Supporting Information

Hydrogen evolution, electron-transfer, hydride-transfer reactions in a nickel-iron hydrogenase model complex: A theoretical study of the distinctive reactivities for the conformational isomers of nickel-iron hydride

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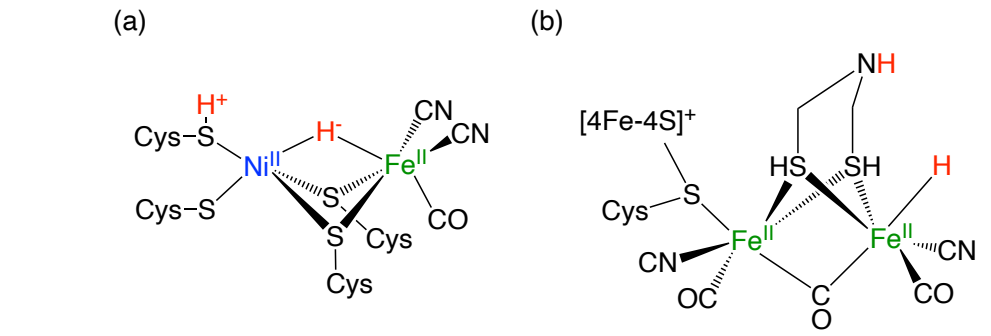

Fig. S1 Metal hydride complexes produced by H_2 activation/evolution by (a) NiFe hydrogenase and (b) FeFe hydrogenase.

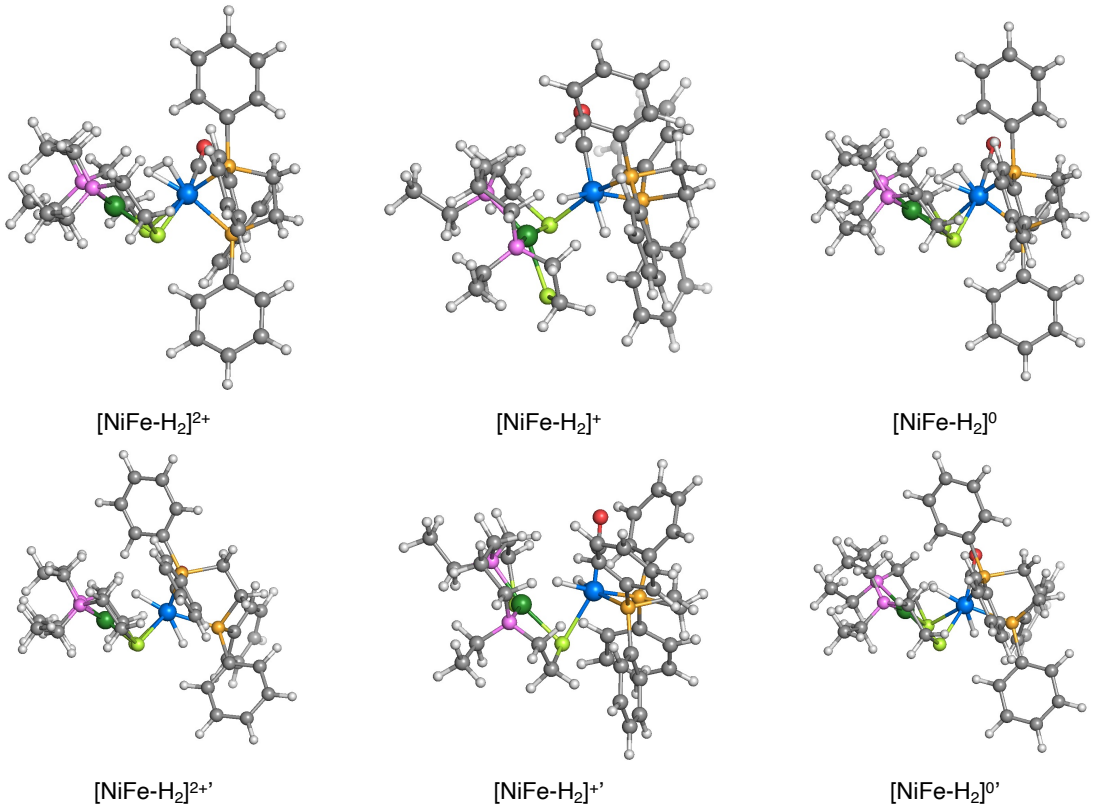

Fig. S2 Structures of intermediates of proton-transfer, hydrogen-atom-transfer, and hydride-transfer reactions occurring between NiFe hydride complexes.

Table S1 Relative energy (kcal/mol) for the singlet spin state. The spin multiplicity of the ground state is shown in bold

$[NiFe\text{-}H_2]^{2+}$			
S = 0	S = 1	S = 2	S = 3
0.0	16.2	32.7	54.1
$[NiFe\text{-}H_2]^{+}$			
S = 1/2	S = 3/2	S = 5/2	S = 7/2
0.0	16.9	24.5	67.8
$[NiFe\text{-}H_2]^{0}$			
S = 0	S = 1	S = 2	S = 3
0.0	1.1	37.2	67.5
$[NiFe]^{0}$			
S = 0	**S = 1**	S = 2	S = 3
0.0	**-4.8**	9.3	46.0
$[NiFe]^{+}$			
S = 1/2	S = 3/2	S = 5/2	S = 7/2
0.0	12.3	33.1	82.1
$[NiFe]^{2+}$			
S = 0	S = 1	S = 2	S = 3
0.0	8.6	25.7	53.1

Table S2 Experimentally determined product yields at specific times for electron transfer, hydride transfer, and H_2 generation reactions in NiFe hydride complexes

	2a	**2b**	**2c**
Electron transfer (1 minute)	57%	27%	33%
Hydride transfer (60 minites)	4%	14%	31%
H_2 evolution (30 minites)	16%	55%	9%

The data is taken from previous study.[11]

[a] $[Fe^{III}(C_5Me_5)_2]^+$ is used as electron acceptor in electron transfer reaction.

