$

²a2

Charge = 0 Multiplicity = 2

C	2.49835	-2.76421	-0.51356
N	2.678	-1.41807	-0.65114
C	3.65989	-1.25638	-1.58572
C	4.10813	-2.53797	-2.05861
C	3.38027	-3.47335	-1.4005
Fe	1.69164	0.02855	0.33536
O	0.43049	-0.04979	-0.95557
C	4.14646	-0.03913	-2.02977
C	3.67743	1.20355	-1.63393
N	2.70014	1.42266	-0.70244
C	2.46915	2.77228	-0.69837
C	3.34583	3.4223	-1.62956
C	4.10189	2.45064	-2.20214
C	1.53612	3.4254	0.08972
C	0.71252	2.82269	1.02975
N	0.64381	1.47625	1.27755
C	-0.19052	1.32369	2.35443
C	-0.68431	2.5999	2.77579
C	-0.13702	3.53131	1.94454
C	-0.53871	0.11261	2.93014
C	-0.10427	-1.12931	2.49968
N	0.7712	-1.35009	1.46744
C	0.85315	-2.70854	1.31825
C	0.01527	-3.35834	2.28303
C	-0.56895	-2.37997	3.0228
C	1.64047	-3.36952	0.38857
S	3.30254	0.07968	1.97302
H	4.03995	1.10997	1.5102
H	-1.26792	-2.48088	3.84466
H	-0.0971	-4.43213	2.37619
H	1.60414	-4.45594	0.39093
H	3.43259	-4.55243	-1.48413
H	4.88205	-2.68407	-2.80277
H	4.9323	-0.05827	-2.78047
H	4.87134	2.55203	-2.9583
H	3.36784	4.49021	-1.81226
H	1.4771	4.50704	-0.00246
H	-0.25994	4.60812	1.96608
H	-1.37	2.75363	3.6005
H	-1.23101	0.13817	3.76732
H	-4.72535	2.09868	-0.53717
C	-4.74756	1.41927	-1.3969
C	-3.50071	0.50542	-1.31648
C	-6.05929	0.65432	-1.37551
H	-4.67299	2.04988	-2.29201
C	-3.70405	-0.61982	-0.31317

C	-6.15985	-0.25692	-0.17028
H	-6.92026	1.32942	-1.38252
C	-2.51347	-1.5013	-0.13093
C	-4.90548	-0.90524	0.22215
O	-7.22009	-0.49962	0.37747
C	-2.18792	-2.16339	-1.47987
H	-1.63823	-0.92698	0.19712
H	-2.70138	-2.25832	0.63751
H	-5.00134	-1.7242	0.9355
H	-2.99682	-2.86626	-1.72637
H	-1.27172	-2.75651	-1.38071
H	-6.16051	0.02424	-2.27119
C	-2.35172	1.37304	-0.89832
H	-1.7579	1.91749	-1.63889
H	-0.38561	0.43365	-0.7258
O	-2.48112	1.91336	0.32339
H	-1.75534	2.52422	0.52845
C	-2.02519	-1.14197	-2.5996
H	-1.9227	-1.6584	-3.56156
H	-1.08061	-0.6067	-2.45085
C	-3.18627	-0.15707	-2.67546
H	-2.98265	0.62556	-3.41969
H	-4.09569	-0.66926	-3.01801

$$\Delta E_{\text{solv}} = -2164.85133897$$

$$\Delta G_{\text{correction}} = 0.472128$$

²a3

Charge = 0 Multiplicity = 2

C	-2.08053	-2.65263	-0.80227
N	-1.63759	-1.85136	0.22354
C	-1.40499	-2.69838	1.28284
C	-1.66985	-4.05122	0.90299
C	-2.08267	-4.02346	-0.39362
Fe	-1.58895	0.16933	0.24089
O	0.40118	-0.20385	-0.5674
C	-0.94357	-2.30167	2.52814
C	-0.65849	-0.99889	2.90104
N	-0.80747	0.10545	2.09428
C	-0.38042	1.16945	2.85354
C	0.05154	0.72493	4.1477
C	-0.12476	-0.62052	4.17875
C	-0.3494	2.48486	2.4213
C	-0.74878	2.926	1.17004
N	-1.23361	2.12563	0.16511
C	-1.54253	2.97449	-0.86662
C	-1.21812	4.32407	-0.51571
C	-0.7222	4.29424	0.74804
C	-2.09345	2.59529	-2.07908
C	-2.4074	1.2993	-2.44729
N	-2.23464	0.19768	-1.65291
C	-2.5817	-0.87452	-2.43205
C	-3.00762	-0.4346	-3.73378
C	-2.90264	0.91604	-3.74193
C	-2.5046	-2.19981	-2.04198
S	-3.63901	0.38419	0.96588
H	-3.42856	0.43829	2.30154
H	-3.12374	1.60678	-4.54718
H	-3.3354	-1.09227	-4.53036
H	-2.82128	-2.95076	-2.76189
H	-2.38398	-4.85359	-1.02191
H	-1.55721	-4.9089	1.55602
H	-0.78947	-3.0789	3.273
H	0.08648	-1.31067	4.98739
H	0.43617	1.37379	4.92594
H	0.01316	3.2335	3.12154
H	-0.37172	5.11984	1.35609
H	-1.3586	5.18004	-1.16516
H	-2.2817	3.38139	-2.80634
H	3.47742	1.89209	0.35365
C	3.73235	0.89842	0.73929
C	2.83792	-0.13554	0.02507
C	5.22032	0.67737	0.54644
H	3.47022	0.91252	1.80562
C	3.42413	-0.57529	-1.29969

C	5.57285	0.62332	-0.92343
H	5.81442	1.45679	1.03104
C	2.68686	-1.66727	-2.01438
C	4.61836	-0.13763	-1.74334
O	6.60419	1.07896	-1.37884
C	2.74236	-2.9152	-1.12085
H	1.6392	-1.40201	-2.2069
H	3.1523	-1.87092	-2.98411
H	4.98631	-0.45199	-2.72079
H	3.794	-3.21017	-1.00256
H	2.23862	-3.75557	-1.61153
H	5.53894	-0.27628	0.99391
C	1.50092	0.63361	-0.17894
H	1.24326	1.11377	0.77344
H	0.51453	-1.09026	-0.19905
O	1.58273	1.65929	-1.09829
H	1.83233	1.28448	-1.95395
C	2.12155	-2.65431	0.2447
H	2.29657	-3.5076	0.91055
H	1.02642	-2.64323	0.1441
C	2.6552	-1.38651	0.92434
H	2.02879	-1.1213	1.78874
H	3.64382	-1.6192	1.34252

$$\Delta E_{\text{solv}} = -2164.95153946$$

$$\Delta G_{\text{correction}} = 0.479453$$

4a1

Charge = 0 Multiplicity = 4

C	-2.32624	2.87566	-0.36353
N	-2.65405	1.55646	-0.48961
C	-3.76306	1.51537	-1.28466
C	-4.15137	2.84441	-1.66435
C	-3.2452	3.68874	-1.10945
Fe	-1.63344	0.00135	0.25138
O	-0.52056	0.04247	-0.96126
C	-4.37762	0.35407	-1.72828
C	-3.91575	-0.93551	-1.51177
N	-2.83022	-1.25925	-0.74662
C	-2.65931	-2.60835	-0.8843
C	-3.65871	-3.14847	-1.76115
C	-4.45279	-2.11215	-2.1334
C	-1.72822	-3.36367	-0.1854
C	-0.88427	-2.88546	0.80432
N	-0.78052	-1.56795	1.17078
C	0.10497	-1.53049	2.21832
C	0.54248	-2.85756	2.53709
C	-0.05548	-3.69676	1.64874
C	0.58935	-0.37608	2.81068
C	0.26622	0.91807	2.4403
N	-0.60564	1.2537	1.43633
C	-0.54579	2.61627	1.32422
C	0.37551	3.15266	2.28483
C	0.86904	2.10008	2.9853
C	-1.32333	3.3699	0.45905
S	-3.15758	-0.12419	2.21237
H	-3.52811	-1.41543	2.08709
H	1.59161	2.10573	3.79238
H	0.5978	4.20619	2.4052
H	-1.18017	4.44772	0.47432
H	-3.20402	4.76958	-1.17092
H	-5.004	3.08449	-2.28804
H	-5.25314	0.46712	-2.36313
H	-5.3196	-2.12623	-2.7831
H	-3.74409	-4.19429	-2.03085
H	-1.71096	-4.43368	-0.37832
H	0.0327	-4.77443	1.57696
H	1.24385	-3.10034	3.32617
H	1.3239	-0.4977	3.60234
H	4.86395	-2.04919	-0.49398
C	4.90242	-1.35316	-1.33956
C	3.5766	-0.58015	-1.36723
C	6.1309	-0.47364	-1.19252
H	4.97601	-1.97226	-2.24397
C	3.58305	0.5749	-0.3879

C	6.02784	0.43666	0.01305
H	7.05146	-1.0598	-1.1166
C	2.31338	1.35505	-0.32878
C	4.69178	0.97468	0.26577
O	7.00312	0.76651	0.66742
H	1.46773	0.71326	-0.05618
H	2.38131	2.14546	0.42649
H	4.641	1.80339	0.97306
H	6.25589	0.1758	-2.07237
C	2.45937	-1.56908	-1.01285
H	2.5181	-2.41524	-1.72175
H	1.46301	-1.11881	-1.12223
O	2.66449	-2.00382	0.32033
H	1.95319	-2.61052	0.55255
C	2.03137	0.88517	-2.80055
H	1.13511	0.26689	-2.67843
H	1.93955	1.35337	-3.78838
C	2.03249	1.95378	-1.71497
H	1.06723	2.4742	-1.69791
H	2.79833	2.71229	-1.9349
C	3.287	0.01791	-2.7633
H	3.21159	-0.79947	-3.49425
H	4.15834	0.61496	-3.06941

$$\Delta E_{\text{solv}} = -2164.8574466$$

$$\Delta G_{\text{correction}} = 0.472831$$

⁴a1-ts

Charge = 0 Multiplicity = 4

C	-2.14599	2.85543	-0.3424
N	-2.42063	1.5353	-0.59192
C	-3.34323	1.52269	-1.60407
C	-3.65226	2.86609	-2.00468
C	-2.90058	3.69048	-1.23324
Fe	-1.61456	-0.03877	0.31089
O	-0.24092	0.03661	-0.78836
C	-3.8802	0.38676	-2.18229
C	-3.51146	-0.91515	-1.87995
N	-2.60661	-1.27292	-0.92103
C	-2.44622	-2.6304	-1.0329
C	-3.29112	-3.13821	-2.07586
C	-3.96157	-2.07673	-2.59207
C	-1.61557	-3.41038	-0.24645
C	-0.85317	-2.95445	0.8212
N	-0.76811	-1.65121	1.22332
C	-0.00063	-1.64089	2.35395
C	0.42295	-2.97384	2.66978
C	-0.09396	-3.79018	1.70984
C	0.36775	-0.50548	3.06091
C	0.04573	0.79609	2.72105
N	-0.71976	1.174	1.64605
C	-0.67944	2.53746	1.608
C	0.11612	3.03841	2.69205
C	0.55496	1.95888	3.38911
C	-1.32577	3.32583	0.66619
S	-3.29848	-0.22929	1.88545
H	-3.81741	-1.40545	1.47559
H	1.18519	1.93486	4.27016
H	0.30241	4.08819	2.88605
H	-1.20644	4.40302	0.75093
H	-2.86249	4.77331	-1.24091
H	-4.35663	3.12836	-2.78513
H	-4.61067	0.52747	-2.97474
H	-4.68652	-2.06323	-3.39721
H	-3.35524	-4.18112	-2.36305
H	-1.5943	-4.47751	-0.4535
H	-0.00058	-4.86616	1.61889
H	1.0453	-3.23956	3.51589
H	0.99804	-0.64834	3.93474
H	4.24632	-2.15586	-1.05264
C	4.26313	-1.31441	-1.75511
C	3.16318	-0.31507	-1.32977
C	5.66042	-0.72068	-1.7583
H	4.01058	-1.72787	-2.74037
C	3.62591	0.56456	-0.18607

C	6.00837	-0.10241	-0.42041
H	6.41683	-1.46912	-2.01269
C	2.6097	1.54994	0.28656
C	4.90283	0.59489	0.23989
O	7.14207	-0.10669	0.02537
H	1.66745	1.0587	0.55906
H	2.96612	2.08548	1.17272
H	5.18318	1.24196	1.07147
H	5.74915	0.07123	-2.51641
C	1.98195	-1.17581	-0.89715
H	1.64069	-1.86184	-1.6919
H	0.86271	-0.50813	-0.7568
O	2.26312	-1.80567	0.29022
H	1.60169	-2.48899	0.473
C	1.87192	1.78595	-2.12011
H	0.85411	1.42212	-1.94756
H	1.80984	2.48084	-2.96653
C	2.34419	2.52338	-0.87336
H	1.59678	3.26604	-0.56927
H	3.27005	3.079	-1.08176
C	2.7788	0.61694	-2.5031
H	2.3131	0.01908	-3.2992
H	3.71599	1.00172	-2.92934

$$\Delta E_{\text{solv}} = -2164.83226528$$

$$\Delta G_{\text{correction}} = 0.469263$$

4a2

Charge = 0 Multiplicity = 4

C	-2.34732	2.85392	-0.35141
N	-2.61783	1.52622	-0.54231
C	-3.64318	1.46907	-1.44656
C	-4.02093	2.79539	-1.84393
C	-3.21005	3.65283	-1.17472
Fe	-1.70359	-0.01491	0.33315
O	-0.44582	0.0276	-0.96595
C	-4.22272	0.30915	-1.92836
C	-3.81246	-0.97745	-1.61738
N	-2.8133	-1.29781	-0.7408
C	-2.64839	-2.65589	-0.82362
C	-3.59137	-3.20534	-1.75427
C	-4.32068	-2.16666	-2.23718
C	-1.72451	-3.40016	-0.10985
C	-0.84686	-2.89772	0.84003
N	-0.71169	-1.57574	1.17016
C	0.15377	-1.52581	2.23022
C	0.59546	-2.84725	2.56187
C	-0.01119	-3.69883	1.68877
C	0.57347	-0.36865	2.86613
C	0.19881	0.91622	2.51636
N	-0.68006	1.24684	1.51497
C	-0.6755	2.6124	1.43589
C	0.21533	3.15724	2.41806
C	0.74714	2.10691	3.09545
C	-1.43366	3.36498	0.55314
S	-3.22676	-0.11966	2.03572
H	-3.89792	-1.22153	1.64138
H	1.46649	2.1202	3.90557
H	0.39867	4.21543	2.56221
H	-1.32885	4.44565	0.6013
H	-3.19555	4.73563	-1.21075
H	-4.80917	3.02436	-2.55117
H	-5.03303	0.41524	-2.64473
H	-5.12184	-2.1861	-2.96634
H	-3.67259	-4.25794	-1.99833
H	-1.72019	-4.47497	-0.2722
H	0.06498	-4.77888	1.63852
H	1.29336	-3.08136	3.35678
H	1.28353	-0.47718	3.68132
H	4.72773	-2.10603	-0.59395
C	4.78152	-1.39513	-1.4268
C	3.52413	-0.50036	-1.36409
C	6.08648	-0.62494	-1.32359
H	4.75013	-1.99442	-2.34607
C	3.67922	0.59562	-0.32248

C	6.12881	0.24445	-0.08447
H	6.95439	-1.2913	-1.31874
C	2.47738	1.46492	-0.1563
C	4.85454	0.87216	0.27362
O	7.16292	0.47395	0.51779
H	1.59937	0.87514	0.13203
H	2.63816	2.2052	0.63475
H	4.91382	1.66846	1.01634
H	6.21855	0.03879	-2.19093
C	2.35512	-1.38275	-1.0248
H	1.91075	-1.9928	-1.81965
H	0.34674	-0.51244	-0.79477
O	2.45264	-1.95791	0.2059
H	1.74612	-2.6041	0.34231
C	2.06794	1.16432	-2.64576
H	1.13389	0.60327	-2.53337
H	1.97982	1.70367	-3.59675
C	2.18202	2.15817	-1.49591
H	1.25543	2.73755	-1.40867
H	2.98794	2.87764	-1.70162
C	3.25133	0.20522	-2.7116
H	3.09003	-0.55467	-3.48906
H	4.16115	0.74788	-3.00375

$$\Delta E_{\text{solv}} = -2164.86794131$$

$$\Delta G_{\text{correction}} = 0.471229$$

4a3

Charge = 0 Multiplicity = 4

C	-2.19708	-2.64185	-0.80424
N	-1.6964	-1.86453	0.21032
C	-1.36329	-2.73738	1.21744
C	-1.63441	-4.08588	0.81723
C	-2.14785	-4.02672	-0.43961
Fe	-1.7166	0.17115	0.30193
O	0.50044	-0.257	-0.75997
C	-0.82077	-2.36909	2.43691
C	-0.519	-1.07138	2.81969
N	-0.71641	0.0537	2.0504
C	-0.23845	1.10475	2.80008
C	0.27072	0.63079	4.0487
C	0.09359	-0.71877	4.06245
C	-0.21936	2.43067	2.39492
C	-0.68635	2.90077	1.17953
N	-1.26554	2.12987	0.20519
C	-1.59536	2.99564	-0.80389
C	-1.20085	4.33212	-0.46504
C	-0.63458	4.27338	0.76591
C	-2.22542	2.6432	-1.98356
C	-2.58425	1.35514	-2.34546
N	-2.37865	0.23376	-1.58426
C	-2.79557	-0.82307	-2.35233
C	-3.29708	-0.3531	-3.60895
C	-3.16796	0.99964	-3.60377
C	-2.70967	-2.15932	-1.99625
S	-3.88941	0.38717	1.24088
H	-3.5353	0.48172	2.53922
H	-3.43073	1.70523	-4.38301
H	-3.68924	-0.98988	-4.39318
H	-3.0815	-2.88911	-2.71094
H	-2.4816	-4.84273	-1.06981
H	-1.45514	-4.96013	1.4321
H	-0.60717	-3.16111	3.15029
H	0.35623	-1.42452	4.84187
H	0.70646	1.26059	4.81546
H	0.20194	3.15705	3.08513
H	-0.21555	5.0796	1.35616
H	-1.34499	5.19726	-1.10115
H	-2.4399	3.43847	-2.69272
H	3.47666	1.90325	0.30311
C	3.74214	0.91618	0.6992
C	2.91056	-0.13812	-0.05803
C	5.2431	0.73783	0.57485
H	3.43062	0.92055	1.75257
C	3.56822	-0.55602	-1.35374

