Supporting Information

Optimized Geometry for model of 1

Ni	0.00000	0.00000	0.00000
Fe	-1.28273	0.00000	2.23634
Fe	1.28273	0.00000	2.24787
O	-1.74858	2.92375	2.21622
H	0.72922	4.17879	-2.58617
H	-1.68605	3.30302	-1.88738
H	2.06048	4.14502	-4.68563
H	-2.27173	2.42590	-0.45245
O	1.53745	2.90056	2.84868
C	1.19771	3.25333	-2.92403
C	-1.63946	2.34645	-1.34695
C	-1.55096	1.77126	2.22589
C	1.95217	3.23303	-4.09724
S	0.06664	2.15710	-0.63146
H	-3.15194	1.25470	-2.43177
C	1.42687	1.77104	2.59515
C	1.04467	2.08570	-2.15991
C	-2.06776	1.20517	-2.25898
O	-1.59529	-0.19389	5.16209
H	-1.55817	1.27171	-3.22754
C	2.59082	2.05392	-4.49814
C	-1.46330	-0.12900	4.00858
H	3.19875	2.04061	-5.40380
C	-2.92256	-0.58575	1.76552
O	-3.99704	-0.92440	1.46774
C	1.69678	0.90338	-2.55701
C	2.48072	0.90117	-3.72099
S	-1.70033	-0.48940	-1.56239
C	1.66853	-0.52549	3.90866
O	1.92704	-0.86798	4.98800
H	-0.64911	-0.45425	-3.75541
C	2.92673	-0.33359	1.59293
H	3.01572	-0.00677	-4.00556
S	1.62652	-0.57887	-1.52135
O	3.99042	-0.53510	1.16163
C	-0.73512	-1.22595	-2.98102
S	0.00625	-1.64329	1.49297
H	-1.33523	-2.05461	-3.38395
C	0.64068	-1.74023	-2.57849
H	1.22916	-1.99671	-3.47210
H	0.57395	-2.63421	-1.94305

Total Energy: -9.62942691 a.u.

Optimized Geometry for model of 1^-

Ni	0.00000	0.00000	0.00000
Fe	1.34560	0.00000	2.33989
Fe	-1.34560	0.00000	2.31436
O	1.95876	-2.90229	2.23495
H	-0.53965	-4.14447	-2.67326
H	1.82079	-3.24293	-1.84693
H	-1.81508	-4.15648	-4.80700
H	2.30349	-2.37062	-0.36563
O	-1.55444	-2.92880	2.78527
C	-1.01893	-3.23035	-3.02909
C	1.73224	-2.29208	-1.29912
C	1.66607	-1.76121	2.27142
C	-1.74458	-3.23865	-4.22041
S	-0.01489	-2.11429	-0.67420
H	3.30896	-1.17492	-2.26135
C	-1.43599	-1.78082	2.58108
C	-0.90856	-2.06086	-2.26046
C	2.21369	-1.13724	-2.16694
O	1.67582	0.27798	5.27777
H	1.77908	-1.20176	-3.17311
C	-2.40853	-2.07601	-4.64078
C	1.51636	0.20143	4.11990
H	-2.99848	-2.08018	-5.55939
C	2.95300	0.59404	1.83949
O	4.04229	0.95659	1.57984
C	-1.57541	-0.88712	-2.68559
C	-2.33652	-0.91859	-3.86730
S	1.77605	0.55055	-1.48512
C	-1.77461	0.49033	3.98362
O	-2.13480	0.78166	5.06022
H	0.85039	0.48323	-3.74197
C	-2.92909	0.34676	1.57139
H	-2.88087	-0.02110	-4.16844
S	-1.56471	0.59685	-1.65355
O	-3.98342	0.58528	1.11052
C	0.89159	1.25932	-2.96713
S	-0.00828	1.58286	1.55240
H	1.49850	2.09511	-3.34637
C	-0.51314	1.75874	-2.64429
H	-1.03848	2.02999	-3.57218
H	-0.48143	2.64556	-1.99346

Total Energy: -9.69519261 a.u.