[b] MB is used as hydride acceptor in the hydride transfer reaction.

[c] CH_3COOH is used as proton donor in the H_2 evolution reaction.

Table S3 Reaction energies (kcal/mol) for coordination of H_2O and CH_3CN to vacant sites of Fe produced by hydride removal and H_2 removal, respectively

	2a + X → **2a**-X	**2b** + X → **2b**-X	**2c** + X → **2c**-X
		H_2O	
ΔG	14.6	6.4	3.3
		CH_3CN	
ΔG	4.2	-2.7	-9.4

Table S4 Reaction barriers (kcal/mol), rate constant (s^{-1}), and kinetic isotope effect for hydride transfer

	ΔG_H	ΔG_D	k_H	k_D	k_H/k_D
2a	21.3	24.4	0.2×10^{-2}	0.8×10^{-5}	187.2
2b	8.0	12.6	0.8×10^{7}	0.4×10^{4}	2354.1
2c	17.4	22.5	0.1×10	0.2×10^{-3}	5474.2

Table S5. Imaginary frequencies (cm^{-1}) of optimized transition states

label	frequency
TS-2a2b^{+}(acetone)	-499.3
TS-2a2c^{+}(acetone)	-47.8
TS-2b2c^{+}(acetone)	-189.7
TS-HD-a^{2+}(water)	-269.0
TS-HD-b^{2+}(water)	-542.3
TS-HD-c^{2+}(water)	-4430.1
TS-HT-a^{2+}(acetonitrile)	-359.7
TS-HT-b^{2+}(acetonitrile)	-879.0
TS-HT-c^{2+}(acetonitrile)	-1051.3
TS-PTa^{+}(water)	-467.6
TS-PTb^{+}(water)	-758.5
TS-PTc^{+}(water)	-595.8

Table S6. Total electronic energy (E_{SCF}), thermal correction to enthalpy (H_{corr}), and thermal correction to free energy (G_{corr}). All are given in a.u.

label	E_{SCF}	H_{corr}	G_{corr}
2a^{+}(acetone)	-3437.5101454	0.824337	0.69449
2a^{+}(acetonitrile)	-3437.5103864	0.824343	0.694976
2a^{+}(water)	-3437.4781160	0.824615	0.694348
2ad^{+}(acetone)	-3437.5057554	0.82399	0.693203
2add^{+}(acetone)	-3437.5028890	0.824459	0.694048
2b^{+}(acetone)	-3437.5022114	0.824166	0.695035
2b^{+}(acetonitrile)	-3437.5025265	0.823982	0.694805
2b^{+}(water)	-3437.4713328	0.824417	0.695475
2bd^{+}(acetone)	-3437.5048390	0.824063	0.694861
2bdd^{+}(acetone)	-3437.5018544	0.824112	0.693168
2c^{+}(acetone)	-3437.5043176	0.824092	0.692302
2c^{+}(acetonitrile)	-3437.5046509	0.824286	0.69382
2c^{+}(water)	-3437.4729372	0.824706	0.695091
2cd^{+}(acetone)	-3437.4968298	0.823683	0.693329
2cdd^{+}(acetone)	-3437.5043053	0.824106	0.691933
3a^{2+}(acetonitrile)	-3436.7712756	0.818508	0.692569
3a^{2+}(water)	-3436.7442795	0.819588	0.692639
3ad^{2+}(acetonitrile)	-4620.7370170	1.155859	0.982146
3b^{2+}(acetonitrile)	-3569.6102010	0.868201	0.730326
3b^{2+}(water)	-3436.7458124	0.819143	0.694351
3c^{2+}(acetonitrile)	-3569.6018212	0.86847	0.731939
3c^{2+}(water)	-3436.7195734	0.818223	0.688685
4a^{2+}(water)	-3437.9168244	0.835226	0.705287
4b^{2+}(water)	-3437.9180518	0.836137	0.706893
4c^{2+}(water)	-3437.9163798	0.836088	0.707501
TS-2a2b^{+}(acetone)	-3437.4571059	0.822135	0.691822
TS-2a2c^{+}(acetone)	-3437.4682316	0.822519	0.693758
TS-2b2c^{+}(acetone)	-3437.4653189	0.82181	0.691647
TS-HD-a^{2+}(water)	-3437.9120168	0.832181	0.702649
TS-HD-b^{2+}(water)	-3437.9146285	0.83201	0.702278
TS-HD-c^{2+}(water)	-3437.8999451	0.831588	0.700124
TS-HT-a^{2+}(acetonitrile)	-4620.7242812	1.148991	0.978147
TS-HT-b^{2+}(acetonitrile)	-4620.7367498	1.147041	0.977048
TS-HT-c^{2+}(acetonitrile)	-4620.7208038	1.146888	0.972981

Table S7 (Continue). Total electronic energy (E_{SCF}), thermal correction to enthalpy (H_{corr}), and thermal correction to free energy (G_{corr}). All are given in a.u.