C	5.66531	0.69512	-0.87742
H	5.79318	1.53283	1.08571
C	2.88731	-1.65866	-2.10544
C	4.76957	-0.08541	-1.74218
O	6.70667	1.17665	-1.28178
C	2.92669	-2.90999	-1.21612
H	1.843	-1.41117	-2.33303
H	3.39837	-1.84763	-3.05518
H	5.18843	-0.38429	-2.7039
H	3.97734	-3.18289	-1.0457
H	2.46793	-3.75911	-1.73495
H	5.56776	-0.20706	1.03655
C	1.55593	0.58774	-0.31825
H	1.26155	1.06113	0.62909
H	0.52509	-1.08795	-0.26858
O	1.65053	1.62783	-1.2262
H	1.91682	1.25938	-2.0792
C	2.23344	-2.66854	0.11775
H	2.3888	-3.52385	0.7864
H	1.14591	-2.66659	-0.04307
C	2.71824	-1.39756	0.82603
H	2.05617	-1.14855	1.66876
H	3.69371	-1.6173	1.28126

$$\Delta E_{\text{solv}} = -2164.97446686$$

$$\Delta G_{\text{correction}} = 0.474432$$

3. Coordinates of all stationary points in Fig. 5

²ferric-peroxo

Charge = 0 Multiplicity = 2

C	1.87395	-2.40519	-0.13099
N	1.74307	-1.04121	-0.10295
C	3.02029	-0.54343	-0.11397
C	3.97046	-1.61486	-0.1662
C	3.25889	-2.77066	-0.18018
Fe	0.03565	0.01274	0.0953
O	0.02258	-0.02804	-2.06011
C	3.35374	0.79808	-0.07879
C	2.44755	1.84319	-0.0502
N	1.07925	1.71167	-0.04464
C	0.58028	2.99186	-0.06427
C	1.65152	3.93844	-0.07608
C	2.8095	3.22601	-0.06391
C	-0.76198	3.3283	-0.08281
C	-1.80898	2.42504	-0.06438
N	-1.67666	1.0612	-0.02907
C	-2.95359	0.56454	0.03567
C	-3.90466	1.63596	0.02017
C	-3.19446	2.79068	-0.04556
C	-3.28548	-0.77516	0.10948
C	-2.37851	-1.82039	0.10037
N	-1.01137	-1.68863	0.03819
C	-0.51345	-2.96953	-0.00246
C	-1.58371	-3.91573	0.04748
C	-2.74003	-3.20293	0.11495
C	0.82645	-3.30719	-0.08691
S	0.13687	0.07989	2.42135
H	-0.30627	-1.17147	2.6587
H	-3.75795	-3.57161	0.1585
H	-1.45483	-4.99136	0.02545
H	1.07385	-4.36513	-0.11123
H	3.62561	-3.78967	-0.21463
H	5.04569	-1.48309	-0.18787
H	4.41016	1.05278	-0.08448
H	3.8283	3.59475	-0.07156
H	1.52151	5.01397	-0.09411
H	-1.01194	4.38569	-0.10151
H	-3.56208	3.80953	-0.0735
H	-4.97956	1.50471	0.05601
H	-4.34069	-1.02922	0.16192
O	-1.04199	-0.24358	-2.65242

$\Delta E_{\text{solv}} = -1660.95093591$

$\Delta G_{\text{correction}} = 0.234765$

⁴ferric-peroxo

Charge = 0 Multiplicity = 4

C	-0.28946	-3.01035	-0.08064
N	0.56048	-1.92978	-0.10315
C	1.82574	-2.45802	-0.13178
C	1.77024	-3.88764	-0.16119
C	0.45607	-4.23065	-0.13089
Fe	0.06262	-0.00139	0.08826
O	-0.19298	-0.06401	-2.0556
C	2.99732	-1.72033	-0.11566
C	3.06909	-0.34197	-0.06937
N	1.98507	0.50427	-0.03777
C	2.5164	1.77272	-0.04249
C	3.94883	1.71866	-0.06856
C	4.2916	0.40687	-0.0851
C	1.77791	2.93991	-0.05189
C	0.39547	3.00745	-0.05434
N	-0.44807	1.92477	-0.04492
C	-1.7189	2.44943	0.00141
C	-1.66763	3.87934	-0.01357
C	-0.35467	4.22589	-0.04645
C	-2.88637	1.71297	0.07905
C	-2.96174	0.33102	0.13013
N	-1.88336	-0.51297	0.10726
C	-2.41006	-1.77881	0.10015
C	-3.84278	-1.72804	0.15165
C	-4.18602	-0.41551	0.16995
C	-1.66814	-2.94351	0.01038
S	0.1347	-0.02644	2.27559
H	-1.13098	-0.40133	2.56285
H	-5.17597	0.02443	0.19278
H	-4.49066	-2.59657	0.1562
H	-2.21257	-3.88453	0.01401
H	0.01625	-5.22094	-0.13278
H	2.63716	-4.53684	-0.19456
H	3.93456	-2.27045	-0.14
H	5.28151	-0.03278	-0.1153
H	4.59682	2.58699	-0.08209
H	2.32452	3.87947	-0.0573
H	0.08208	5.21743	-0.05938
H	-2.53666	4.52621	0.00768
H	-3.8223	2.26557	0.10305
O	-1.20242	0.24177	-2.68865

$\Delta E_{\text{solv}} = -1660.97022846$

$\Delta G_{\text{correction}} = 0.23522$

19-OH

Charge = 0 Multiplicity = 1

H	1.24576	2.01568	0.11315
C	0.92493	1.28968	0.86949
C	-0.35938	0.62538	0.35558
C	2.0631	0.32028	1.13069
H	0.69288	1.86926	1.77325
C	-0.05483	-0.4685	-0.64809
C	2.36329	-0.537	-0.08045
H	2.97876	0.83474	1.43598
C	-1.25627	-1.13363	-1.23928
C	1.18815	-0.93931	-0.85879
O	3.48456	-0.9364	-0.33853
C	-2.03932	-1.80039	-0.09787
H	-1.8957	-0.40671	-1.75807
H	-0.95724	-1.87716	-1.9851
H	1.35771	-1.72664	-1.59382
H	-1.42163	-2.60904	0.31702
H	-2.94613	-2.27754	-0.4875
H	1.81318	-0.36471	1.95513
C	-1.21113	1.72288	-0.29089
H	-1.31637	2.54747	0.4359
H	-2.22587	1.36305	-0.51561
O	-0.56071	2.14994	-1.47079
H	-1.05907	2.88317	-1.84225
C	-2.3893	-0.81018	1.00654
H	-2.85002	-1.33721	1.8504
H	-3.16108	-0.11836	0.64449
C	-1.17277	-0.02735	1.49731
H	-1.47878	0.74694	2.21473
H	-0.50603	-0.7024	2.05135

$\Delta E_{\text{solv}} = -579.023497485$

$\Delta G_{\text{correction}} = 0.217473$

²b1

Charge = 0 Multiplicity = 2

C	-3.72028	0.41871	-1.63148
N	-2.96499	-0.40779	-0.83578
C	-3.40838	-1.6829	-1.07777
C	-4.47272	-1.65558	-2.03356
C	-4.6789	-0.35159	-2.36151
Fe	-1.55458	0.15361	0.45322
O	-0.20785	-0.34201	-1.07907
C	-2.9138	-2.82811	-0.47428
C	-1.96877	-2.84933	0.53691
N	-1.33477	-1.7446	1.05045
C	-0.63057	-2.18767	2.14343
C	-0.79279	-3.6016	2.29218
C	-1.60437	-4.01537	1.2841
C	0.15389	-1.38971	2.95765
C	0.43683	-0.05674	2.71247
N	-0.05174	0.66885	1.64876
C	0.6095	1.87457	1.67853
C	1.5264	1.90524	2.77539
C	1.39528	0.72112	3.43407
C	0.38306	2.93273	0.81483
C	-0.64683	2.98523	-0.10779
N	-1.55094	1.98068	-0.34158
C	-2.45984	2.48616	-1.2365
C	-2.1202	3.83697	-1.56876
C	-0.98325	4.13837	-0.88844
C	-3.50793	1.77668	-1.79628
S	-3.16012	0.66424	2.02394
H	-2.453	1.59669	2.69548
H	-0.41914	5.06326	-0.88978
H	-2.68051	4.46078	-2.25492
H	-4.16721	2.3083	-2.47702
H	-5.39839	0.06144	-3.05832
H	-4.99422	-2.53218	-2.39909
H	-3.3485	-3.7783	-0.77264
H	-1.9541	-5.01787	1.06882
H	-0.33037	-4.19522	3.07167
H	0.633	-1.85761	3.81351
H	1.92986	0.37638	4.31163
H	2.19095	2.7335	2.98813
H	1.04352	3.79054	0.89719
O	-0.39207	0.19415	-2.19735
H	3.0216	-0.3889	1.65615
C	3.8924	-0.44766	0.9898
C	3.42972	-0.9777	-0.38151
C	4.54416	0.92231	0.9601
H	4.5632	-1.1855	1.44858

C	2.98216	0.13878	-1.29699
C	4.57511	-1.75515	-1.06693
C	3.65361	1.9363	0.27607
H	4.78834	1.27903	1.96565
C	2.64805	-0.25334	-2.70182
C	2.98828	1.43781	-0.92393
C	4.30446	-2.13278	-2.51799
H	4.79733	-2.65021	-0.46959
H	5.48188	-1.13176	-1.02132
O	3.57412	3.09853	0.64947
C	3.87295	-0.9244	-3.33446
H	1.81888	-0.96519	-2.73004
H	2.33308	0.62438	-3.27572
H	2.58216	2.19673	-1.59471
H	5.20471	-2.58415	-2.95303
H	3.51994	-2.89465	-2.55687
H	4.69442	-0.19514	-3.39311
H	3.64382	-1.21239	-4.36696
O	1.64396	-2.66043	-1.05327
H	0.84922	-2.17999	-1.31462
H	5.49313	0.89237	0.40407
C	2.24389	-1.91568	-0.01934
H	1.48951	-1.31183	0.49938
H	2.63312	-2.64039	0.71248

$$\Delta E_{\text{solv}} = -2239.99998606$$

$$\Delta G_{\text{correction}} = 0.477928$$

²b1-ts

Charge = 0 Multiplicity = 2

C	-3.54188	-0.3047	-2.12247
N	-2.81182	-0.85111	-1.10206
C	-2.95912	-2.20659	-1.21025
C	-3.79308	-2.52231	-2.33482
C	-4.16109	-1.34228	-2.89565
Fe	-1.76906	0.14112	0.29187
O	-0.36064	-0.03581	-0.98871
C	-2.42335	-3.14673	-0.34463
C	-1.67444	-2.86889	0.78666
N	-1.26952	-1.61077	1.17885
C	-0.62679	-1.78404	2.38732
C	-0.59333	-3.17153	2.73121
C	-1.23076	-3.84381	1.7347
C	-0.05081	-0.7632	3.12575
C	-0.02644	0.57325	2.75558
N	-0.60328	1.09265	1.62436
C	-0.3376	2.43818	1.65156
C	0.47004	2.75931	2.79021
C	0.65159	1.60424	3.48358
C	-0.8401	3.37318	0.76299
C	-1.7296	3.10968	-0.26499
N	-2.2243	1.87513	-0.58531
C	-3.03378	2.0617	-1.67322
C	-3.08167	3.45384	-2.02121
C	-2.26546	4.10258	-1.15309
C	-3.66452	1.05066	-2.37982
S	-3.56378	0.26082	1.66402
H	-4.27708	1.19601	1.00267
H	-2.03047	5.15937	-1.10858
H	-3.65575	3.86414	-2.84346
H	-4.27994	1.34337	-3.22674
H	-4.79285	-1.17355	-3.75964
H	-4.06345	-3.52687	-2.63804
H	-2.64859	-4.19108	-0.54522
H	-1.40491	-4.90984	1.64819
H	-0.13298	-3.57335	3.62608
H	0.43435	-1.03308	4.06041
H	1.19218	1.4509	4.41037
H	0.82407	3.75424	3.03309
H	-0.53663	4.40719	0.90544
O	0.65686	0.8401	-0.93429
H	3.32407	1.26917	1.11242
C	4.10211	0.5008	0.9911
C	3.58758	-0.55077	-0.00792
C	5.38365	1.18619	0.56113
H	4.21342	0.03527	1.97933

C	3.74806	-0.07677	-1.4452
C	4.36447	-1.89256	0.11385
C	5.24284	1.81086	-0.81115
H	5.69222	1.95591	1.2738
C	3.24621	-1.02384	-2.484
C	4.44616	1.03074	-1.76195
C	4.02583	-2.90882	-0.97268
H	4.19409	-2.31869	1.11147
H	5.43492	-1.64486	0.06521
O	5.81911	2.83604	-1.12506
C	4.07659	-2.313	-2.37459
H	2.1843	-1.25088	-2.33712
H	3.34925	-0.58319	-3.4807
H	4.51834	1.34304	-2.8038
H	4.72335	-3.7522	-0.90019
H	3.03142	-3.32483	-0.78858
H	5.11687	-2.07866	-2.64201
H	3.72847	-3.04582	-3.11118
O	1.4554	-1.76726	-0.15874
H	0.52055	-1.72901	0.13166
H	6.21434	0.46713	0.51131
C	2.13146	-0.73119	0.3558
H	1.42747	0.36801	-0.28406
H	1.8551	-0.47105	1.38571

$$\Delta E_{\text{solv}} = -2239.973679$$

$$\Delta G_{\text{correction}} = 0.471799$$

4b1

Charge = 0 Multiplicity = 4

C	0.27167	-1.81055	-2.27062
N	0.3039	-0.51387	-1.81436
C	-0.59782	0.17373	-2.58399
C	-1.23143	-0.70823	-3.51579
C	-0.70356	-1.94443	-3.30977
Fe	1.55477	0.26628	-0.45325
O	0.25787	-0.55497	0.93924
C	-0.8852	1.52196	-2.45752
C	-0.35695	2.35156	-1.49045
N	0.58598	1.9818	-0.55306
C	0.7297	3.0789	0.26804
C	-0.13399	4.13842	-0.15957
C	-0.79796	3.69314	-1.25612
C	1.60052	3.15903	1.33704
C	2.49001	2.16573	1.70971
N	2.59521	0.9392	1.10644
C	3.64222	0.30356	1.73454
C	4.18876	1.14468	2.75522
C	3.46696	2.29535	2.7476
C	4.08832	-0.97305	1.45271
C	3.52336	-1.83303	0.5232
N	2.47337	-1.52017	-0.29612
C	2.14676	-2.68415	-0.94188
C	3.03223	-3.73914	-0.5453
C	3.8964	-3.20661	0.35702
C	1.10736	-2.828	-1.84581
S	3.01973	0.89897	-1.9716
H	3.67876	-0.26231	-2.1697
H	4.70194	-3.6961	0.89125
H	2.98176	-4.75693	-0.91335
H	0.96109	-3.81066	-2.28689
H	-0.92998	-2.87026	-3.82527
H	-1.99052	-0.40563	-4.22796
H	-1.6398	1.94283	-3.11471
H	-1.5653	4.18885	-1.83594
H	-0.21493	5.09999	0.33342
H	1.61722	4.08691	1.90269
H	3.58338	3.16957	3.37696
H	5.01946	0.87329	3.39572
H	4.9215	-1.35028	2.04017
O	0.57063	-1.4128	1.79851
H	-3.09424	-1.23644	-1.4873
C	-3.95431	-1.07357	-0.82178
C	-3.45834	-1.1449	0.63194
C	-4.60608	0.24048	-1.20488
H	-4.63527	-1.9141	-1.00886