label	E_{SCF}	H_{corr}	G_{corr}
TS-PT-a$^+$(water)	-3743.1612580	0.912745	0.76415
TS-PT-b$^+$(water)	-3743.1609015	0.913241	0.76599
TS-PT-c$^+$(water)	-3743.1641398	0.913525	0.766868
CH_3COOH-H_2O(water)	-305.6838927	0.091747	0.051747
CH_3COO-H_2O(water)	-305.2266496	0.078754	0.039644
H_2(water)	-1.1748220	0.013032	-0.001822
H_2O(water)	-76.4755123	0.024229	0.002747
MBH(acetonitrile)	-1183.9750398	0.333988	0.264365
MB(acetonitrile)	-1183.2224384	0.324199	0.257719
MeCN(acetonitrile)	-132.8155918	0.048157	0.019518

XYZ coordinate

$2a^+$ (acetone)

Ni	1.624992	-1.290651	-0.854392
Fe	-0.395313	-0.152485	0.373523
S	0.230338	0.073748	-1.959142
S	-0.304708	-2.341246	-0.504100
P	-0.334146	1.922028	1.039856
P	-2.637180	0.080301	0.197710
O	-0.442528	-0.980914	3.148803
N	3.189464	-0.155889	-1.405088
N	2.579702	-2.721776	0.193841
C	-0.453855	-0.638797	2.020477
C	-1.986689	2.262337	1.868052
H	-1.920228	1.748407	2.850750
H	-2.116957	3.347833	2.053914
C	-3.135621	1.700896	1.018532
H	-3.381507	2.406939	0.200658
H	-4.060473	1.567734	1.615432
C	-0.175017	3.264812	-0.221263
C	-1.103344	3.316743	-1.289548
H	-1.910271	2.573593	-1.371073
C	-0.977538	4.288427	-2.295589
H	-1.708890	4.314663	-3.119081
C	0.089974	5.206119	-2.265280
H	0.194984	5.959568	-3.062191
C	1.027639	5.147478	-1.219366
H	1.872773	5.854004	-1.193025
C	0.896032	4.185614	-0.200445
H	1.642086	4.150518	0.608014
C	0.904723	2.379352	2.330086
C	0.727651	3.515287	3.153661
H	-0.160675	4.155837	3.037910
C	1.693968	3.843931	4.120190
H	1.546469	4.729114	4.759558
C	2.846351	3.048972	4.269989
H	3.602052	3.311089	5.027827
C	3.028628	1.919208	3.452041
H	3.926684	1.290496	3.564052
C	2.060088	1.584341	2.489950
H	2.182996	0.692683	1.853546
C	-3.553866	0.068216	-1.407874
C	-3.079155	-0.769611	-2.443476
H	-2.182005	-1.385279	-2.280908
C	-3.746924	-0.825421	-3.679556
H	-3.365733	-1.485551	-4.475240
C	-4.890207	-0.036771	-3.900172
H	-5.409963	-0.074156	-4.871029
C	-5.370356	0.798787	-2.874290
H	-6.270253	1.413485	-3.037882
C	-4.711440	0.849066	-1.633201
H	-5.115818	1.496904	-0.839934
C	-3.489538	-1.243382	1.163114
C	-3.779954	-2.486413	0.554256
H	-3.615722	-2.626739	-0.525495
C	-4.284462	-3.551551	1.320247
H	-4.510221	-4.513184	0.831493
C	-4.504697	-3.391206	2.701304
H	-4.901555	-4.226693	3.300024
C	-4.216217	-2.157340	3.312499
H	-4.385532	-2.021887	4.393048
C	-3.706929	-1.090031	2.551372
H	-3.469048	-0.139004	3.053289
C	1.476228	1.368415	-2.385687
H	1.737395	1.211211	-3.451879
H	1.017104	2.370172	-2.303645
C	2.670169	1.252836	-1.471764
H	3.483553	1.947568	-1.779035
H	2.367071	1.523832	-0.440359
C	3.607137	-0.685267	-2.754268
H	2.689476	-0.773825	-3.366560
H	3.957341	-1.721137	-2.589561
C	4.671997	0.117739	-3.504530
H	4.873278	-0.389232	-4.470749
H	4.338395	1.149848	-3.735507
H	5.633503	0.174551	-2.955129
C	4.323305	-0.145934	-0.433593
H	3.961462	0.404119	0.457886
H	5.156936	0.450425	-0.863227
C	4.821023	-1.517535	0.002848
H	5.734312	-1.355333	0.612278
H	5.143744	-2.137606	-0.858831
C	3.816202	-2.245403	0.884670
H	4.298203	-3.109032	1.391423
H	3.475414	-1.553439	1.681810
C	2.861123	-3.830123	-0.788408
H	3.526419	-3.404849	-1.563391
H	1.906435	-4.053294	-1.302133
C	3.469436	-5.113365	-0.218851
H	3.605729	-5.832331	-1.052928
H	4.464809	-4.950300	0.241610
H	2.810636	-5.598335	0.529882
C	1.633113	-3.143786	1.283536
H	1.516325	-2.260125	1.937420
H	2.091412	-3.953279	1.894322
C	0.279329	-3.562358	0.753745
H	-0.462948	-3.611796	1.575783
H	0.302064	-4.552395	0.254124
H	1.153095	-0.282668	0.550358

$2a^+$ (acetonitrile)

Ni	1.620945	-1.289057	-0.864006
Fe	-0.396899	-0.153998	0.369439
S	0.226708	0.079823	-1.964251
S	-0.310374	-2.339255	-0.517020
P	-0.324129	1.917473	1.043749
P	-2.638003	0.088143	0.201251
O	-0.449204	-0.991386	3.141850
N	3.185640	-0.153772	-1.408545
N	2.574197	-2.724610	0.179276
C	-0.456982	-0.645213	2.014310
C	-1.973117	2.260940	1.877450
H	-1.905225	1.742483	2.857558
H	-2.098664	3.345894	2.069097
C	-3.128154	1.706274	1.031534
H	-3.377335	2.416038	0.217942
H	-4.049799	1.572252	1.632989
C	-0.160890	3.266910	-0.209715
C	-1.098305	3.335760	-1.269038
H	-1.914732	2.602785	-1.347034
C	-0.971035	4.312233	-2.270341
H	-1.710161	4.351933	-3.086319
C	0.106599	5.218202	-2.244175
H	0.212202	5.975726	-3.037081
C	1.052973	5.142882	-1.207107
H	1.905642	5.840365	-1.183986

C	0.920208	4.176045	-0.192989
H	1.673667	4.127366	0.607869
C	0.917739	2.360365	2.336078
C	0.758020	3.508721	3.146134
H	-0.115981	4.165995	3.015811
C	1.723528	3.827957	4.116557
H	1.589894	4.723475	4.744470
C	2.857723	3.010423	4.284124
H	3.613313	3.265259	5.044566
C	3.022042	1.867634	3.480433
H	3.905635	1.221404	3.606463
C	2.054394	1.542292	2.513829
H	2.164266	0.640370	1.889197
C	-3.560778	0.085176	-1.400758
C	-3.091354	-0.749773	-2.441114
H	-2.194477	-1.367189	-2.283513
C	-3.764054	-0.800321	-3.674836
H	-3.387244	-1.458284	-4.474387
C	-4.907202	-0.009238	-3.887990
H	-5.430889	-0.042629	-4.856841
C	-5.381940	0.823678	-2.857263
H	-6.281627	1.440103	-3.015312
C	-4.717972	0.868760	-1.618565
H	-5.117646	1.514610	-0.821317
C	-3.491335	-1.238310	1.162696
C	-3.788295	-2.477153	0.548230
H	-3.630160	-2.611628	-0.533197
C	-4.290107	-3.546073	1.310873
H	-4.520229	-4.504313	0.817590
C	-4.501368	-3.393790	2.694318
H	-4.895683	-4.232246	3.290508
C	-4.207014	-2.163945	3.311112
H	-4.369405	-2.034802	4.393486
C	-3.700412	-1.092908	2.553271
H	-3.457600	-0.145305	3.059237
C	1.474321	1.373489	-2.388802
H	1.735802	1.217206	-3.455006
H	1.015898	2.375586	-2.306387
C	2.667680	1.255536	-1.474128
H	3.482052	1.949689	-1.779799
H	2.365074	1.525565	-0.442430
C	3.607632	-0.680360	-2.757528
H	2.693267	-0.759389	-3.375955
H	3.949701	-1.719339	-2.595563
C	4.682555	0.118922	-3.496939
H	4.888508	-0.384904	-4.463726
H	4.357164	1.154065	-3.725900
H	5.639835	0.167667	-2.939481
C	4.316247	-0.145952	-0.432816
H	3.949933	0.398641	0.460285
H	5.149336	0.454787	-0.857148
C	4.816232	-1.518939	-0.003524
H	5.728088	-1.358264	0.608470
H	5.141584	-2.133210	-0.868366
C	3.811935	-2.254157	0.872785
H	4.293690	-3.122446	1.371874
H	3.472130	-1.568481	1.675716
C	2.852783	-3.829870	-0.807512
H	3.532573	-3.408156	-1.571657
H	1.901219	-4.037522	-1.333589
C	3.436844	-5.125202	-0.240274
H	3.576868	-5.838397	-1.078724
H	4.427155	-4.978684	0.236441
H	2.760383	-5.607975	0.493960
C	1.626888	-3.148940	1.267258
H	1.509897	-2.266915	1.923254
H	2.084933	-3.959857	1.876097
C	0.273296	-3.566049	0.735771
H	-0.468607	-3.619066	1.557850
H	0.297092	-4.554012	0.232368
H	1.151053	-0.288303	0.543709

$2a^{+}$ (water)

Ni	1.598365	-1.260633	-0.913111
Fe	-0.405536	-0.164061	0.348129
S	0.196866	0.148448	-1.979476
S	-0.336596	-2.327336	-0.597157
P	-0.316589	1.882731	1.090693
P	-2.645202	0.091468	0.221644
O	-0.460269	-1.073133	3.095046
N	3.169891	-0.107826	-1.426513
N	2.548810	-2.714637	0.110844
C	-0.461435	-0.700793	1.972014
C	-1.950389	2.201651	1.960110
H	-1.867559	1.647606	2.919375
H	-2.067668	3.279651	2.190770
C	-3.119683	1.679919	1.112840
H	-3.379139	2.418118	0.328216
H	-4.032682	1.526026	1.722391
C	-0.160044	3.264170	-0.125737
C	-1.106770	3.365697	-1.174041
H	-1.929763	2.641231	-1.263067
C	-0.979339	4.364756	-2.152523
H	-1.724565	4.430770	-2.960745
C	0.106931	5.259814	-2.114911
H	0.212860	6.034067	-2.890990
C	1.062701	5.150923	-1.089750
H	1.923073	5.838009	-1.059577
C	0.930247	4.161825	-0.097694
H	1.692316	4.084217	0.692456
C	0.946554	2.272332	2.376986
C	0.815410	3.405236	3.213059
H	-0.048230	4.079913	3.105076
C	1.797307	3.685434	4.178839
H	1.687504	4.568516	4.828026
C	2.918611	2.844584	4.314837
H	3.686982	3.069289	5.071476
C	3.054291	1.717609	3.484251
H	3.927671	1.053754	3.584003
C	2.070317	1.430780	2.522500
H	2.159376	0.543462	1.874400
C	-3.591236	0.134229	-1.363771
C	-3.139283	-0.671581	-2.434333
H	-2.241985	-1.295749	-2.308312
C	-3.829396	-0.682884	-3.659102
H	-3.466871	-1.318143	-4.482773
C	-4.971233	0.119454	-3.833067
H	-5.508013	0.117197	-4.794928
C	-5.427387	0.924253	-2.772373
H	-6.324983	1.550098	-2.899922
C	-4.746525	0.930015	-1.542287
H	-5.131287	1.554515	-0.721411
C	-3.461519	-1.272664	1.159567
C	-3.711967	-2.509881	0.521350
H	-3.553611	-2.616659	-0.562946