C	-2.85858	0.1701	1.07022
C	-4.62204	-1.47282	1.5974
C	-3.70746	1.4182	-0.90286
H	-4.88526	0.26784	-2.263
C	-2.38945	0.23175	2.48788
C	-2.91066	1.2889	0.31333
C	-4.28267	-1.32331	3.07869
H	-4.97813	-2.49124	1.38888
H	-5.46091	-0.80404	1.35125
O	-3.71989	2.43531	-1.5827
C	-3.61313	0.00901	3.38852
H	-1.64963	-0.54334	2.70635
H	-1.91399	1.1979	2.69298
H	-2.44134	2.20686	0.67023
H	-5.19907	-1.42925	3.67257
H	-3.61897	-2.13809	3.37894
H	-4.3211	0.83605	3.23264
H	-3.31449	0.0542	4.44243
O	-1.9727	-2.80212	1.8385
H	-1.10337	-2.42733	2.03172
H	-5.53972	0.39339	-0.64328
C	-2.41445	-2.29472	0.60287
H	-1.56763	-1.97773	-0.0241
H	-2.89883	-3.13081	0.0761

$$\Delta E_{\text{solv}} = -2240.01544763$$

$$\Delta G_{\text{correction}} = 0.476042$$

4b1-ts

Charge = 0 Multiplicity = 4

C	0.26184	1.37343	-2.61226
N	0.81499	1.48338	-1.36042
C	0.78537	2.81464	-1.05002
C	0.17923	3.55881	-2.1137
C	-0.13061	2.66733	-3.08996
Fe	1.62343	0.01113	-0.2513
O	-0.1105	-0.17176	0.46658
C	1.29197	3.37545	0.10937
C	1.9573	2.68683	1.10549
N	2.19828	1.33528	1.11843
C	2.87711	1.08567	2.28486
C	3.08183	2.30585	3.00849
C	2.50257	3.2957	2.28334
C	3.27011	-0.16384	2.72802
C	2.99966	-1.35779	2.08085
N	2.31981	-1.47623	0.90032
C	2.27282	-2.81741	0.62263
C	2.92612	-3.55778	1.66188
C	3.3828	-2.65171	2.564
C	1.69596	-3.38905	-0.49652
C	1.11089	-2.69676	-1.54659
N	1.02395	-1.33492	-1.64239
C	0.39497	-1.07454	-2.83082
C	0.09022	-2.30189	-3.50553
C	0.52937	-3.31004	-2.7046
C	0.06823	0.18912	-3.30078
S	3.60326	0.21536	-1.30399
H	3.29402	-0.3745	-2.47704
H	0.48166	-4.37896	-2.87839
H	-0.39996	-2.37	-4.46988
H	-0.40452	0.25173	-4.27803
H	-0.59948	2.85208	-4.04967
H	0.00951	4.62826	-2.09248
H	1.15669	4.44479	0.24397
H	2.43915	4.35291	2.51169
H	3.59363	2.37657	3.96096
H	3.81171	-0.21435	3.66894
H	3.92965	-2.82869	3.48256
H	3.02416	-4.63694	1.6799
H	1.72381	-4.47357	-0.57055
O	-0.4844	-1.38707	0.92672
H	-1.8478	0.16183	-1.20873
C	-2.91815	0.3937	-1.155
C	-3.5247	-0.4143	0.00714
C	-3.05919	1.89601	-1.01205
H	-3.35294	0.04428	-2.10182

C	-3.26227	0.26317	1.34497
C	-5.06605	-0.54497	-0.13397
C	-2.50259	2.38866	0.30566
H	-2.55929	2.42522	-1.82836
C	-3.80366	-0.46124	2.53347
C	-2.74353	1.5012	1.44457
C	-5.76743	-1.14427	1.08264
H	-5.29763	-1.12488	-1.03766
H	-5.45489	0.46801	-0.31539
O	-1.98663	3.48723	0.4272
C	-5.33346	-0.49928	2.39368
H	-3.41441	-1.48494	2.58747
H	-3.51307	0.04832	3.45795
H	-2.55603	1.93289	2.42801
H	-6.85239	-1.03998	0.95773
H	-5.57036	-2.21877	1.12537
H	-5.70948	0.53248	2.44504
H	-5.77755	-1.03007	3.24385
O	-3.39473	-2.80541	0.62017
H	-2.94647	-3.62064	0.3679
H	-4.11597	2.20088	-1.05019
C	-2.83212	-1.76322	-0.08226
H	-1.51778	-1.5405	0.49905
H	-2.53204	-2.03984	-1.10353

$$\Delta E_{\text{solv}} = -2239.97269273$$

$$\Delta G_{\text{correction}} = 0.470568$$

4b2

Charge = 0 Multiplicity = 4

C	-0.22867	0.56217	-2.80157
N	0.59107	0.93799	-1.77039
C	0.70286	2.30247	-1.84773
C	-0.09104	2.79742	-2.93399
C	-0.65051	1.71695	-3.53883
Fe	1.50211	-0.25875	-0.4446
O	0.21112	0.29228	0.78167
C	1.5235	3.08461	-1.0521
C	2.42585	2.60211	-0.11808
N	2.59768	1.28544	0.20255
C	3.58495	1.24183	1.14584
C	4.07916	2.56622	1.3974
C	3.34754	3.41148	0.62785
C	3.98006	0.10897	1.83806
C	3.36996	-1.13129	1.75646
N	2.3353	-1.45316	0.92113
C	1.96964	-2.73267	1.23628
C	2.79791	-3.23247	2.29575
C	3.67728	-2.24554	2.60572
C	0.98696	-3.4632	0.58925
C	0.28165	-3.03467	-0.52438
N	0.40706	-1.79935	-1.11237
C	-0.389	-1.82184	-2.23042
C	-1.02325	-3.09983	-2.35224
C	-0.62491	-3.84494	-1.28002
C	-0.66338	-0.73017	-3.04018
S	3.17991	-0.70571	-1.89605
H	3.00998	-2.04387	-1.9564
H	-0.88791	-4.86794	-1.03603
H	-1.69379	-3.3801	-3.15685
H	-1.3224	-0.89003	-3.88952
H	-1.30721	1.69079	-4.40049
H	-0.17954	3.84301	-3.20487
H	1.49714	4.1593	-1.21189
H	3.41375	4.49067	0.55942
H	4.86899	2.80565	2.09936
H	4.78496	0.22126	2.55979
H	4.46029	-2.2507	3.35463
H	2.71208	-4.22131	2.73051
H	0.79183	-4.47033	0.94833
O	0.66558	0.44767	2.08956
H	-1.75486	1.39015	-0.74267
C	-2.75069	1.70901	-0.4198
C	-3.51202	0.48521	0.13864
C	-2.55545	2.83531	0.58771
H	-3.25863	2.06537	-1.32438

C	-3.30874	0.31454	1.63369
C	-5.01286	0.56217	-0.19598
C	-1.82331	2.26703	1.77585
H	-1.9764	3.65805	0.15873
C	-4.11154	-0.77564	2.26769
C	-2.4301	1.0732	2.33165
C	-5.88617	-0.46572	0.51715
H	-5.13671	0.48587	-1.28417
H	-5.35039	1.5735	0.07683
O	-0.79281	2.77209	2.22793
C	-5.59989	-0.52085	2.01125
H	-3.84632	-1.75177	1.83739
H	-3.89575	-0.82997	3.34014
H	-2.15379	0.80142	3.35124
H	-6.94254	-0.22862	0.34131
H	-5.71765	-1.45586	0.08181
H	-5.88849	0.42792	2.48675
H	-6.20377	-1.30001	2.49107
O	-3.47706	-1.87532	-0.6118
H	-2.82639	-2.55156	-0.85625
H	-3.52145	3.24329	0.91638
C	-2.8102	-0.7087	-0.43109
H	0.22263	1.29308	2.35108
H	-1.73695	-0.77738	-0.24929

$$\Delta E_{\text{solv}} = -2239.98956937$$

$$\Delta G_{\text{correction}} = 0.476238$$

4. Coordinates of all stationary points in Fig. 7 and Fig. S1

²c1

Charge = 0 Multiplicity = 2

C	-0.7291	-0.70814	1.86602
N	0.38337	-1.13146	1.18055
C	0.38575	-2.50047	1.28076
C	-0.7726	-2.94523	1.99572
C	-1.45437	-1.83295	2.37254
Fe	1.83351	0.02495	0.39906
O	0.86413	-0.32525	-1.36958
C	1.39927	-3.33043	0.83677
C	2.58968	-2.90414	0.2739
N	2.92297	-1.59692	0.00759
C	4.17783	-1.6328	-0.55315
C	4.64787	-2.9804	-0.61446
C	3.6586	-3.76918	-0.11405
C	4.85782	-0.53821	-1.05797
C	4.35706	0.74945	-1.11108
N	3.13787	1.1448	-0.62282
C	3.04229	2.48723	-0.89092
C	4.21244	2.93561	-1.58418
C	5.03258	1.86113	-1.7106
C	1.99813	3.30734	-0.50766
C	0.90806	2.9056	0.24483
N	0.6786	1.6237	0.68915
C	-0.47417	1.69027	1.44206
C	-0.97038	3.03048	1.47141
C	-0.1211	3.77881	0.71455
C	-1.11386	0.611	2.02491
S	2.92349	0.2753	2.39153
H	2.20293	1.3078	2.87501
H	-0.17568	4.83755	0.49052
H	-1.87913	3.32917	1.98209
H	-2.01131	0.81865	2.6012
H	-2.37638	-1.76181	2.93683
H	-1.01209	-3.98335	2.19277
H	1.2722	-4.39929	0.98549
H	3.64426	-4.84757	-0.01063
H	5.61084	-3.27801	-1.0118
H	5.84393	-0.71188	-1.47983
H	6.01022	1.80847	-2.17453
H	4.37677	3.95363	-1.91637
H	2.05469	4.35609	-0.78583
H	-2.58123	1.99766	-0.83415
C	-3.59096	1.64659	-1.08521
C	-3.57779	0.09804	-1.163
C	-4.55107	2.24345	-0.06791

H	-3.78652	2.04543	-2.0853
C	-3.99765	-0.55901	0.13931
C	-4.54981	-0.37864	-2.268
C	-2.1087	-0.23556	-1.52158
C	-4.30121	1.62036	1.28153
H	-4.43889	3.32995	-0.00271
C	-4.19639	-2.04427	0.13229
C	-4.27666	0.15961	1.2453
C	-4.7391	-1.88767	-2.32171
H	-4.19057	0.00541	-3.22711
H	-5.52208	0.10407	-2.08246
O	-1.88902	0.30269	-2.79603
O	-4.15455	2.26064	2.31336
C	-5.18114	-2.43735	-0.97441
H	-3.24232	-2.54765	-0.04743
H	-4.56516	-2.3705	1.11231
H	-4.51828	-0.34887	2.18041
H	-5.47864	-2.13633	-3.0928
H	-3.79964	-2.36107	-2.62541
H	-6.17827	-2.04485	-0.72485
H	-5.28127	-3.52858	-1.00754
H	-0.93433	0.4034	-2.92068
O	-1.82797	-1.61393	-1.47136
H	-0.86474	-1.69263	-1.46119
H	-1.46105	0.27095	-0.78454
H	-5.59478	2.04198	-0.34905
O	0.90763	0.55396	-2.2776

$$\Delta E_{\text{solv}} = -2315.2320344$$

$$\Delta G_{\text{correction}} = 0.480176$$

²c1-ts

Charge = 0 Multiplicity = 2

C	-0.72317	-0.86369	1.87235
N	0.4128	-1.22204	1.19155
C	0.47944	-2.58916	1.25995
C	-0.66496	-3.10307	1.95223
C	-1.40322	-2.03219	2.34313
Fe	1.77179	0.01042	0.36483
O	0.81014	-0.30322	-1.24439
C	1.53777	-3.3587	0.80996
C	2.7037	-2.86542	0.25115
N	2.96665	-1.5427	-0.00872
C	4.21039	-1.50998	-0.59116
C	4.74968	-2.83244	-0.6686
C	3.81176	-3.67304	-0.15762
C	4.8222	-0.37928	-1.10155
C	4.25918	0.88419	-1.12702
N	3.03807	1.2165	-0.60417
C	2.87874	2.55863	-0.83512
C	4.01294	3.07274	-1.54335
C	4.87384	2.03722	-1.71477
C	1.81477	3.32622	-0.40182
C	0.76072	2.86605	0.37017
N	0.58431	1.56754	0.77628
C	-0.55286	1.5639	1.54878
C	-1.08817	2.88751	1.64708
C	-0.28173	3.6905	0.90047
C	-1.15656	0.43522	2.07916
S	2.85269	0.278	2.32212
H	2.00632	1.14866	2.90954
H	-0.37446	4.75454	0.71811
H	-1.99346	3.1368	2.18929
H	-2.05744	0.58514	2.66812
H	-2.33243	-2.01548	2.9
H	-0.85596	-4.15511	2.12712
H	1.46495	-4.43486	0.9421
H	3.85312	-4.7515	-0.06229
H	5.71959	-3.07695	-1.0848
H	5.80575	-0.49976	-1.54737
H	5.84276	2.03695	-2.19946
H	4.12793	4.10508	-1.85117
H	1.82491	4.38342	-0.65261
H	-2.50493	1.98629	-0.59708
C	-3.50221	1.67241	-0.92734
C	-3.49428	0.14552	-1.16773
C	-4.51175	2.16034	0.09996
H	-3.64759	2.17786	-1.88701
C	-3.96356	-0.64779	0.02987

C	-4.39069	-0.20735	-2.37683
C	-1.98653	-0.16242	-1.51958
C	-4.32477	1.39756	1.38618
H	-4.40611	3.23347	0.28547
C	-4.15833	-2.12197	-0.15019
C	-4.28269	-0.05182	1.19821
C	-4.60645	-1.69812	-2.59439
H	-3.95471	0.26288	-3.26578
H	-5.36479	0.27954	-2.21173
O	-1.59449	0.59604	-2.54386
O	-4.23712	1.92541	2.48594
C	-5.10543	-2.37813	-1.32825
H	-3.19771	-2.60365	-0.35443
H	-4.56093	-2.55639	0.77248
H	-4.55549	-0.65772	2.06401
H	-5.3238	-1.84661	-3.41094
H	-3.66718	-2.15887	-2.91492
H	-6.10617	-1.99876	-1.07296
H	-5.21838	-3.45747	-1.48306
H	-0.15768	0.62224	-2.56467
O	-1.75223	-1.54849	-1.6697
H	-0.78975	-1.64419	-1.70945
H	-1.40118	0.16407	-0.61706
H	-5.54043	1.9927	-0.25057
O	0.81575	0.67938	-2.18087

$$\Delta E_{\text{solv}} = -2315.20131509$$

$$\Delta G_{\text{correction}} = 0.478947$$

²c2

Charge = 0 Multiplicity = 2

C	-0.73677	-0.86217	1.76904
N	0.42868	-1.22314	1.14452
C	0.49524	-2.58894	1.23103
C	-0.6717	-3.09892	1.88764
C	-1.43179	-2.02636	2.22895
Fe	1.81241	0.00224	0.34785
O	0.84604	-0.23294	-1.23784
C	1.56361	-3.36146	0.80977
C	2.7358	-2.87799	0.25337
N	3.00376	-1.55995	-0.01477
C	4.24737	-1.53845	-0.59374
C	4.78033	-2.86528	-0.66779
C	3.8398	-3.69686	-0.14965
C	4.87471	-0.40917	-1.09014
C	4.3367	0.86575	-1.09213
N	3.11913	1.209	-0.56905
C	2.98958	2.55751	-0.76645
C	4.14179	3.06902	-1.44777
C	4.98158	2.02046	-1.64326
C	1.92558	3.33476	-0.34281
C	0.83505	2.88062	0.37875
N	0.63308	1.58195	0.7663
C	-0.54734	1.57538	1.4587
C	-1.09074	2.89985	1.53468
C	-0.23606	3.70757	0.85208
C	-1.18491	0.4389	1.9417
S	2.84985	0.25181	2.3285
H	1.99245	1.11155	2.91598
H	-0.31269	4.77395	0.67625
H	-2.02345	3.14835	2.02914
H	-2.1133	0.58651	2.48742
H	-2.38246	-2.00652	2.7481
H	-0.86483	-4.14912	2.07115
H	1.4872	-4.43642	0.95124
H	3.87518	-4.77478	-0.0462
H	5.74914	-3.11662	-1.08247
H	5.85823	-0.53811	-1.53419
H	5.95445	2.01301	-2.11986
H	4.28102	4.10701	-1.72519
H	1.95999	4.39543	-0.5777
H	-2.77794	2.08637	-0.62662
C	-3.75122	1.68335	-0.92909
C	-3.62259	0.15734	-1.15136
C	-4.77525	2.10278	0.11506
H	-3.96029	2.1619	-1.8912
C	-4.07423	-0.66727	0.03042