C	-4.164164	-3.613090	1.265242
H	-4.357990	-4.570036	0.754886
C	-4.371147	-3.497200	2.652840
H	-4.725342	-4.363078	3.234222
C	-4.123259	-2.269220	3.292661
H	-4.282516	-2.168801	4.378170
C	-3.666623	-1.163033	2.553883
H	-3.456028	-0.217775	3.078219
C	1.456308	1.441853	-2.369342
H	1.721628	1.301876	-3.436843
H	1.006699	2.446524	-2.271247
C	2.648926	1.300201	-1.456469
H	3.460987	2.004602	-1.744624
H	2.348558	1.544458	-0.417953
C	3.586790	-0.603046	-2.787958
H	2.667045	-0.698355	-3.396781
H	3.959971	-1.634428	-2.645801
C	4.628866	0.236072	-3.529717
H	4.849943	-0.259214	-4.497216
H	4.263145	1.258213	-3.755230
H	5.584369	0.319451	-2.973738
C	4.304725	-0.123584	-0.456098
H	3.951800	0.418199	0.444109
H	5.144676	0.469496	-0.877922
C	4.789178	-1.506183	-0.039676
H	5.698676	-1.359394	0.578639
H	5.113084	-2.113986	-0.909419
C	3.774259	-2.242686	0.822793
H	4.250541	-3.110242	1.328387
H	3.421352	-1.558893	1.621861
C	2.844221	-3.792323	-0.898662
H	3.474838	-3.331305	-1.682461
H	1.885156	-4.039088	-1.393244
C	3.510183	-5.062356	-0.367284
H	3.626429	-5.772929	-1.210987
H	4.520558	-4.872337	0.047393
H	2.899339	-5.566307	0.408943
C	1.597501	-3.171183	1.181045
H	1.482227	-2.310813	1.865202
H	2.051751	-4.001253	1.766302
C	0.242280	-3.572450	0.638455
H	-0.501353	-3.630893	1.458910
H	0.262336	-4.553456	0.121782
H	1.142969	-0.301176	0.510214

2ad^{+} (acetone)

Ni	2.001154	-0.818315	-0.865424
Fe	-0.239138	-0.201405	0.405201
S	0.334433	0.268184	-1.881715
S	0.352667	-2.272295	-0.553356
P	-0.854441	1.796932	1.071027
P	-2.461727	-0.637632	0.322751
O	0.119983	-1.069968	3.145911
N	3.266311	0.658838	-1.357882
N	3.262507	-2.077129	0.059418
C	-0.071052	-0.710442	2.039203
C	-2.361978	1.503633	2.149433
H	-2.032917	0.936936	3.044654
H	-2.790746	2.470819	2.483307
C	-3.361926	0.691533	1.310847
H	-3.850998	1.351909	0.565280
H	-4.162540	0.244226	1.933481
C	-1.582955	3.021993	-0.117223
C	-2.090735	2.577081	-1.357160
H	-1.943778	1.530511	-1.666065
C	-2.774578	3.462514	-2.208541
H	-3.163011	3.097008	-3.172432
C	-2.958918	4.803789	-1.829330
H	-3.490507	5.500243	-2.497487
C	-2.465285	5.253331	-0.589877
H	-2.612489	6.301304	-0.282827
C	-1.787914	4.368182	0.266245
H	-1.421725	4.730887	1.239757
C	0.343907	2.759623	2.081417
C	1.183612	3.723277	1.474509
H	1.037842	3.997281	0.417693
C	2.203660	4.344154	2.215150
H	2.848843	5.093986	1.729861
C	2.398081	4.012428	3.568790
H	3.198187	4.499669	4.148633
C	1.562408	3.059422	4.180003
H	1.703644	2.799256	5.241365
C	0.541934	2.433442	3.442718
H	-0.093418	1.682798	3.936820
C	-3.431711	-0.794933	-1.242018
C	-2.774500	-1.283658	-2.393907
H	-1.713260	-1.567807	-2.338410
C	-3.467700	-1.408111	-3.611107
H	-2.942437	-1.790956	-4.500873
C	-4.822046	-1.038268	-3.692279
H	-5.363902	-1.127713	-4.647528
C	-5.484821	-0.556104	-2.547612
H	-6.548169	-0.272216	-2.603269
C	-4.797515	-0.438773	-1.327122
H	-5.337868	-0.072181	-0.440408
C	-2.813572	-2.225574	1.192513
C	-2.783990	-3.445059	0.477233
H	-2.683767	-3.441866	-0.619245
C	-2.886103	-4.669838	1.159781
H	-2.864654	-5.612973	0.590142
C	-3.019396	-4.692745	2.560764
H	-3.100216	-5.653555	3.093966
C	-3.052443	-3.481853	3.276842
H	-3.159633	-3.490178	4.373631
C	-2.945951	-2.254207	2.599445
H	-2.955590	-1.317075	3.177829
C	1.211067	1.879114	-2.114717
H	1.432787	1.967171	-3.197926
H	0.530993	2.710199	-1.841837
C	2.454189	1.917517	-1.257808
H	2.156880	1.994725	-0.194591
H	3.082319	2.803795	-1.500579
C	3.718168	0.354489	-2.763259
H	4.266796	-0.605647	-2.714195
H	2.808859	0.149329	-3.359648
C	4.573695	1.420079	-3.451777
H	4.814509	1.065030	-4.475061
H	4.040568	2.387212	-3.554749
H	5.535404	1.602578	-2.930891
C	4.419146	0.829352	-0.423806
H	5.088885	1.620768	-0.823658
H	3.994300	1.215873	0.524849
C	5.207486	-0.439204	-0.127073
H	6.104805	-0.140332	0.453706
H	5.594255	-0.916667	-1.051128

C	4.417613	-1.413446	0.735834
H	3.993954	-0.859462	1.597761
H	5.086023	-2.197325	1.152222
C	3.709108	-3.040978	-1.011378
H	4.194821	-2.433153	-1.798992
H	2.793087	-3.453175	-1.475735
C	4.634916	-4.175901	-0.569278
H	4.831889	-4.824787	-1.447517
H	5.615713	-3.812771	-0.201203
H	4.178301	-4.812411	0.216041
C	2.467405	-2.741066	1.150886
H	2.209399	-1.935344	1.862642
H	3.103854	-3.475768	1.692990
C	1.199390	-3.394458	0.644049
H	0.507209	-3.606764	1.483734
H	1.390516	-4.347803	0.110506
H	1.295394	0.065823	0.596095

2add$^+$ (acetone)

Ni	-2.039930	-1.068701	-0.289033
Fe	0.426476	-0.075991	-0.306735
S	-0.806422	-0.972038	1.578171
S	-0.284381	-2.247361	-0.938175
P	2.362898	-0.801532	0.644662
P	0.967429	1.950800	0.410234
O	1.263626	0.363933	-3.042117
N	-3.546674	-0.117616	0.637397
N	-2.893019	-1.377511	-2.084158
C	0.960107	0.226044	-1.911094
C	2.822893	0.497260	1.907019
H	2.118148	0.378518	2.756384
H	3.855349	0.336164	2.279897
C	2.652125	1.868464	1.243052
H	3.405193	2.008916	0.439922
H	2.778593	2.700912	1.963779
C	3.916563	-0.881274	-0.365968
C	4.121397	0.086357	-1.376949
H	3.343701	0.833126	-1.592244
C	5.318655	0.111076	-2.113811
H	5.459430	0.874229	-2.896062
C	6.325681	-0.836480	-1.857797
H	7.260174	-0.823874	-2.441444
C	6.133845	-1.799348	-0.849800
H	6.920287	-2.541370	-0.636794
C	4.942505	-1.818969	-0.103519
H	4.817196	-2.570591	0.690948
C	2.329898	-2.403141	1.541999
C	2.312730	-3.596981	0.779943
H	2.429295	-3.552047	-0.314184
C	2.159431	-4.842432	1.410063
H	2.155364	-5.762933	0.804383
C	2.008588	-4.914165	2.808179
H	1.884403	-5.891257	3.302118
C	2.018306	-3.732902	3.570991
H	1.903170	-3.780287	4.665907
C	2.176709	-2.483340	2.943923
H	2.179393	-1.573254	3.562026
C	1.145233	3.256116	-0.887827
C	0.243371	3.267401	-1.975612
H	-0.522059	2.478964	-2.053615
C	0.320380	4.274154	-2.953456
H	-0.389484	4.272492	-3.796207
C	1.305313	5.274180	-2.859622
H	1.372281	6.058731	-3.630429
C	2.204570	5.270563	-1.777257
H	2.975813	6.053477	-1.696416
C	2.122000	4.272584	-0.790000
H	2.823283	4.298348	0.058369
C	-0.053408	2.874804	1.659594
C	-1.149375	3.656497	1.227427
H	-1.378736	3.741727	0.153492
C	-1.957166	4.332470	2.157195
H	-2.807685	4.935703	1.801319
C	-1.680042	4.242483	3.533823
H	-2.312775	4.773700	4.262674
C	-0.585888	3.476403	3.972835
H	-0.356590	3.402209	5.047914
C	0.221530	2.794368	3.044254
H	1.064086	2.194125	3.419221
C	-1.926579	0.144030	2.530990
H	-2.436241	-0.493516	3.282562
H	-1.326095	0.895699	3.077851
C	-2.891432	0.830729	1.596064
H	-2.334802	1.548788	0.968781
H	-3.660021	1.405192	2.160417
C	-4.335796	-1.196307	1.334148
H	-4.767318	-1.836025	0.541697
H	-3.607376	-1.834245	1.870881
C	-5.435233	-0.727487	2.289648
H	-5.933028	-1.623802	2.713858
H	-5.033658	-0.139177	3.139649
H	-6.216100	-0.124711	1.783085
C	-4.401436	0.723197	-0.254688
H	-5.237094	1.144963	0.344509
H	-3.767673	1.577367	-0.569765
C	-4.937101	0.027847	-1.498641
H	-5.631949	0.737359	-1.994401
H	-5.550137	-0.862598	-1.248697
C	-3.836329	-0.296300	-2.499300
H	-3.215250	0.609666	-2.655302
H	-4.274077	-0.562737	-3.485553
C	-3.566334	-2.724165	-1.998986
H	-4.320583	-2.652998	-1.193455
H	-2.807572	-3.440282	-1.630557
C	-4.213197	-3.248078	-3.282363
H	-4.635007	-4.252769	-3.072995
H	-5.046511	-2.607507	-3.635608
H	-3.482687	-3.362326	-4.108978
C	-1.768941	-1.360604	-3.082570
H	-1.354131	-0.335305	-3.052366
H	-2.165511	-1.535097	-4.107673
C	-0.680934	-2.354412	-2.741892
H	0.233689	-2.144562	-3.331112
H	-0.978766	-3.404061	-2.940380
H	-0.989298	0.428280	-0.758443