C	-4.41622	-0.26665	-2.40657
C	-2.06815	-0.04665	-1.41961
C	-4.50484	1.35559	1.3961
H	-4.73906	3.18081	0.29726
C	-4.19015	-2.15031	-0.1553
C	-4.41154	-0.09269	1.20434
C	-4.51112	-1.76918	-2.62244
H	-3.96726	0.23214	-3.27334
H	-5.43115	0.14823	-2.30033
O	-1.652	0.71798	-2.40868
O	-4.38785	1.8896	2.48868
C	-5.04788	-2.46908	-1.3834
H	-3.19504	-2.58373	-0.29486
H	-4.62098	-2.59932	0.74745
H	-4.65603	-0.71281	2.06839
H	-5.15767	-1.97338	-3.48464
H	-3.52204	-2.16657	-2.87196
H	-6.08315	-2.14751	-1.19568
H	-5.08799	-3.55409	-1.53342
H	-0.01658	0.77092	-2.53127
O	-1.72243	-1.40923	-1.48504
H	-0.75576	-1.42169	-1.57933
H	-1.59429	0.35812	-0.47984
H	-5.79535	1.86117	-0.2158
O	0.92113	0.77639	-2.18191

$$\Delta E_{\text{solv}} = -2315.21362732$$

$$\Delta G_{\text{correction}} = 0.481165$$

²c2-ts

Charge = 0 Multiplicity = 2

C	0.71866	0.74499	1.84921
N	-0.40398	1.16864	1.18607
C	-0.41068	2.53514	1.29291
C	0.75301	2.98048	2.0007
C	1.44731	1.86851	2.35545
Fe	-1.82022	0.02414	0.32803
O	-0.84187	0.22777	-1.25428
C	-1.42716	3.36314	0.84987
C	-2.60596	2.94337	0.25609
N	-2.93206	1.64282	-0.02988
C	-4.16351	1.68626	-0.6344
C	-4.62868	3.03841	-0.70769
C	-3.6594	3.81874	-0.16319
C	-4.83769	0.59311	-1.14935
C	-4.36261	-0.70719	-1.1553
N	-3.17072	-1.11179	-0.62033
C	-3.09495	-2.45994	-0.83818
C	-4.2597	-2.91189	-1.54001
C	-5.05084	-1.82489	-1.73051
C	-2.06564	-3.28635	-0.41962
C	-0.96475	-2.89098	0.31974
N	-0.71341	-1.60963	0.73818
C	0.44452	-1.67032	1.4631
C	0.93061	-3.01814	1.51906
C	0.06049	-3.77263	0.79561
C	1.11071	-0.57489	2.00148
S	-2.90726	-0.23248	2.29008
H	-2.07802	-1.11475	2.88411
H	0.09558	-4.8374	0.59768
H	1.84287	-3.31353	2.02621
H	2.01358	-0.77505	2.57317
H	2.37455	1.79651	2.91215
H	0.98563	4.01788	2.21016
H	-1.3038	4.43142	1.00809
H	-3.64468	4.89622	-0.05017
H	-5.57541	3.34048	-1.13928
H	-5.80619	0.77427	-1.6081
H	-6.01578	-1.76826	-2.21986
H	-4.43995	-3.93872	-1.83498
H	-2.14135	-4.34085	-0.67242
H	4.0527	-1.98786	-2.22815
C	4.45821	-1.52688	-1.32203
C	4.01148	-0.08069	-1.25467
C	4.08519	-2.33457	-0.09219
H	5.55221	-1.51534	-1.44075
C	4.37951	0.58761	0.00449

C	4.3012	0.67129	-2.54337
C	2.17577	-0.21466	-1.14122
C	4.25929	-1.58778	1.21321
H	3.03442	-2.65339	-0.14915
C	4.47692	2.08266	0.03823
C	4.52119	-0.15313	1.13896
C	4.26172	2.1883	-2.447
H	3.63121	0.29849	-3.3264
H	5.31271	0.36363	-2.85694
O	1.74368	-0.94916	-2.06889
O	4.13036	-2.15826	2.29071
C	5.05314	2.67334	-1.24318
H	3.45651	2.46969	0.17506
H	5.04482	2.3934	0.92325
H	4.75525	0.33271	2.08706
H	4.65942	2.62047	-3.37272
H	3.22436	2.5271	-2.36292
H	6.10911	2.38281	-1.34594
H	5.04363	3.76738	-1.18412
H	0.03624	-0.92238	-2.4038
O	1.76261	1.10767	-1.03224
H	0.83151	1.12242	-1.32876
H	2.20047	-0.66598	-0.1246
H	4.65481	-3.26784	-0.02626
O	-0.92325	-0.79482	-2.19869

$$\Delta E_{\text{solv}} = -2315.21253813$$

$$\Delta G_{\text{correction}} = 0.481165$$

²c3

Charge = 0 Multiplicity = 2

C	0.71862	0.74504	1.84926
N	-0.40403	1.16866	1.18609
C	-0.41076	2.53517	1.29294
C	0.75289	2.98053	2.00077
C	1.44721	1.86859	2.35554
Fe	-1.82021	0.02413	0.32802
O	-0.84184	0.22778	-1.25427
C	-1.42726	3.36314	0.84988
C	-2.60603	2.94334	0.25608
N	-2.9321	1.64278	-0.0299
C	-4.16354	1.68619	-0.63442
C	-4.62875	3.03833	-0.70771
C	-3.65949	3.81868	-0.16321
C	-4.8377	0.59303	-1.14937
C	-4.36258	-0.70726	-1.15533
N	-3.17067	-1.11183	-0.62036
C	-3.09485	-2.45998	-0.83823
C	-4.25959	-2.91195	-1.54007
C	-5.05076	-1.82498	-1.73056
C	-2.06552	-3.28635	-0.41967
C	-0.96465	-2.89096	0.3197
N	-0.71337	-1.60961	0.73818
C	0.44456	-1.67027	1.46311
C	0.93069	-3.01807	1.51906
C	0.06061	-3.77258	0.79558
C	1.1107	-0.57482	2.00151
S	-2.90728	-0.23253	2.29005
H	-2.07798	-1.11473	2.88411
H	0.09574	-4.83734	0.59763
H	1.84294	-3.31344	2.02622
H	2.01356	-0.77496	2.57323
H	2.37442	1.79661	2.91228
H	0.98547	4.01794	2.21024
H	-1.30392	4.43142	1.0081
H	-3.6448	4.89616	-0.05019
H	-5.57548	3.34038	-1.13931
H	-5.8062	0.77416	-1.60813
H	-6.0157	-1.76837	-2.2199
H	-4.4398	-3.93878	-1.83506
H	-2.14119	-4.34085	-0.6725
H	4.05269	-1.98797	-2.22798
C	4.45819	-1.52691	-1.32188
C	4.01144	-0.08072	-1.25463
C	4.08515	-2.33451	-0.09199
H	5.55218	-1.51537	-1.44059
C	4.37947	0.58767	0.00448

C	4.3012	0.67117	-2.54338
C	2.17577	-0.21465	-1.14122
C	4.25929	-1.58764	1.21336
H	3.03437	-2.65329	-0.14892
C	4.47687	2.08273	0.03811
C	4.52117	-0.15299	1.139
C	4.26175	2.18818	-2.44713
H	3.63123	0.29833	-3.3264
H	5.31271	0.36346	-2.85692
O	1.74369	-0.94925	-2.06881
O	4.13045	-2.15806	2.2909
C	5.05315	2.6733	-1.24333
H	3.45645	2.46975	0.17485
H	5.04472	2.39354	0.92314
H	4.75524	0.33292	2.08707
H	4.6595	2.62028	-3.37287
H	3.22441	2.52701	-2.36311
H	6.10912	2.38275	-1.34602
H	5.04365	3.76734	-1.18434
H	0.03628	-0.92241	-2.40376
O	1.7626	1.10771	-1.03244
H	0.8315	1.1224	-1.32896
H	2.20038	-0.66584	-0.12454
H	4.65473	-3.26781	-0.02601
O	-0.92321	-0.79482	-2.19867

$$\Delta E_{\text{solv}} = -2315.26292178$$

$$\Delta G_{\text{correction}} = 0.471928$$

²c3-ts

Charge = 0 Multiplicity = 2

C	4.0104	-0.16844	-0.30918
N	2.95528	0.70102	-0.24665
C	3.35016	1.8195	-0.92847
C	4.68383	1.64896	-1.43811
C	5.09782	0.41805	-1.04446
Fe	1.19082	0.39267	0.67857
O	0.56447	-0.13869	-1.07386
C	2.58017	2.96063	-1.08775
C	1.32324	3.16963	-0.54001
N	0.63238	2.26487	0.21839
C	-0.50556	2.9075	0.6273
C	-0.54581	4.23848	0.09148
C	0.58557	4.39783	-0.64111
C	-1.49577	2.3407	1.41321
C	-1.52027	1.02312	1.85119
N	-0.56432	0.08474	1.57548
C	-1.03124	-1.09417	2.10493
C	-2.30652	-0.88605	2.73194
C	-2.60502	0.43103	2.58493
C	-0.36279	-2.30524	2.06336
C	0.91621	-2.50126	1.5569
N	1.69686	-1.52563	1.00491
C	2.91118	-2.10631	0.75234
C	2.88487	-3.48983	1.13341
C	1.64134	-3.73891	1.62186
C	3.99864	-1.46819	0.17518
S	2.16377	1.05854	2.59211
H	1.21152	0.69947	3.48146
H	1.2459	-4.66756	2.01714
H	3.72208	-4.17239	1.04019
H	4.90303	-2.05654	0.03791
H	6.04702	-0.06866	-1.23645
H	5.22453	2.39002	-2.0153
H	3.01359	3.77809	-1.65935
H	0.9099	5.26866	-1.19872
H	-1.36055	4.93622	0.24002
H	-2.33974	2.97328	1.67968
H	-3.48143	0.96893	2.93089
H	-2.88031	-1.65694	3.23512
H	-0.85709	-3.16389	2.51265
H	-1.50732	-0.77129	-1.5804
C	-2.47692	-0.17895	-2.22497
C	-3.55323	-0.75531	-1.54416
C	-2.15084	1.28606	-2.07234
H	-2.23621	-0.63589	-3.19152
C	-4.25671	-0.02557	-0.52653

C	-3.9221	-2.17727	-1.84167
C	2.22693	-2.26653	-2.40935
C	-3.14434	2.08323	-1.26536
H	-1.17338	1.39143	-1.56069
C	-5.23811	-0.72482	0.37739
C	-4.03006	1.31669	-0.39203
C	-4.58517	-2.89035	-0.67307
H	-3.03721	-2.71943	-2.199
H	-4.61433	-2.17184	-2.69957
O	1.1767	-2.86682	-2.3085
O	-3.21239	3.30027	-1.3268
C	-5.74543	-2.05598	-0.15638
H	-4.72242	-0.89756	1.33351
H	-6.06664	-0.04752	0.61366
H	-4.62159	1.90311	0.31115
H	-4.91712	-3.88664	-0.9833
H	-3.85045	-3.04468	0.13024
H	-6.4656	-1.89026	-0.97027
H	-6.29389	-2.58603	0.62934
H	0.00075	-1.91007	-1.5067
O	3.35339	-2.82904	-2.83112
H	3.16403	-3.76614	-3.00278
H	2.36089	-1.20246	-2.17409
H	-1.99274	1.7734	-3.04008
O	-0.43404	-1.19537	-0.9721

$$\Delta E_{\text{solv}} = -2315.24293582$$

$$\Delta G_{\text{correction}} = 0.471013$$

²c4

Charge = 0 Multiplicity = 2

C	1.86944	-2.55809	1.23565
N	1.99478	-1.44151	0.45437
C	2.78163	-1.80613	-0.60431
C	3.16247	-3.18399	-0.485
C	2.60251	-3.64914	0.6615
Fe	1.03588	0.33533	0.7014
O	-0.19069	-0.19034	-0.27257
C	3.14854	-0.97211	-1.6495
C	2.81285	0.36335	-1.78346
N	2.03627	1.07509	-0.90211
C	1.93744	2.33667	-1.42267
C	2.67863	2.43002	-2.64606
C	3.21821	1.2053	-2.87189
C	1.18624	3.36003	-0.86971
C	0.39138	3.26188	0.26219
N	0.23922	2.13638	1.0266
C	-0.66975	2.4632	1.99752
C	-1.09442	3.82328	1.84306
C	-0.43041	4.32109	0.76737
C	-1.10819	1.60662	2.99498
C	-0.69005	0.29847	3.18055
N	0.21436	-0.35449	2.38909
C	0.34703	-1.60331	2.92648
C	-0.47888	-1.7363	4.08964
C	-1.13102	-0.55655	4.24351
C	1.12439	-2.62392	2.40088
S	3.1217	0.92251	1.8247
H	3.20627	2.20243	1.40613
H	-1.84754	-0.27415	5.00544
H	-0.55451	-2.6339	4.69097
H	1.11038	-3.57482	2.92748
H	2.66611	-4.64234	1.08938
H	3.78721	-3.7136	-1.1945
H	3.75819	-1.40862	-2.43691
H	3.83718	0.88337	-3.70076
H	2.74626	3.32269	-3.25561
H	1.17122	4.30625	-1.40217
H	-0.49266	5.31064	0.33121
H	-1.80674	4.32377	2.48828
H	-1.83878	1.99838	3.69899
H	-1.26385	-1.52421	0.4309
C	-2.17857	-0.58547	-2.8068
C	-3.03258	-0.56065	-1.7631
C	-1.22427	0.50974	-3.10081
H	-2.18979	-1.44198	-3.48376
C	-3.01327	0.59529	-0.86701

C	-4.06203	-1.65237	-1.57355
C	-0.08689	-2.82497	-2.01641
C	-1.44801	1.80163	-2.34603
H	-0.20494	0.19118	-2.8192
C	-3.79362	0.52419	0.4101
C	-2.28674	1.70679	-1.16945
C	-4.70504	-1.70796	-0.19299
H	-3.61341	-2.62049	-1.82767
H	-4.85129	-1.4904	-2.3241
O	-0.7735	-3.74063	-1.63554
O	-0.90179	2.84226	-2.69965
C	-5.0596	-0.31441	0.29971
H	-3.13269	0.05316	1.15699
H	-3.99319	1.53604	0.78285
H	-2.33282	2.58687	-0.52807
H	-5.59369	-2.34878	-0.22911
H	-4.00115	-2.16296	0.511
H	-5.77103	0.17018	-0.38587
H	-5.55889	-0.36258	1.27402
H	-1.53587	-2.99588	0.10032
O	0.58499	-2.82544	-3.17721
H	0.4039	-3.67584	-3.60953
H	0.07241	-1.87392	-1.47877
H	-1.15416	0.71846	-4.17545
O	-1.70641	-2.32071	0.77046

$$\Delta E_{\text{solv}} = -2315.32715949$$

$$\Delta G_{\text{correction}} = 0.469862$$

⁴c1

Charge = 0 Multiplicity = 4

C	-0.68322	-0.30685	1.91168
N	0.35518	-0.9182	1.24506
C	0.14797	-2.26596	1.38995
C	-1.05928	-2.50742	2.11963
C	-1.56342	-1.29219	2.46037
Fe	1.92009	-0.02181	0.39167
O	0.84192	-0.14599	-1.37652
C	1.02632	-3.25195	0.97022
C	2.26831	-3.01977	0.4103
N	2.77808	-1.77699	0.10573
C	4.03438	-2.01167	-0.41122
C	4.32078	-3.41438	-0.40216
C	3.22036	-4.03972	0.08852
C	4.85791	-1.04729	-0.95873
C	4.51209	0.28293	-1.13301
N	3.33323	0.84441	-0.71865
C	3.38057	2.15774	-1.12239
C	4.59888	2.41133	-1.82992
C	5.30918	1.25293	-1.82036
C	2.43083	3.11852	-0.82805
C	1.32696	2.93134	-0.00938
N	0.98736	1.74746	0.58724
C	-0.14041	2.01258	1.32036
C	-0.5033	3.39623	1.20374
C	0.4011	3.96126	0.36166
C	-0.89612	1.05842	1.98211
S	2.98557	0.31464	2.2883
H	2.65308	1.59967	2.5335
H	0.44825	4.9862	0.01312
H	-1.37718	3.83744	1.66815
H	-1.764	1.40817	2.53483
H	-2.46206	-1.06603	3.0215
H	-1.45406	-3.48982	2.35001
H	0.74479	-4.28549	1.15497
H	3.05534	-5.10115	0.23056
H	5.24508	-3.85511	-0.75614
H	5.8251	-1.36852	-1.33638
H	6.28496	1.05663	-2.24843
H	4.8732	3.36747	-2.25935
H	2.59121	4.1164	-1.22842
H	-1.93045	1.3307	-0.93502
C	-2.96735	1.32764	-1.3041
C	-3.56327	-0.08153	-1.09799
C	-3.7079	2.44587	-0.59356
H	-2.8982	1.52973	-2.37883
C	-4.12333	-0.25047	0.29805