2b$^+$ (acetone)

Ni	2.009857	-1.018259	-0.969549
Fe	-0.498766	0.108410	-0.228005
S	1.111097	0.793008	-1.854357
S	0.014065	-1.856533	-1.390017
P	-0.993909	2.110006	0.544797
P	-2.444312	-0.586980	0.456268
O	0.864206	-0.737381	2.237286
N	3.546400	0.081513	-0.265725
N	2.722012	-2.870243	-0.528078

C	0.411317	-0.370084	1.208221
C	-2.423992	1.908839	1.740148
H	-1.980680	1.567760	2.698040
H	-2.915337	2.885467	1.926074
C	-3.392927	0.871012	1.172961
H	-3.961654	1.292221	0.316648
H	-4.122923	0.512161	1.926847
C	-1.608912	3.390149	-0.642264
C	-2.109830	4.623613	-0.161658
H	-2.113488	4.838298	0.919428
C	-2.593868	5.589725	-1.059024
H	-2.983655	6.545818	-0.674199
C	-2.579819	5.337585	-2.444616
H	-2.959888	6.096744	-3.147109
C	-2.080462	4.115488	-2.928066
H	-2.066553	3.911753	-4.010869
C	-1.598891	3.144557	-2.030505
H	-1.214863	2.180395	-2.399731
C	0.267285	3.022208	1.547784
C	0.924868	4.175578	1.063760
H	0.623140	4.625074	0.105094
C	1.971889	4.760951	1.798330
H	2.477479	5.656474	1.402872
C	2.370459	4.208990	3.028478
H	3.192409	4.667386	3.601251
C	1.708677	3.071185	3.527161
H	2.007070	2.635437	4.494154
C	0.667271	2.480659	2.792812
H	0.175853	1.581091	3.192166
C	-2.439486	-1.869244	1.787641
C	-2.614026	-3.237961	1.481874
H	-2.850612	-3.547346	0.451934
C	-2.486960	-4.214357	2.485022
H	-2.626292	-5.277405	2.230418
C	-2.186371	-3.836664	3.806445
H	-2.088851	-4.602151	4.592949
C	-2.011223	-2.475684	4.118864
H	-1.775656	-2.170605	5.151169
C	-2.129829	-1.498237	3.116190
H	-1.968483	-0.441065	3.376204
C	-3.664508	-1.266144	-0.756906
C	-3.395799	-1.273551	-2.140696
H	-2.424952	-0.898180	-2.500306
C	-4.361796	-1.743391	-3.049478
H	-4.138575	-1.747702	-4.128515
C	-5.605916	-2.203140	-2.582692
H	-6.362325	-2.570822	-3.294688
C	-5.883878	-2.191263	-1.202243
H	-6.858737	-2.545937	-0.830708
C	-4.919044	-1.727747	-0.292398
H	-5.143407	-1.729791	0.786554
C	2.329854	2.032859	-1.237472
H	3.033169	2.253035	-2.066370
H	1.799276	2.971732	-0.989646
C	3.010333	1.467188	-0.015877
H	2.264790	1.376089	0.796801
H	3.823950	2.129741	0.351827
C	4.625692	0.092558	-1.316920
H	4.137834	0.382045	-2.267432
H	4.954078	-0.951660	-1.456578
C	5.839550	0.983186	-1.045861
H	6.551397	0.865646	-1.888884
H	5.576444	2.058573	-0.984464
H	6.377887	0.700118	-0.118516
C	4.016756	-0.426489	1.061498
H	4.852757	0.215749	1.415197
H	3.174908	-0.271404	1.762867
C	4.436078	-1.889803	1.106522
H	4.799447	-2.083118	2.137810
H	5.310968	-2.081434	0.451678
C	3.307952	-2.888897	0.851741
H	2.474599	-2.688689	1.554938
H	3.679930	-3.919326	1.054111
C	3.751116	-3.307455	-1.537047
H	4.705962	-2.812082	-1.287377
H	3.922243	-4.398991	-1.394896
C	3.378181	-2.992545	-2.981291
H	4.181156	-3.356534	-3.654916
H	2.430269	-3.476523	-3.290557
H	3.262103	-1.899061	-3.131360
C	1.594414	-3.882465	-0.573237
H	1.846034	-4.733636	0.097194
H	1.541263	-4.282248	-1.603952
C	0.257035	-3.271315	-0.221063
H	0.206472	-2.902111	0.820786
H	-0.558910	-4.006542	-0.368837
H	-1.484044	0.469940	-1.354066

$2b^{+}$ (acetonitrile)