C	-4.71639	-0.33544	-2.09737
C	-2.36446	-1.03062	-1.37997
C	-3.81687	2.14874	0.88153
H	-3.21584	3.41223	-0.73776
C	-4.81071	-1.54515	0.59686
C	-4.16832	0.76468	1.18705
C	-5.52763	-1.59888	-1.82675
H	-4.2912	-0.35566	-3.10691
H	-5.38427	0.53832	-2.05925
O	-1.90532	-0.8592	-2.70105
O	-3.6803	2.99836	1.75095
C	-5.98833	-1.69208	-0.37897
H	-4.12954	-2.39115	0.47101
H	-5.16842	-1.54916	1.63312
H	-4.55783	0.58894	2.19154
H	-6.39616	-1.61969	-2.49676
H	-4.92402	-2.47601	-2.07383
H	-6.71951	-0.89796	-0.16738
H	-6.50571	-2.64133	-0.19654
H	-1.18638	-0.21278	-2.70095
O	-2.71981	-2.37456	-1.24528
H	-1.97928	-2.87542	-1.6069
H	-1.55122	-0.77479	-0.67414
H	-4.72906	2.55116	-0.98881
O	0.41639	0.80891	-2.06699

$$\Delta E_{\text{solv}} = -2315.24285579$$

$$\Delta G_{\text{correction}} = 0.480932$$

⁴c1-ts

Charge = 0 Multiplicity = 4

C	-0.63012	-0.54486	2.10555
N	0.42794	-1.04202	1.38135
C	0.36359	-2.40049	1.50051
C	-0.78214	-2.77616	2.27564
C	-1.38703	-1.62409	2.66654
Fe	1.81639	0.01429	0.38763
O	0.6634	-0.31647	-1.11636
C	1.32372	-3.28454	1.02771
C	2.50057	-2.92452	0.40117
N	2.86022	-1.63867	0.06226
C	4.08733	-1.74142	-0.54613
C	4.52015	-3.10707	-0.55882
C	3.53051	-3.8406	0.01161
C	4.75759	-0.69481	-1.15405
C	4.26351	0.59188	-1.28521
N	3.07668	1.03436	-0.76305
C	2.96286	2.34768	-1.14108
C	4.08738	2.72678	-1.94292
C	4.90281	1.6429	-2.01772
C	1.95838	3.21366	-0.74537
C	0.94434	2.91288	0.15114
N	0.74833	1.68838	0.72684
C	-0.32669	1.8319	1.56492
C	-0.80245	3.18515	1.53661
C	-0.02364	3.85013	0.64207
C	-0.95023	0.79352	2.24113
S	2.99648	0.38783	2.23885
H	2.32494	1.45304	2.72365
H	-0.08653	4.88759	0.33528
H	-1.66051	3.53971	2.09539
H	-1.80902	1.04873	2.85641
H	-2.27493	-1.49755	3.27441
H	-1.06434	-3.79722	2.50289
H	1.1605	-4.34324	1.21168
H	3.48841	-4.91246	0.16427
H	5.45711	-3.45097	-0.98033
H	5.71839	-0.91289	-1.6128
H	5.85295	1.54677	-2.52937
H	4.23212	3.71093	-2.37229
H	1.99953	4.23024	-1.12811
H	-1.94182	1.51258	-0.70151
C	-2.97815	1.48788	-1.06732
C	-3.43392	0.02157	-1.16692
C	-3.82568	2.34667	-0.14553
H	-2.93514	1.91291	-2.07457
C	-3.95783	-0.50809	0.14282

C	-4.54497	-0.14685	-2.22747
C	-2.11841	-0.73422	-1.66823
C	-3.91031	1.73072	1.22853
H	-3.43158	3.3643	-0.06668
C	-4.49248	-1.90556	0.14583
C	-4.10733	0.28306	1.2279
C	-5.191	-1.52697	-2.25747
H	-4.12472	0.11401	-3.20565
H	-5.31724	0.60685	-2.00857
O	-1.66398	-0.20113	-2.78535
O	-3.87302	2.38534	2.26161
C	-5.63747	-1.98356	-0.87536
H	-3.71526	-2.62462	-0.12658
H	-4.85383	-2.16497	1.14746
H	-4.47084	-0.14359	2.16427
H	-6.04827	-1.51111	-2.94199
H	-4.48313	-2.25278	-2.66824
H	-6.4648	-1.3492	-0.52474
H	-6.03178	-3.00575	-0.91451
H	-0.35233	0.26162	-2.58381
O	-2.29562	-2.13934	-1.74205
H	-1.86186	-2.3912	-2.56733
H	-1.37189	-0.57205	-0.83372
H	-4.85216	2.43826	-0.53126
O	0.58655	0.53355	-2.15236

$$\Delta E_{\text{solv}} = -2315.19015601$$

$$\Delta G_{\text{correction}} = 0.476485$$

⁴c2

Charge = 0 Multiplicity = 4

C	0.75354	0.6983	1.81668
N	-0.38815	1.138	1.20287
C	-0.38843	2.50271	1.34381
C	0.79265	2.92694	2.03548
C	1.49885	1.80596	2.33372
Fe	-1.82155	0.01348	0.33562
O	-0.84032	0.24292	-1.23686
C	-1.39886	3.34705	0.92054
C	-2.57165	2.95418	0.2948
N	-2.90604	1.6661	-0.02774
C	-4.11792	1.7388	-0.66149
C	-4.56373	3.09799	-0.72336
C	-3.60092	3.85358	-0.13323
C	-4.80175	0.65953	-1.19729
C	-4.36177	-0.6516	-1.18345
N	-3.19349	-1.08793	-0.61629
C	-3.15911	-2.43969	-0.81611
C	-4.32423	-2.86424	-1.53343
C	-5.07334	-1.75433	-1.75844
C	-2.15566	-3.2916	-0.38173
C	-1.03567	-2.91472	0.33389
N	-0.74144	-1.63135	0.72512
C	0.43801	-1.71142	1.41159
C	0.89567	-3.06971	1.47036
C	-0.01729	-3.81373	0.79218
C	1.14168	-0.62848	1.92695
S	-2.89924	-0.20455	2.30502
H	-1.95602	-0.89132	2.98242
H	-0.01434	-4.88174	0.60984
H	1.81926	-3.3764	1.94972
H	2.05638	-0.84655	2.47148
H	2.44526	1.71666	2.85413
H	1.03338	3.95811	2.26516
H	-1.26762	4.41018	1.10516
H	-3.57522	4.92805	0.00344
H	-5.49388	3.42135	-1.17496
H	-5.75438	0.86174	-1.67992
H	-6.02485	-1.673	-2.27002
H	-4.53177	-3.8887	-1.8182
H	-2.26347	-4.34717	-0.61742
H	4.05752	-1.96011	-2.27768
C	4.41221	-1.50534	-1.34757
C	3.88025	-0.07354	-1.2562
C	4.03102	-2.35615	-0.15195
H	5.50627	-1.44333	-1.42098
C	4.32448	0.55745	0.04218

C	4.33111	0.71083	-2.50311
C	2.28533	-0.1515	-1.22882
C	4.22163	-1.65193	1.17363
H	2.97732	-2.66399	-0.21398
C	4.44902	2.04707	0.11508
C	4.50319	-0.21767	1.13642
C	4.32233	2.22546	-2.37409
H	3.72506	0.37807	-3.35388
H	5.35979	0.38899	-2.72556
O	1.77406	-0.91661	-2.15683
O	4.08869	-2.25051	2.23489
C	5.08104	2.65958	-1.13074
H	3.43015	2.449	0.21725
H	4.98856	2.32913	1.02734
H	4.77233	0.23351	2.09285
H	4.77076	2.66739	-3.27219
H	3.29206	2.59111	-2.32376
H	6.13355	2.34839	-1.20555
H	5.09265	3.75155	-1.03887
H	0.07854	-0.87691	-2.38785
O	1.794	1.15985	-1.11188
H	0.82665	1.10142	-1.23174
H	2.07344	-0.65887	-0.23736
H	4.59351	-3.29586	-0.11779
O	-0.88506	-0.80327	-2.1547

$$\Delta E_{\text{solv}} = -2315.21308762$$

$$\Delta G_{\text{correction}} = 0.479806$$

⁴c2-ts

Charge = 0 Multiplicity = 4

C	0.71681	0.73646	1.85889
N	-0.40281	1.1603	1.19312
C	-0.40957	2.52699	1.29846
C	0.75204	2.97172	2.01063
C	1.44434	1.85949	2.36847
Fe	-1.81961	0.01421	0.32832
O	-0.84587	0.24859	-1.25346
C	-1.42255	3.3564	0.85039
C	-2.60145	2.93935	0.25392
N	-2.93296	1.64032	-0.02932
C	-4.16236	1.68586	-0.63378
C	-4.62347	3.03913	-0.71115
C	-3.65113	3.81767	-0.1685
C	-4.83896	0.59172	-1.14592
C	-4.36417	-0.70783	-1.15159
N	-3.17116	-1.11515	-0.61765
C	-3.09691	-2.46279	-0.83887
C	-4.26267	-2.91224	-1.54043
C	-5.05324	-1.82443	-1.72784
C	-2.06686	-3.29048	-0.42474
C	-0.96497	-2.89506	0.31204
N	-0.7143	-1.61341	0.7335
C	0.44276	-1.67597	1.46192
C	0.92899	-3.02383	1.51312
C	0.06068	-3.77668	0.78627
C	1.10816	-0.58456	2.00705
S	-2.89942	-0.21414	2.29899
H	-2.03701	-1.04709	2.91717
H	0.09647	-4.84088	0.58559
H	1.84072	-3.32031	2.02066
H	2.01082	-0.78794	2.578
H	2.36989	1.78716	2.92789
H	0.98449	4.00906	2.22065
H	-1.29675	4.4246	1.00725
H	-3.63268	4.89541	-0.05841
H	-5.56896	3.34341	-1.14392
H	-5.80752	0.77265	-1.60457
H	-6.01846	-1.76617	-2.21646
H	-4.44377	-3.93831	-1.83751
H	-2.14282	-4.34453	-0.679
H	4.04983	-1.9884	-2.23021
C	4.4592	-1.52435	-1.32736
C	4.00662	-0.07966	-1.25914
C	4.09699	-2.33167	-0.09399
H	5.55231	-1.5083	-1.453
C	4.38497	0.5919	-0.00353

C	4.28599	0.67105	-2.55109
C	2.17769	-0.21832	-1.12959
C	4.27256	-1.58096	1.20923
H	3.04837	-2.6579	-0.14547
C	4.47988	2.08713	0.02667
C	4.53565	-0.14659	1.13084
C	4.24223	2.18802	-2.4568
H	3.61243	0.29481	-3.32939
H	5.29658	0.36639	-2.87041
O	1.73484	-0.95437	-2.05139
O	4.14421	-2.14857	2.28823
C	5.04297	2.67725	-1.26086
H	3.45981	2.47203	0.17179
H	5.05491	2.40065	0.90607
H	4.77501	0.34107	2.07666
H	4.6302	2.62006	-3.38671
H	3.20458	2.52374	-2.36398
H	6.09878	2.38951	-1.37273
H	5.03093	3.77135	-1.20345
H	0.01856	-0.90181	-2.41379
O	1.75899	1.10103	-1.01352
H	0.8264	1.11304	-1.30761
H	2.21272	-0.67147	-0.1142
H	4.6735	-3.26079	-0.02855
O	-0.9386	-0.76754	-2.20819

$$\Delta E_{\text{solv}} = -2315.19433451$$

$$\Delta G_{\text{correction}} = 0.477572$$

⁴c3

Charge = 0 Multiplicity = 4

C	0.63567	0.70918	1.61721
N	-0.51382	1.17189	1.02662
C	-0.47797	2.53656	1.14215
C	0.73296	2.94371	1.78923
C	1.41777	1.81	2.09347
Fe	-2.02679	0.06126	0.27423
O	-1.11468	0.2181	-1.37073
C	-1.48196	3.39876	0.73619
C	-2.6877	3.01572	0.17825
N	-3.07484	1.7238	-0.08299
C	-4.32176	1.81017	-0.65068
C	-4.72957	3.17913	-0.73525
C	-3.71547	3.92613	-0.22614
C	-5.07169	0.73918	-1.10121
C	-4.66783	-0.58327	-1.06382
N	-3.47658	-1.03219	-0.56208
C	-3.48916	-2.39446	-0.71605
C	-4.71285	-2.80721	-1.33639
C	-5.44568	-1.68471	-1.54932
C	-2.48205	-3.25784	-0.33018
C	-1.3031	-2.88443	0.29271
N	-0.95985	-1.60277	0.63515
C	0.26362	-1.69043	1.24928
C	0.69891	-3.0549	1.29817
C	-0.27112	-3.79253	0.69565
C	0.99746	-0.62155	1.73506
S	-2.97862	-0.08789	2.32511
H	-2.00143	-0.77431	2.95211
H	-0.29944	-4.86341	0.53223
H	1.64544	-3.37112	1.72242
H	1.92664	-0.85705	2.24549
H	2.36946	1.7112	2.60221
H	1.0038	3.97259	1.99489
H	-1.31799	4.46255	0.88614
H	-3.65389	5.00352	-0.12837
H	-5.67487	3.51389	-1.14553
H	-6.04677	0.95493	-1.5295
H	-6.42737	-1.59272	-1.99853
H	-4.96603	-3.83429	-1.57081
H	-2.63004	-4.31689	-0.52406
H	5.33978	-1.96526	-2.05508
C	5.42556	-1.64561	-1.00867
C	5.33465	-0.15379	-0.92122
C	4.39962	-2.37298	-0.14761
H	6.4446	-1.94403	-0.70793
C	4.8869	0.44367	0.25421

C	5.83696	0.64533	-2.08061
C	2.03554	-0.03177	-1.84714
C	4.21708	-1.7675	1.22442
H	3.41333	-2.32725	-0.63438
C	4.84893	1.94464	0.39044
C	4.45729	-0.34684	1.3255
C	5.4958	2.12761	-2.00656
H	5.46482	0.20296	-3.01672
H	6.93161	0.51317	-2.14405
O	1.56813	-1.15116	-1.90279
O	3.7904	-2.42489	2.17302
C	5.74527	2.66226	-0.60586
H	3.80663	2.27174	0.24884
H	5.09793	2.22252	1.42223
H	4.23629	0.11333	2.28859
H	6.07044	2.68423	-2.75451
H	4.43725	2.27685	-2.26433
H	6.8003	2.51092	-0.33631
H	5.57063	3.74256	-0.56212
H	-0.24924	-1.24489	-2.14053
O	1.38795	1.09024	-1.63956
H	0.41482	0.88634	-1.50135
H	3.11338	0.16365	-1.97052
H	4.63136	-3.43647	-0.04197
O	-1.17598	-0.92033	-2.19601

$$\Delta E_{\text{solv}} = -2315.26668346$$

$$\Delta G_{\text{correction}} = 0.473576$$

⁴c3-ts

Charge = 0 Multiplicity = 4

C	-1.94331	0.17248	2.3079
N	-0.67665	-0.28358	2.04305
C	-0.53086	-1.44207	2.76566
C	-1.72048	-1.70483	3.51773
C	-2.59947	-0.70743	3.22723
Fe	0.72514	0.63674	0.94936
O	-0.09861	-0.40617	-0.89271
C	0.55876	-2.2979	2.69282
C	1.69717	-2.08739	1.93143
N	1.93615	-0.97452	1.16718
C	3.21573	-1.11076	0.69546
C	3.77089	-2.36246	1.122
C	2.82727	-2.97007	1.88809
C	3.88725	-0.16736	-0.06728
C	3.35862	1.03772	-0.50861
N	2.08383	1.47901	-0.26453
C	1.96373	2.68017	-0.91701
C	3.18855	2.99612	-1.58978
C	4.05445	1.97892	-1.33493
C	0.81906	3.46202	-0.96032
C	-0.38306	3.16782	-0.33674
N	-0.60378	2.08801	0.4698
C	-1.91126	2.16731	0.86055
C	-2.53952	3.31816	0.27095
C	-1.58586	3.94442	-0.46609
C	-2.53183	1.29236	1.73755
S	1.63614	1.82706	2.84127
H	0.53665	1.81753	3.6226
H	-1.67563	4.85211	-1.05185
H	-3.58035	3.58649	0.40682
H	-3.57443	1.48645	1.97694
H	-3.60849	-0.56777	3.59844
H	-1.86089	-2.55758	4.17192
H	0.51922	-3.20479	3.29145
H	2.88836	-3.9216	2.40336
H	4.7651	-2.71414	0.87187
H	4.91067	-0.39672	-0.3542
H	5.0792	1.86718	-1.67024
H	3.35545	3.89017	-2.17916
H	0.86798	4.37914	-1.54243
H	-1.21977	0.2953	-2.42247
C	-2.43621	-0.2615	-2.82471
C	-2.1703	-1.42276	-2.1151
C	-3.49819	0.70611	-2.37493
H	-2.20935	-0.2835	-3.89501
C	-2.76568	-1.64276	-0.80977

C	-1.30291	-2.48213	-2.73016
C	2.30825	-1.28622	-2.54769
C	-4.15605	0.40531	-1.04195
H	-3.11876	1.73662	-2.3146
C	-2.27091	-2.77788	0.03692
C	-3.73606	-0.80602	-0.35524
C	-0.65478	-3.43235	-1.73506
H	-0.55881	-2.00593	-3.38132
H	-1.94311	-3.06399	-3.41434
O	1.83478	-0.45866	-3.30058
O	-4.98079	1.17096	-0.56384
C	-1.69097	-3.94394	-0.74856
H	-1.47376	-2.36303	0.66766
H	-3.05788	-3.0978	0.72879
H	-4.20481	-0.98944	0.61082
H	-0.1711	-4.25804	-2.26943
H	0.13066	-2.90078	-1.18289
H	-2.48662	-4.48218	-1.28431
H	-1.2452	-4.66658	-0.05608
H	0.54519	0.36156	-2.52812
O	3.37601	-2.01824	-2.83927
H	3.68591	-1.74737	-3.71939
H	1.89837	-1.527	-1.55844
H	-4.29827	0.76187	-3.12587
O	-0.18592	0.61519	-1.90298

$$\Delta E_{\text{solv}} = -2315.2739718$$

$$\Delta G_{\text{correction}} = 0.468373$$

4c4

Charge = 0 Multiplicity = 4

C	-1.71477	0.44598	2.40764
N	-0.47051	-0.0501	2.11007
C	-0.29255	-1.14452	2.919
C	-1.44058	-1.32771	3.75594
C	-2.32206	-0.34147	3.43872
Fe	0.85646	0.73828	0.83649
O	-0.05784	-0.59663	-0.72372
C	0.80103	-1.9983	2.88831
C	1.91627	-1.85216	2.07849
N	2.10814	-0.82878	1.18852
C	3.3675	-1.00125	0.67987
C	3.96743	-2.18211	1.23164
C	3.06368	-2.71425	2.09605
C	3.96818	-0.16445	-0.24924
C	3.37827	0.94579	-0.83901
N	2.10956	1.4011	-0.58608
C	1.92341	2.48827	-1.40354
C	3.09599	2.71028	-2.19651
C	3.99937	1.75701	-1.84384
C	0.76954	3.25462	-1.47736
C	-0.37689	3.0637	-0.721
N	-0.52648	2.10756	0.243
C	-1.7892	2.26499	0.74248
C	-2.46317	3.33888	0.06518
C	-1.58284	3.83698	-0.8429
C	-2.334	1.51239	1.771
S	1.86664	2.17731	2.49739
H	0.7692	2.38642	3.25323
H	-1.72406	4.65877	-1.53573
H	-3.48403	3.64442	0.26131
H	-3.35102	1.75083	2.07313
H	-3.30486	-0.15451	3.85662
H	-1.5501	-2.11983	4.48765
H	0.78955	-2.84221	3.57394
H	3.16305	-3.60002	2.71267
H	4.95875	-2.5449	0.98565
H	4.98157	-0.40995	-0.55799
H	5.00464	1.60981	-2.2218
H	3.20658	3.50566	-2.92437
H	0.76772	4.07812	-2.1875
H	-1.13926	-0.04596	-2.25848
C	-2.99342	-0.52173	-2.66879
C	-2.6205	-1.58515	-1.91982
C	-3.77046	0.62293	-2.11729
H	-2.77668	-0.52397	-3.73994
C	-2.97298	-1.62611	-0.49485

C	-1.90911	-2.76482	-2.53735
C	2.2067	-1.71725	-2.37927
C	-4.31542	0.44423	-0.71126
H	-3.15169	1.53768	-2.08556
C	-2.34683	-2.66834	0.38377
C	-3.82174	-0.70598	0.02598
C	-1.08693	-3.58788	-1.55513
H	-1.2994	-2.42879	-3.38659
H	-2.67679	-3.41808	-2.98047
O	1.65003	-1.02869	-3.21667
O	-5.07175	1.27109	-0.22245
C	-1.9273	-3.93934	-0.33861
H	-1.44574	-2.19875	0.804
H	-2.99842	-2.87566	1.23997
H	-4.12616	-0.77344	1.06924
H	-0.7109	-4.4894	-2.05234
H	-0.21681	-3.00618	-1.22744
H	-2.81123	-4.51646	-0.64789
H	-1.3672	-4.58325	0.34849
H	0.4587	-0.16069	-2.5665
O	3.25561	-2.47655	-2.64729
H	3.47928	-2.35467	-3.58509
H	1.88817	-1.78822	-1.33173
H	-4.59733	0.89825	-2.78383
O	-0.23538	0.23887	-1.95463

$$\Delta E_{\text{solv}} = -2315.28782342$$

$$\Delta G_{\text{correction}} = 0.471799$$

5. Coordinates of all stationary points in Fig. 4

21

Charge = 0 Multiplicity = 2

C	0.06163	-2.21771	1.74338
N	1.04153	-1.87844	0.85219
C	1.54819	-3.05865	0.3777
C	0.84196	-4.16516	0.95291
C	-0.07137	-3.64238	1.81455
Fe	1.56489	-0.04725	0.26472
O	0.7354	-0.07613	-1.15596
C	2.65556	-3.17328	-0.45078
C	3.44218	-2.12535	-0.90427
N	3.195	-0.80429	-0.65516
C	4.1798	-0.10475	-1.29661
C	5.09511	-1.01167	-1.92882
C	4.63187	-2.26581	-1.69402
C	4.24148	1.27749	-1.39792
C	3.3104	2.17205	-0.89872
N	2.20826	1.82818	-0.15954
C	1.50342	2.98789	0.03581
C	2.19259	4.09069	-0.57157
C	3.31908	3.58741	-1.1367
C	0.32976	3.08278	0.76516
C	-0.27656	2.03981	1.45453
N	0.11334	0.72929	1.40049
C	-0.70152	0.06232	2.28177
C	-1.59928	0.97951	2.91875
C	-1.35256	2.20412	2.38893
C	-0.71854	-1.31145	2.45035
S	3.13783	0.26871	2.12001
H	2.5483	1.33668	2.69617
H	-1.86294	3.14166	2.56881
H	-2.35138	0.69857	3.64671
H	-1.44471	-1.71965	3.14904
H	-0.77904	-4.16416	2.44782
H	1.04843	-5.20729	0.74014
H	2.95562	-4.17842	-0.73733
H	5.05046	-3.21099	-2.01829
H	5.97098	-0.71114	-2.49119
H	5.07029	1.69329	-1.96576
H	4.09131	4.11508	-1.68354
H	1.84833	5.11761	-0.5511
H	-0.13966	4.05992	0.84404
H	-1.29168	0.9097	-1.4314
C	-2.28405	0.87637	-1.90119
C	-3.11857	-0.23454	-1.22657
C	-2.88084	2.27031	-1.82135

H	-2.09453	0.59023	-2.94153
C	-3.86929	0.28495	-0.02011
C	-4.13736	-0.82987	-2.22361
C	-2.05192	-1.28721	-0.80818
C	-3.14618	2.63522	-0.38163
H	-2.22014	3.01722	-2.27194
C	-4.81189	-0.66675	0.64784
C	-3.79901	1.57198	0.37984
C	-5.18346	-1.74956	-1.60143
H	-3.57624	-1.35243	-3.00717
H	-4.64492	0.01196	-2.71905
O	-1.31074	-1.72656	-1.91313
O	-2.89387	3.73382	0.09394
C	-5.85141	-1.12375	-0.38533
H	-4.27824	-1.54418	1.02673
H	-5.30098	-0.17598	1.4975
H	-4.31071	1.88471	1.29129
H	-5.9398	-2.00051	-2.35584
H	-4.71057	-2.69111	-1.30972
H	-6.44887	-0.25246	-0.6924
H	-6.55308	-1.82787	0.07769
H	-0.47605	-1.22268	-1.90034
O	-2.63202	-2.4168	-0.2077
H	-1.94169	-3.09162	-0.22425
H	-1.36644	-0.78891	-0.10392
H	-3.83696	2.32411	-2.36335

$$\Delta E_{\text{solv}} = -2240.0900127$$

$$\Delta G_{\text{correction}} = 0.480417$$

21-ts

Charge = 0 Multiplicity = 2

C	-0.07941	-1.68245	1.9752
N	0.96545	-1.62111	1.09915
C	1.36141	-2.91535	0.89335
C	0.52462	-3.8121	1.63518
C	-0.36935	-3.04475	2.31161
Fe	1.73547	0.02081	0.25461
O	0.73519	-0.1132	-1.12513
C	2.45305	-3.30205	0.13406
C	3.32691	-2.4478	-0.52171
N	3.21416	-1.08653	-0.54959
C	4.26587	-0.63516	-1.29806
C	5.07121	-1.73859	-1.73455
C	4.48401	-2.86594	-1.2579
C	4.49928	0.68923	-1.63697
C	3.70291	1.76796	-1.29495
N	2.57175	1.69606	-0.52873
C	2.06569	2.96217	-0.48157
C	2.90159	3.86021	-1.22753
C	3.92394	3.11952	-1.72461
C	0.92799	3.33484	0.22037
C	0.15815	2.50351	1.01527
N	0.38853	1.16468	1.21525
C	-0.59811	0.73858	2.05427
C	-1.46021	1.82772	2.40999
C	-0.99423	2.92318	1.75712
C	-0.80695	-0.5878	2.42449
S	3.22607	0.32798	2.05613
H	2.67153	1.43825	2.58419
H	-1.41329	3.92154	1.74495
H	-2.33432	1.74869	3.04508
H	-1.63913	-0.78819	3.09537
H	-1.16558	-3.35816	2.97554
H	0.62984	-4.89041	1.64154
H	2.65722	-4.36786	0.06668
H	4.797	-3.89545	-1.38332
H	5.96629	-1.64718	-2.33794
H	5.37262	0.89377	-2.25154
H	4.75734	3.44376	-2.33613
H	2.72029	4.92241	-1.33976
H	0.62497	4.37741	0.15993
H	-1.60162	1.04717	-0.55954
C	-2.41582	1.02126	-1.29501
C	-3.26098	-0.24725	-1.0636
C	-3.18302	2.32553	-1.18177
H	-1.91055	0.94128	-2.26354
C	-4.36143	-0.02685	-0.05843

C	-3.86895	-0.75311	-2.38659
C	-2.19117	-1.29733	-0.51997
C	-3.90788	2.41343	0.14135
H	-2.52369	3.19245	-1.29308
C	-5.33114	-1.15016	0.14864
C	-4.55641	1.16627	0.5483
C	-4.89188	-1.87052	-2.2291
H	-3.04412	-1.06213	-3.03904
H	-4.34867	0.10748	-2.87854
O	-1.20217	-1.51277	-1.38697
O	-4.02183	3.45122	0.77462
C	-5.9585	-1.52082	-1.20176
H	-4.82658	-2.03097	0.55564
H	-6.10476	-0.84678	0.8628
H	-5.33348	1.26848	1.30749
H	-5.35696	-2.07959	-3.20056
H	-4.38431	-2.79154	-1.92554
H	-6.55713	-0.67103	-1.56195
H	-6.65946	-2.35334	-1.06895
H	-0.194	-0.76312	-1.24952
O	-2.78341	-2.5203	-0.11856
H	-2.16727	-3.19122	-0.43949
H	-1.82026	-0.80644	0.41261
H	-3.93998	2.40819	-1.97635

$$\Delta E_{\text{solv}} = -2240.07927332$$

$$\Delta G_{\text{correction}} = 0.470591$$

Charge = 0 Multiplicity = 2

C	-0.0748	-1.70051	1.8734
N	0.95454	-1.63711	0.97779
C	1.30534	-2.93336	0.7067
C	0.44046	-3.83269	1.41323
C	-0.40777	-3.06746	2.14805
Fe	1.83163	0.02033	0.24459
O	0.81136	-0.08041	-1.21193
C	2.3958	-3.32014	-0.05153
C	3.3309	-2.46498	-0.61697
N	3.28385	-1.10044	-0.56361
C	4.38892	-0.65126	-1.233
C	5.16793	-1.76283	-1.69351
C	4.50412	-2.8887	-1.32293
C	4.67168	0.67757	-1.5091
C	3.85477	1.75301	-1.20368
N	2.67667	1.67425	-0.51464
C	2.16822	2.93926	-0.4775
C	3.04265	3.84254	-1.1694
C	4.0979	3.10821	-1.60657
C	1.01145	3.31583	0.19206
C	0.23114	2.48779	0.97798
N	0.45864	1.14855	1.18587
C	-0.5292	0.7227	2.02519
C	-1.38585	1.81728	2.37884
C	-0.92199	2.90922	1.71701
C	-0.75869	-0.60521	2.37986
S	3.17671	0.14876	2.1022
H	2.5833	1.19777	2.70764
H	-1.34066	3.90773	1.69903
H	-2.25726	1.74153	3.01855
H	-1.56543	-0.80094	3.08192
H	-1.2027	-3.38393	2.81279
H	0.50437	-4.91328	1.3646
H	2.56018	-4.3873	-0.17734
H	4.77572	-3.92202	-1.50261
H	6.09478	-1.67784	-2.248
H	5.58545	0.88654	-2.05957
H	4.96618	3.43963	-2.16342
H	2.86621	4.90538	-1.28372
H	0.71385	4.35937	0.12593
H	-1.61773	0.87256	-0.38391
C	-2.36602	0.89318	-1.18417
C	-3.36976	-0.25165	-0.96553
C	-2.98568	2.27899	-1.20783
H	-1.79555	0.7027	-2.09894
C	-4.5187	0.13947	-0.07529

C	-3.91391	-0.78409	-2.305
C	-2.45995	-1.40771	-0.26594
C	-3.81692	2.52844	0.02845
H	-2.22081	3.05678	-1.29693
C	-5.61862	-0.86222	0.10495
C	-4.63527	1.38492	0.43827
C	-5.06189	-1.77718	-2.18146
H	-3.07831	-1.21029	-2.87214
H	-4.25883	0.09199	-2.87687
O	-1.41907	-1.71304	-0.97278
O	-3.87804	3.61114	0.58799
C	-6.16569	-1.2549	-1.27344
H	-5.25122	-1.7603	0.6091
H	-6.41234	-0.4325	0.72568
H	-5.46135	1.61761	1.11169
H	-5.4636	-1.99395	-3.17893
H	-4.68656	-2.72724	-1.7884
H	-6.63847	-0.3747	-1.73345
H	-6.95952	-2.0021	-1.15841
H	0.02677	-0.66899	-1.14542
O	-3.23168	-2.52534	0.1457
H	-2.70454	-3.28742	-0.12878
H	-2.16056	-0.87993	0.68563
H	-3.65074	2.39774	-2.07673

$$\Delta E_{\text{solv}} = -2240.08172563$$

$$\Delta G_{\text{correction}} = 0.476213$$

2-ts

Charge = 0 Multiplicity = 2

C	-6.14548	-1.25026	-1.45392
C	-5.685	-0.85614	-0.04656
C	-4.56703	0.13821	-0.14318
C	-3.40428	-0.21478	-0.99542
C	-3.83206	-0.7941	-2.343
C	-4.98763	-1.7838	-2.28382
C	-4.6684	1.35559	0.44771
C	-3.81889	2.50196	0.11515
C	-2.93862	2.29361	-1.0956
C	-2.35524	0.88987	-1.1213
C	-2.46359	-1.48111	-0.1708
O	-3.28054	-2.5593	0.19628
O	-3.894	3.56243	0.71388
O	-1.45652	-1.75685	-0.89278
O	0.77283	-0.0988	-1.18124
Fe	1.83545	0.02836	0.2477
S	3.22434	0.18148	2.06788
N	0.99323	-1.63435	1.01354
C	-0.02018	-1.70233	1.92835
C	-0.32826	-3.07145	2.22225
C	0.51736	-3.8317	1.48003
C	1.35695	-2.92713	0.74905
C	-0.69975	-0.61226	2.44792
C	-0.49535	0.71344	2.07748
N	0.47154	1.14735	1.21524
C	0.22338	2.48122	1.00247
C	-0.91873	2.89412	1.76297
C	-1.35692	1.80094	2.44088
C	2.43719	-3.3077	-0.02789
C	3.34569	-2.44572	-0.62318
N	3.28072	-1.08036	-0.58564
C	4.35963	-0.6236	-1.29187
C	5.14189	-1.73017	-1.75926
C	4.50567	-2.86063	-1.35591
C	4.61528	0.7049	-1.59358
C	3.7907	1.77144	-1.27835
N	2.6344	1.68429	-0.55502
C	2.11111	2.94383	-0.5121
C	2.95311	3.85127	-1.23854
C	4.00378	3.12614	-1.7009
C	0.97181	3.31293	0.18836
H	2.56874	1.14583	2.74555
H	-1.34971	3.88751	1.74685
H	-2.21367	1.71991	3.09973
H	-1.4919	-0.81248	3.16521
H	-1.10627	-3.39294	2.90441

H	0.59469	-4.91171	1.43946
H	2.61418	-4.37372	-0.14559
H	4.78746	-3.8922	-1.53011
H	6.05154	-1.63888	-2.34067
H	5.51021	0.91981	-2.1719
H	4.85109	3.46307	-2.28611
H	2.76006	4.91088	-1.35627
H	0.66035	4.35253	0.12358
H	-1.63823	0.80968	-0.297
H	-1.75567	0.72665	-2.02232
H	-2.15045	3.05252	-1.10983
H	-2.95449	-1.22846	-2.83396
H	-4.13194	0.06622	-2.96465
H	-5.35026	-1.75506	0.48052
H	-6.51334	-0.42678	0.52694
H	-5.50771	1.56998	1.11034
H	-5.32244	-2.0128	-3.30252
H	-4.64336	-2.73282	-1.85926
H	-6.58152	-0.3708	-1.9498
H	-6.94975	-1.99191	-1.38788
H	0.01212	-0.71011	-1.08428
H	-2.90493	-3.32038	-0.26807
H	-2.2772	-0.88791	0.75587
H	-3.56107	2.47571	-1.9849

$$\Delta E_{\text{solv}} = -2240.08168053$$

$$\Delta G_{\text{correction}} = 0.475803$$

Charge = 0 Multiplicity = 2

C	0.47952	-2.94164	1.75303
N	-0.4479	-2.26671	1.00466
C	-1.66157	-2.49733	1.58851
C	-1.49739	-3.34118	2.73725
C	-0.17324	-3.6289	2.82985
Fe	-0.0893	-1.10325	-0.58874
O	-0.04522	0.37103	0.44996
C	-2.87865	-2.03124	1.11533
C	-3.05923	-1.31448	-0.05593
N	-2.05749	-0.88992	-0.88712
C	-2.67118	-0.34117	-1.98272
C	-4.09558	-0.4006	-1.82472
C	-4.33609	-0.98742	-0.62286
C	-2.01848	0.24755	-3.05322
C	-0.64785	0.44509	-3.13867
N	0.27015	-0.00477	-2.22861
C	1.47783	0.52417	-2.60217
C	1.31455	1.32806	-3.77812
C	0.00198	1.25993	-4.12446
C	2.69206	0.25758	-1.99152
C	2.88378	-0.63453	-0.94709
N	1.88948	-1.30852	-0.29371
C	2.50293	-2.12601	0.61393
C	3.92605	-1.97881	0.51669
C	4.16256	-1.04062	-0.43794
C	1.84892	-2.91067	1.55098
S	-0.05417	-3.01944	-1.84321
H	0.84176	-2.62262	-2.77083
H	5.11377	-0.65068	-0.78059
H	4.64441	-2.5257	1.11677
H	2.46467	-3.5036	2.22237
H	0.3339	-4.2405	3.56666
H	-2.30614	-3.67431	3.37696
H	-3.769	-2.30001	1.67821
H	-5.29054	-1.20865	-0.15949
H	-4.81124	-0.03062	-2.54952
H	-2.63316	0.65364	-3.85246
H	-0.50081	1.73643	-4.95792
H	2.11581	1.86775	-4.26866
H	3.57091	0.75386	-2.3942
C	-1.34109	2.8791	-0.6481
C	-1.57059	2.72406	0.81285
C	-0.12067	3.69897	-1.03929
C	-0.55446	2.97952	1.72998
C	-2.88162	2.14048	1.21962
C	3.23524	1.24922	1.63951

C	1.05457	3.49023	-0.11248
H	0.19013	3.49696	-2.06857
C	-0.74858	2.69718	3.19845
C	0.71708	3.34061	1.28387
C	-2.85265	1.5029	2.59891
H	-3.19614	1.4173	0.45398
H	-3.65216	2.93105	1.18455
O	2.33468	0.59738	2.11396
O	2.21783	3.4914	-0.51743
C	-2.19683	2.44917	3.59189
H	-0.146	1.80842	3.44188
H	-0.31169	3.51074	3.79159
H	1.53029	3.43091	2.00362
H	-3.866	1.2283	2.91473
H	-2.27684	0.56853	2.54532
H	-2.74935	3.4	3.60949
H	-2.24499	2.05146	4.61172
O	4.50077	1.18369	2.06537
H	4.52799	0.50677	2.76114
H	3.13772	1.98943	0.8274
H	-0.36003	4.77235	-0.99264
H	-1.22369	1.85433	-1.02586
H	-2.24927	3.25863	-1.13873
H	0.712	0.42131	1.06197

$$\Delta E_{\text{solv}} = -2240.11268962$$

$$\Delta G_{\text{correction}} = 0.470755$$

23-ts

Charge = 0 Multiplicity = 2

C	-1.76135	-2.9573	-0.74687
N	-2.03414	-1.87661	0.0471
C	-2.70837	-2.36424	1.13117
C	-2.87385	-3.78652	1.01425
C	-2.28792	-4.15455	-0.15273
Fe	-1.54615	0.05757	-0.28996
O	0.04055	-0.25173	0.70643
C	-3.15826	-1.60596	2.20047
C	-3.01426	-0.23592	2.34022
N	-2.40741	0.59734	1.44034
C	-2.52424	1.85933	1.95067
C	-3.21001	1.82226	3.21143
C	-3.51296	0.52136	3.45321
C	-2.0622	3.01143	1.33522
C	-1.39759	3.05608	0.12042
N	-1.08061	1.9624	-0.64703
C	-0.38346	2.45235	-1.72571
C	-0.27239	3.8787	-1.6384
C	-0.90431	4.25375	-0.49546
C	0.16762	1.69026	-2.74018
C	0.06296	0.31343	-2.85937
N	-0.58069	-0.50871	-1.97207
C	-0.49978	-1.77154	-2.49847
C	0.24031	-1.74677	-3.72601
C	0.59276	-0.4525	-3.94892
C	-1.04964	-2.9123	-1.93377
S	-3.49609	0.20533	-1.40163
H	-3.45939	1.51654	-1.72485
H	1.15572	-0.03753	-4.77655
H	0.45121	-2.61731	-4.33638
H	-0.90572	-3.84947	-2.4659
H	-2.20602	-5.14499	-0.58488
H	-3.3771	-4.41076	1.74335
H	-3.67809	-2.13239	2.99734
H	-4.03598	0.09669	4.30215
H	-3.43057	2.69177	3.81964
H	-2.23683	3.95628	1.84399
H	-1.02346	5.25023	-0.08605
H	0.25102	4.49657	-2.35829
H	0.72996	2.21705	-3.50592
C	1.93166	1.38891	1.53211
C	2.92292	0.42881	1.87936
C	2.30734	2.45519	0.53413
C	4.0318	0.19947	1.01674
C	2.67663	-0.43073	3.07912
C	2.46231	-1.55929	-1.1935

C	3.23456	1.96935	-0.55473
H	1.43973	2.94686	0.09002
C	5.01083	-0.90835	1.31471
C	4.16183	0.92317	-0.15067
C	3.48552	-1.71855	3.10577
H	1.59836	-0.62875	3.14467
H	2.90419	0.16851	3.97658
O	2.06038	-2.11151	-0.19805
O	3.23274	2.43748	-1.6861
C	4.93259	-1.43035	2.74076
H	4.80215	-1.73947	0.62256
H	6.02511	-0.57539	1.06463
H	4.9433	0.66778	-0.8671
H	3.40891	-2.18916	4.09156
H	3.0625	-2.43226	2.38676
H	5.3486	-0.68665	3.43556
H	5.55563	-2.32508	2.84564
O	3.45499	-2.01641	-1.95938
H	3.74803	-2.85957	-1.577
H	2.07877	-0.61062	-1.59942
H	2.85882	3.25273	1.06111
H	1.03872	0.66171	1.05209
H	1.34319	1.7498	2.38479
H	0.55073	-1.03267	0.43357

$$\Delta E_{\text{solv}} = -2240.12645549$$

$$\Delta G_{\text{correction}} = 0.467005$$

Charge = 0 Multiplicity = 2

C	-3.2411	0.7159	1.28229
N	-2.06345	1.35437	0.99232
C	-1.91832	2.31621	1.95649
C	-3.02753	2.28211	2.87155
C	-3.85235	1.29374	2.44888
Fe	-0.8231	1.00049	-0.54036
O	0.29571	-0.21032	0.70712
C	-0.86237	3.20694	2.04009
C	0.19987	3.28947	1.15281
N	0.38758	2.47892	0.06653
C	1.52184	2.93357	-0.55145
C	2.06535	4.04974	0.16692
C	1.24834	4.26524	1.23063
C	2.08635	2.37625	-1.68818
C	1.60609	1.26217	-2.35769
N	0.48249	0.55645	-2.00221
C	0.39423	-0.47486	-2.90604
C	1.48257	-0.41654	-3.84085
C	2.23288	0.66412	-3.50253
C	-0.60483	-1.43452	-2.92374
C	-1.69081	-1.48891	-2.06115
N	-1.92038	-0.6209	-1.02334
C	-3.13668	-0.97946	-0.49853
C	-3.6654	-2.11141	-1.1989
C	-2.76288	-2.43433	-2.16422
C	-3.75374	-0.35915	0.57777
S	-2.01813	2.33592	-1.82078
H	-1.28588	2.30512	-2.95784
H	-2.81591	-3.23104	-2.89707
H	-4.60641	-2.59652	-0.96685
H	-4.71212	-0.75958	0.90027
H	-4.79117	0.96609	2.87993
H	-3.14502	2.94226	3.723
H	-0.87944	3.92197	2.85929
H	1.33062	5.02222	2.00191
H	2.96233	4.58864	-0.116
H	2.98922	2.84201	-2.07706
H	3.13306	1.03651	-3.97836
H	1.63622	-1.11725	-4.65376
H	-0.55526	-2.18948	-3.70531
C	2.76352	-1.96041	-0.80413
C	3.18178	-1.33494	0.31496
C	1.93341	-3.18977	-0.78586
C	2.75522	-1.84482	1.62518
C	4.05511	-0.10925	0.2472
C	-1.59811	-3.05931	1.28901

C	1.51954	-3.71097	0.57629
H	1.02575	-3.05673	-1.39628
C	2.98056	-1.00715	2.85661
C	2.03332	-2.99228	1.72505
C	3.81866	0.84421	1.4089
H	3.91082	0.3865	-0.71939
H	5.10948	-0.42703	0.26708
O	-1.0514	-2.23307	1.98473
O	0.73356	-4.64626	0.677
C	4.019	0.09641	2.71725
H	2.00826	-0.53979	3.07852
H	3.18806	-1.65774	3.71407
H	1.68942	-3.33998	2.69837
H	4.49262	1.70498	1.33491
H	2.7973	1.24781	1.36182
H	5.03314	-0.32761	2.74479
H	3.94924	0.7722	3.57631
O	-2.47551	-3.94709	1.7388
H	-2.5581	-3.81077	2.69655
H	-1.45624	-3.18257	0.2061
H	2.46226	-4.00303	-1.30598
H	1.00819	-0.62375	0.20179
H	3.04307	-1.55505	-1.7775
H	-0.1965	-0.92184	1.16664

$$\Delta E_{\text{solv}} = -2240.19510359$$

$$\Delta G_{\text{correction}} = 0.472679$$

Charge = 0 Multiplicity = 4

C	0.11164	-2.17401	1.74017
N	1.06485	-1.85227	0.81343
C	1.47158	-3.03308	0.24697
C	0.7378	-4.12438	0.81748
C	-0.08937	-3.59369	1.75842
Fe	1.61261	-0.02863	0.22131
O	0.70422	-0.10344	-1.16219
C	2.5288	-3.15084	-0.64153
C	3.37048	-2.11595	-1.03444
N	3.19948	-0.80662	-0.69456
C	4.28721	-0.13544	-1.17388
C	5.18576	-1.05369	-1.81415
C	4.60287	-2.27927	-1.75235
C	4.42805	1.24554	-1.16527
C	3.4514	2.15143	-0.77131
N	2.2613	1.80885	-0.19704
C	1.53397	2.96218	-0.09395
C	2.28399	4.06254	-0.62967
C	3.48679	3.5649	-1.01917
C	0.32638	3.07434	0.58369
C	-0.2572	2.06394	1.33651
N	0.18208	0.76772	1.36357
C	-0.60552	0.11748	2.29034
C	-1.51824	1.04691	2.88714
C	-1.32421	2.24477	2.27887
C	-0.6321	-1.25324	2.46885
S	2.87216	0.05126	2.33282
H	2.71559	1.36375	2.60127
H	-1.86501	3.17316	2.41148
H	-2.25194	0.78771	3.6413
H	-1.35813	-1.64914	3.17449
H	-0.78834	-4.1072	2.40793
H	0.86961	-5.16546	0.54818
H	2.77272	-4.15033	-0.99334
H	4.97618	-3.22208	-2.13362
H	6.12867	-0.77878	-2.27116
H	5.3355	1.65433	-1.60344
H	4.32361	4.09441	-1.45851
H	1.9341	5.08704	-0.66599
H	-0.15779	4.0472	0.60504
H	-1.32084	0.88333	-1.46534
C	-2.31965	0.84228	-1.92055
C	-3.15472	-0.23606	-1.19556
C	-2.9032	2.24371	-1.88401
H	-2.14588	0.51747	-2.95215
C	-3.89045	0.33399	-0.00319

C	-4.18505	-0.8649	-2.1593
C	-2.09017	-1.27775	-0.74414
C	-3.14776	2.66133	-0.45518
H	-2.24063	2.96753	-2.36825
C	-4.83102	-0.5859	0.71005
C	-3.80536	1.63389	0.34932
C	-5.23068	-1.75319	-1.49209
H	-3.63329	-1.42159	-2.9259
H	-4.69225	-0.04076	-2.68397
O	-1.35527	-1.75829	-1.835
O	-2.87289	3.77141	-0.01954
C	-5.88284	-1.07688	-0.29461
H	-4.29729	-1.45051	1.11746
H	-5.30908	-0.06029	1.54492
H	-4.3041	1.9834	1.25461
H	-5.99589	-2.02805	-2.22901
H	-4.76037	-2.68563	-1.16881
H	-6.47876	-0.21476	-0.62933
H	-6.58356	-1.75846	0.20226
H	-0.52067	-1.25268	-1.84399
O	-2.67237	-2.3829	-0.10201
H	-1.988	-3.06439	-0.10741
H	-1.40013	-0.75588	-0.05981
H	-3.86494	2.28711	-2.41671

$$\Delta E_{\text{solv}} = -2240.08868371$$

$$\Delta G_{\text{correction}} = 0.480087$$

41-ts

Charge = 0 Multiplicity = 4

C	-0.04194	-1.68573	1.98601
N	0.96708	-1.62026	1.07137
C	1.30898	-2.91534	0.78898
C	0.47625	-3.81827	1.53137
C	-0.35722	-3.05387	2.28292
Fe	1.74968	0.0416	0.23791
O	0.70716	-0.13666	-1.10896
C	2.36302	-3.29369	-0.02406
C	3.26672	-2.4333	-0.6348
N	3.20616	-1.07077	-0.5831
C	4.30758	-0.61535	-1.25045
C	5.09311	-1.71953	-1.71988
C	4.43615	-2.85026	-1.35265
C	4.57677	0.71887	-1.52131
C	3.74873	1.78865	-1.22156
N	2.57188	1.69713	-0.5318
C	2.04033	2.95326	-0.52075
C	2.8948	3.86106	-1.2319
C	3.9668	3.14056	-1.65016
C	0.88806	3.31879	0.16375
C	0.14673	2.49498	0.99274
N	0.41501	1.16728	1.22198
C	-0.54097	0.73863	2.09796
C	-1.41394	1.82064	2.45168
C	-0.99448	2.90811	1.75485
C	-0.73874	-0.58746	2.47392
S	3.16056	0.18537	2.1207
H	2.59721	1.26076	2.70801
H	-1.43852	3.89518	1.72623
H	-2.26707	1.73915	3.1144
H	-1.5534	-0.78621	3.16641
H	-1.13195	-3.37155	2.96995
H	0.54643	-4.89859	1.48916
H	2.53209	-4.36016	-0.15212
H	4.71474	-3.88136	-1.53368
H	6.01887	-1.62715	-2.27477
H	5.48723	0.93689	-2.07451
H	4.82946	3.47869	-2.21147
H	2.69722	4.91757	-1.36712
H	0.56554	4.35398	0.08031
H	-1.57774	1.00792	-0.50259
C	-2.3627	0.98268	-1.26892
C	-3.2506	-0.25527	-1.03265
C	-3.09541	2.31017	-1.22232
H	-1.82218	0.86034	-2.21374
C	-4.37874	0.02648	-0.07357

C	-3.82725	-0.78203	-2.36151
C	-2.23382	-1.31406	-0.41958
C	-3.86194	2.45735	0.07173
H	-2.40735	3.15437	-1.33504
C	-5.38353	-1.06513	0.1334
C	-4.56159	1.24231	0.48996
C	-4.88931	-1.86353	-2.20889
H	-2.99001	-1.13558	-2.97463
H	-4.26204	0.07713	-2.89576
O	-1.21112	-1.58211	-1.23895
O	-3.96309	3.51563	0.67273
C	-5.97751	-1.45547	-1.22657
H	-4.91502	-1.94706	0.57955
H	-6.17071	-0.72236	0.81413
H	-5.35938	1.38807	1.21981
H	-5.32919	-2.08417	-3.1895
H	-4.42003	-2.79038	-1.86492
H	-6.5397	-0.59948	-1.62844
H	-6.70602	-2.26418	-1.09465
H	-0.23125	-0.81406	-1.16778
O	-2.87281	-2.51503	-0.02558
H	-2.24794	-3.20419	-0.28468
H	-1.8866	-0.81457	0.5167
H	-3.82124	2.38984	-2.04561

$$\Delta E_{\text{solv}} = -2240.07795074$$

$$\Delta G_{\text{correction}} = 0.471287$$

Charge = 0 Multiplicity = 4

C	-0.07018	-1.72087	1.87063
N	0.95001	-1.64552	0.9666
C	1.29728	-2.93747	0.67288
C	0.43797	-3.84679	1.37426
C	-0.40168	-3.09172	2.12926
Fe	1.82445	0.0241	0.24595
O	0.79922	-0.08409	-1.20554
C	2.38336	-3.31267	-0.09752
C	3.31951	-2.45026	-0.65043
N	3.27743	-1.08629	-0.57433
C	4.38482	-0.62935	-1.23343
C	5.16181	-1.73534	-1.71036
C	4.49248	-2.86531	-1.36184
C	4.66633	0.70367	-1.49221
C	3.84199	1.77203	-1.18304
N	2.65961	1.68129	-0.50159
C	2.14303	2.94337	-0.45925
C	3.01428	3.85567	-1.14308
C	4.07765	3.13116	-1.57701
C	0.98579	3.31021	0.21433
C	0.21633	2.47474	1.00311
N	0.4547	1.13622	1.20453
C	-0.52586	0.69996	2.04865
C	-1.38582	1.78829	2.4131
C	-0.93417	2.88583	1.75168
C	-0.75024	-0.63082	2.39404
S	3.17255	0.1083	2.10387
H	2.51893	1.07057	2.78654
H	-1.35971	3.8814	1.73909
H	-2.25166	1.70383	3.05918
H	-1.55377	-0.83374	3.09771
H	-1.19017	-3.41717	2.79732
H	0.50011	-4.92654	1.30892
H	2.54586	-4.37784	-0.24144
H	4.76094	-3.8962	-1.55917
H	6.0902	-1.64407	-2.26124
H	5.58184	0.92156	-2.0363
H	4.94703	3.47171	-2.12654
H	2.83115	4.91784	-1.25262
H	0.68063	4.35181	0.15271
H	-1.59585	0.86378	-0.39014
C	-2.33889	0.87918	-1.19556
C	-3.35328	-0.25366	-0.96546
C	-2.94691	2.26915	-1.2426
H	-1.76436	0.67072	-2.10371
C	-4.49493	0.15921	-0.07523

C	-3.90942	-0.78973	-2.29855
C	-2.45494	-1.4116	-0.26109
C	-3.77654	2.54468	-0.01095
H	-2.17559	3.03906	-1.34332
C	-5.60175	-0.83123	0.1223
C	-4.60085	1.41313	0.41963
C	-5.06799	-1.76904	-2.16146
H	-3.08132	-1.23028	-2.86593
H	-4.24679	0.08548	-2.87608
O	-1.41487	-1.73027	-0.96603
O	-3.83098	3.63743	0.52953
C	-6.16078	-1.22971	-1.24983
H	-5.23865	-1.72822	0.63153
H	-6.38777	-0.38924	0.7442
H	-5.42266	1.66177	1.09258
H	-5.47843	-1.98727	-3.15506
H	-4.70053	-2.72064	-1.76496
H	-6.62847	-0.34855	-1.71319
H	-6.9606	-1.96878	-1.12427
H	0.02579	-0.68845	-1.14392
O	-3.23521	-2.52262	0.15391
H	-2.71086	-3.28892	-0.11397
H	-2.14988	-0.88445	0.68836
H	-3.60997	2.37968	-2.11403

$$\Delta E_{\text{solv}} = -2240.080935$$

$$\Delta G_{\text{correction}} = 0.474811$$

42-ts

Charge = 0 Multiplicity = 4

C	-6.14484	-1.24444	-1.46092
C	-5.68859	-0.85027	-0.05223
C	-4.5678	0.14121	-0.14561
C	-3.40341	-0.21502	-0.99343
C	-3.82667	-0.79556	-2.34162
C	-4.98527	-1.78199	-2.28583
C	-4.66785	1.35914	0.44473
C	-3.815	2.5034	0.11353
C	-2.93096	2.29168	-1.09396
C	-2.35074	0.8866	-1.11549
C	-2.46714	-1.48416	-0.16215
O	-3.28838	-2.56003	0.20122
O	-3.8901	3.56484	0.71059
O	-1.45859	-1.76203	-0.88115
O	0.77304	-0.10915	-1.1819
Fe	1.83413	0.03223	0.24643
S	3.22355	0.16746	2.06792
N	0.98618	-1.62747	1.01781
C	-0.02135	-1.68982	1.9384
C	-0.33527	-3.05732	2.23452
C	0.50038	-3.82221	1.48579
C	1.34075	-2.9221	0.74978
C	-0.69375	-0.59485	2.45819
C	-0.4865	0.72799	2.08125
N	0.47726	1.15578	1.21123
C	0.22894	2.4885	0.99084
C	-0.90974	2.90701	1.75309
C	-1.3451	1.81896	2.44103
C	2.41556	-3.30816	-0.0319
C	3.32984	-2.45127	-0.62635
N	3.27592	-1.08578	-0.58472
C	4.36028	-0.63513	-1.28529
C	5.13569	-1.74604	-1.75393
C	4.48849	-2.87288	-1.3575
C	4.62407	0.69279	-1.58394
C	3.80064	1.7619	-1.27526
N	2.63869	1.67951	-0.55932
C	2.1172	2.94034	-0.52524
C	2.965	3.84298	-1.25069
C	4.01828	3.11452	-1.70179
C	0.97678	3.31465	0.17045
H	2.56927	1.12831	2.75195
H	-1.34055	3.90038	1.73182
H	-2.19908	1.74323	3.1041
H	-1.48396	-0.7892	3.17922
H	-1.11063	-3.3747	2.92162

H	0.571	-4.90264	1.44433
H	2.58529	-4.37512	-0.15185
H	4.76259	-3.90602	-1.53474
H	6.04804	-1.66007	-2.3319
H	5.52274	0.90439	-2.15766
H	4.87017	3.44792	-2.28235
H	2.77429	4.90231	-1.37459
H	0.66645	4.35417	0.09961
H	-1.63846	0.80521	-0.28731
H	-1.74714	0.72086	-2.01335
H	-2.14097	3.04875	-1.1063
H	-2.94812	-1.23322	-2.82794
H	-4.12136	0.06437	-2.96631
H	-5.35789	-1.74957	0.4768
H	-6.51797	-0.41849	0.51794
H	-5.50855	1.57588	1.10482
H	-5.31678	-2.01119	-3.30557
H	-4.64531	-2.73151	-1.85893
H	-6.57657	-0.36428	-1.9593
H	-6.95136	-1.98384	-1.39728
H	0.01312	-0.72106	-1.08168
H	-2.91428	-3.32163	-0.26349
H	-2.28383	-0.89034	0.76434
H	-3.54979	2.47406	-1.98574

$$\Delta E_{\text{solv}} = -2240.08152431$$

$$\Delta G_{\text{correction}} = 0.475174$$

Charge = 0 Multiplicity = 4

C	-3.97706	-1.38668	-3.38321
C	-4.2727	-1.40328	-1.89029
C	-3.78775	-0.16785	-1.16953
C	-2.92227	0.72306	-1.79279
C	-2.33075	0.46695	-3.13801
C	-2.54034	-0.95546	-3.63309
C	-4.1614	0.03314	0.17036
C	-3.87874	1.25068	0.89506
C	-3.37797	2.39563	0.03819
C	-2.44283	1.9342	-1.06809
C	-1.70445	-2.40266	0.08118
O	-2.51621	-3.21417	0.76804
O	-4.0801	1.37495	2.1023
O	-1.0378	-2.74802	-0.8626
O	0.10232	-0.09685	-0.8062
Fe	1.43362	0.17212	0.39977
S	3.15678	0.51144	1.85617
N	1.95545	-1.77048	0.22308
C	1.59933	-2.80106	1.0512
C	2.22693	-4.01538	0.61984
C	2.97332	-3.70757	-0.47154
C	2.82001	-2.29986	-0.69715
C	0.73031	-2.70078	2.12412
C	0.05718	-1.54965	2.50103
N	0.22388	-0.31242	1.93241
C	-0.72138	0.50106	2.50617
C	-1.5054	-0.2435	3.44715
C	-1.00724	-1.50738	3.46055
C	3.51144	-1.57831	-1.65515
C	3.48098	-0.20124	-1.80057
N	2.73736	0.66234	-1.04133
C	2.98075	1.91698	-1.53257
C	3.92767	1.84445	-2.60566
C	4.23096	0.53148	-2.7774
C	2.35912	3.0798	-1.10964
C	1.36151	3.15125	-0.15283
N	0.85818	2.08798	0.54615
C	-0.10896	2.59367	1.37304
C	-0.22652	4.00953	1.17948
C	0.6898	4.35636	0.23876
C	-0.87381	1.85427	2.25887
H	2.47095	0.39314	3.01168
H	-2.34381	0.1664	3.99624
H	-1.34977	-2.36112	4.03318
H	0.51482	-3.60889	2.6816
H	2.10323	-4.977	1.10375

H	3.59658	-4.36154	-1.0697
H	4.15967	-2.13517	-2.32663
H	4.90218	0.08283	-3.50008
H	4.29376	2.69983	-3.16095
H	2.65647	4.00743	-1.59162
H	0.90469	5.33894	-0.16442
H	-0.9217	4.64584	1.71476
H	-1.6652	2.36734	2.79828
H	-1.45255	1.67397	-0.66224
H	-2.24637	2.74687	-1.78094
H	-2.91823	3.15455	0.6772
H	-1.26181	0.71936	-3.09054
H	-2.7579	1.18818	-3.8566
H	-3.81297	-2.29306	-1.43591
H	-5.34803	-1.52353	-1.70708
H	-4.69066	-0.75121	0.71303
H	-2.28175	-1.03235	-4.69486
H	-1.85904	-1.63108	-3.099
H	-4.66027	-0.68823	-3.88782
H	-4.17756	-2.37289	-3.81659
H	-0.00351	-1.0277	-1.0652
H	-2.44292	-4.09525	0.36644
H	-1.75044	-1.38099	0.48769
H	-4.26867	2.86664	-0.4057

$$\Delta E_{\text{solv}} = -2240.13971941$$

$$\Delta G_{\text{correction}} = 0.471571$$

43-ts

Charge = 0 Multiplicity = 4

C	-1.20491	-2.94691	-1.04607
N	-1.68539	-2.01361	-0.16387
C	-2.37014	-2.71443	0.79502
C	-2.27781	-4.1212	0.53497
C	-1.56344	-4.26452	-0.61101
Fe	-1.57398	-0.0066	-0.33709
O	0.04283	-0.07862	0.83534
C	-3.10382	-2.15264	1.82603
C	-3.29006	-0.79492	2.03432
N	-2.7517	0.20589	1.27001
C	-3.15413	1.38498	1.84097
C	-3.98843	1.11851	2.97409
C	-4.06766	-0.23295	3.098
C	-2.76537	2.6504	1.43163
C	-1.88812	2.92513	0.39635
N	-1.29589	1.98597	-0.40374
C	-0.50699	2.67702	-1.28272
C	-0.58249	4.0847	-1.01392
C	-1.44922	4.23918	0.01954
C	0.24244	2.11255	-2.30056
C	0.2864	0.76411	-2.61245
N	-0.40166	-0.22888	-1.95976
C	-0.07154	-1.40103	-2.59028
C	0.82944	-1.13883	-3.67187
C	1.06129	0.20158	-3.67726
C	-0.46713	-2.66695	-2.18328
S	-3.5072	0.11776	-1.662
H	-2.91322	0.14005	-2.87286
H	1.70006	0.77373	-4.33972
H	1.24815	-1.8985	-4.3215
H	-0.13961	-3.50907	-2.78803
H	-1.30126	-5.17776	-1.13232
H	-2.72831	-4.89142	1.14983
H	-3.59816	-2.8336	2.51402
H	-4.60192	-0.81141	3.8425
H	-4.4416	1.88029	3.59749
H	-3.16456	3.49646	1.98522
H	-1.76619	5.15596	0.50274
H	-0.01635	4.83741	-1.54736
H	0.86075	2.78359	-2.88892
C	2.03941	1.2122	1.90077
C	3.19978	0.41044	1.72579
C	1.97514	2.54512	1.19065
C	4.03116	0.59736	0.58783
C	3.47385	-0.67271	2.72716
C	2.0441	-2.04774	-0.28367

C	2.74692	2.62174	-0.11043
H	0.94364	2.86691	1.01001
C	5.19555	-0.32804	0.33842
C	3.7644	1.61237	-0.31102
C	4.51069	-1.70207	2.29896
H	2.52613	-1.15938	2.99547
H	3.80657	-0.18436	3.65789
O	1.5634	-2.50734	0.72181
O	2.55897	3.52905	-0.91606
C	5.6796	-1.03012	1.598
H	4.89328	-1.08414	-0.40221
H	6.00747	0.23249	-0.13892
H	4.37171	1.71795	-1.21014
H	4.84544	-2.27672	3.16947
H	4.04943	-2.43105	1.61973
H	6.14796	-0.30135	2.27504
H	6.45966	-1.75781	1.34809
O	2.90625	-2.7008	-1.07359
H	3.03051	-3.58392	-0.68899
H	1.84952	-1.03712	-0.67506
H	2.40017	3.32666	1.84173
H	1.07564	0.5457	1.36574
H	1.65861	1.23012	2.92816
H	0.23243	-1.0001	1.07704

$$\Delta E_{\text{solv}} = -2240.13764805$$

$$\Delta G_{\text{correction}} = 0.466383$$

Charge = 0 Multiplicity = 4

C	-2.05875	-1.67489	-1.90349
N	-2.19504	-0.61403	-1.04791
C	-3.4827	-0.6655	-0.58255
C	-4.1665	-1.79597	-1.14179
C	-3.27793	-2.4316	-1.95059
Fe	-0.83889	0.85129	-0.7094
O	-0.00338	-0.61182	0.88077
C	-4.02732	0.21231	0.34211
C	-3.34112	1.24259	0.96723
N	-2.03191	1.57918	0.73227
C	-1.7372	2.59266	1.60806
C	-2.88294	2.89608	2.41207
C	-3.88079	2.06577	2.00736
C	-0.51623	3.2447	1.70329
C	0.58987	3.01076	0.90195
N	0.65872	2.066	-0.08666
C	1.89	2.22019	-0.66998
C	2.62099	3.27205	-0.02115
C	1.81608	3.75738	0.95977
C	2.36986	1.45909	-1.72242
C	1.69815	0.39842	-2.31317
N	0.44144	-0.03445	-1.97347
C	0.21085	-1.15969	-2.7233
C	1.33951	-1.4299	-3.56342
C	2.25917	-0.45892	-3.31394
C	-0.93514	-1.94003	-2.67115
S	-1.731	2.38291	-2.33062
H	-1.0415	1.9633	-3.41118
H	3.24141	-0.32995	-3.75411
H	1.41007	-2.26307	-4.25322
H	-0.97106	-2.81091	-3.32132
H	-3.43099	-3.32107	-2.55084
H	-5.19339	-2.06608	-0.92454
H	-5.0669	0.06091	0.62312
H	-4.89717	2.00443	2.37873
H	-2.9121	3.65821	3.18198
H	-0.43385	4.03397	2.44649
H	2.01789	4.5598	1.66008
H	3.6322	3.56315	-0.27726
H	3.37857	1.67112	-2.06773
C	2.96304	-0.48401	2.61945
C	2.66208	-1.59853	1.92367
C	3.79491	0.61774	2.07487
C	3.13313	-1.7262	0.53854
C	1.88056	-2.72835	2.55425
C	-2.6071	-2.40404	1.84573

C	4.3872	0.40252	0.69529
H	3.21551	1.55531	2.02988
C	2.60338	-2.84508	-0.31326
C	3.97217	-0.80361	0.00245
C	1.17437	-3.63679	1.55713
H	1.1728	-2.32346	3.28812
H	2.58518	-3.34038	3.13797
O	-1.95493	-1.68634	2.56456
O	5.12589	1.23746	0.18939
C	2.13999	-4.06656	0.46531
H	1.73637	-2.43602	-0.85522
H	3.33459	-3.10102	-1.08835
H	4.32837	-0.91677	-1.02098
H	0.75122	-4.50246	2.07969
H	0.33728	-3.09735	1.09749
H	3.0004	-4.58884	0.90845
H	1.6679	-4.78128	-0.21793
O	-3.80247	-2.89766	2.15936
H	-4.03468	-2.55535	3.03804
H	-2.30315	-2.75557	0.84729
H	4.61119	0.86499	2.76781
H	0.80914	-0.31753	1.30928
H	2.59768	-0.38131	3.64298
H	-0.61886	-0.87246	1.58702

$$\Delta E_{\text{solv}} = -2240.21257541$$

$$\Delta G_{\text{correction}} = 0.468335$$