Ni	2.008944	-1.024230	-0.970177
Fe	-0.499822	0.107187	-0.226579
S	1.111875	0.787786	-1.854062
S	0.010355	-1.859552	-1.386854
P	-0.987207	2.110834	0.547603
P	-2.447763	-0.580651	0.458683
O	0.850678	-0.742854	2.243357
N	3.544759	0.074277	-0.262963
N	2.720899	-2.875113	-0.530690
C	0.404419	-0.373878	1.212110
C	-2.415054	1.913378	1.745320
H	-1.970270	1.570339	2.701745
H	-2.902204	2.891819	1.932643
C	-3.389479	0.879016	1.180976
H	-3.961221	1.302811	0.328073
H	-4.117102	0.521786	1.937840
C	-1.601066	3.392298	-0.638999
C	-2.101271	4.626108	-0.158455
H	-2.105394	4.840409	0.922692
C	-2.582845	5.593316	-1.056142
H	-2.971776	6.549751	-0.671410
C	-2.566977	5.342047	-2.441967
H	-2.944884	6.102151	-3.144514
C	-2.067919	4.119725	-2.925433
H	-2.052150	3.916612	-4.008304
C	-1.588793	3.147887	-2.027437
H	-1.204067	2.183853	-2.396245
C	0.277476	3.022098	1.547660
C	0.933439	4.175205	1.060650
H	0.630327	4.622465	0.101500
C	1.981582	4.762736	1.791889
H	2.485557	5.657755	1.393316
C	2.383286	4.212983	3.022030
H	3.206176	4.672797	3.592242
C	1.723760	3.074952	3.523455
H	2.025314	2.640790	4.490144

C	0.681146	2.482135	2.792357
H	0.192361	1.582200	3.194184
C	-2.447082	-1.868864	1.784152
C	-2.614262	-3.236001	1.466930
H	-2.843688	-3.538452	0.433298
C	-2.487520	-4.219822	2.462841
H	-2.620265	-5.281403	2.198960
C	-2.195012	-3.851046	3.788698
H	-2.097921	-4.622258	4.569590
C	-2.028040	-2.491641	4.112658
H	-1.799336	-2.193584	5.148517
C	-2.146454	-1.506497	3.117237
H	-1.992430	-0.450809	3.387498
C	-3.671588	-1.252423	-0.755522
C	-3.401361	-1.263527	-2.139037
H	-2.427451	-0.895313	-2.497891
C	-4.369149	-1.728550	-3.048538
H	-4.144447	-1.735894	-4.127226
C	-5.616713	-2.179965	-2.582558
H	-6.374679	-2.543668	-3.294854
C	-5.895929	-2.165089	-1.202275
H	-6.873235	-2.513727	-0.831559
C	-4.929185	-1.706546	-0.291760
H	-5.154355	-1.706955	0.787045
C	2.332841	2.025829	-1.238110
H	3.039381	2.241871	-2.065252
H	1.804789	2.967104	-0.994015
C	3.008606	1.459953	-0.014103
H	2.260669	1.368483	0.796345
H	3.821311	2.121993	0.356188
C	4.627904	0.085363	-1.310299
H	4.141053	0.360544	-2.265476
H	4.966939	-0.957024	-1.437444
C	5.831223	0.991247	-1.043047
H	6.551648	0.868115	-1.877793
H	5.557107	2.064700	-1.000344
H	6.364103	0.727329	-0.106913
C	4.010953	-0.434385	1.065539
H	4.847117	0.206694	1.420794
H	3.167593	-0.277507	1.764769
C	4.428531	-1.898089	1.112101
H	4.786800	-2.091834	2.145010
H	5.306054	-2.090538	0.461125
C	3.300516	-2.895632	0.851893
H	2.464283	-2.694682	1.551352
H	3.670130	-3.926668	1.054900
C	3.754324	-3.310949	-1.535924
H	4.708223	-2.816619	-1.280879
H	3.923696	-4.402777	-1.395003
C	3.388419	-2.993133	-2.981355
H	4.196960	-3.350807	-3.651541
H	2.445015	-3.481517	-3.297753
H	3.268273	-1.899594	-3.128313
C	1.593469	-3.886516	-0.581724
H	1.846560	-4.743118	0.081159
H	1.537709	-4.277959	-1.615474
C	0.257180	-3.277279	-0.221914
H	0.211730	-2.910259	0.820965
H	-0.558546	-4.012834	-0.367746
H	-1.482930	0.470544	-1.354213

$2b^{+}$ (water)

Ni	1.915163	-1.131363	-0.976571
Fe	-0.517340	0.146639	-0.260318
S	1.146815	0.731637	-1.871792
S	-0.124768	-1.843350	-1.428213
P	-0.871153	2.174865	0.522975
P	-2.501434	-0.415612	0.427214
O	0.755732	-0.834753	2.197408
N	3.508210	-0.131536	-0.249043
N	2.505210	-3.021268	-0.537660
C	0.349029	-0.414301	1.166549
C	-2.368337	2.108899	1.649384
H	-1.998549	1.780585	2.641488
H	-2.798687	3.123506	1.770060
C	-3.378004	1.116711	1.071694
H	-3.885162	1.546349	0.181834
H	-4.157022	0.823580	1.804498
C	-1.302306	3.522038	-0.669281
C	-1.671681	4.801408	-0.189720
H	-1.678278	5.007318	0.892997
C	-2.020359	5.821566	-1.089777
H	-2.307636	6.813403	-0.706235
C	-2.001685	5.577441	-2.476667
H	-2.274698	6.379208	-3.181003
C	-1.634541	4.308914	-2.958700
H	-1.618534	4.111252	-4.042266
C	-1.287966	3.284320	-2.058617
H	-1.006101	2.285424	-2.426906
C	0.433905	2.937072	1.591814
C	1.232048	4.016970	1.152422
H	1.009278	4.520298	0.199204
C	2.324856	4.455244	1.921480
H	2.942658	5.291813	1.558670
C	2.628389	3.829522	3.143088
H	3.488439	4.169507	3.741234
C	1.822384	2.770534	3.601407
H	2.044825	2.280486	4.562421
C	0.734580	2.325813	2.832826
H	0.131178	1.482282	3.200193
C	-2.562632	-1.642930	1.806155
C	-2.763044	-3.016682	1.542063
H	-2.994459	-3.353420	0.519714
C	-2.665045	-3.963138	2.576319
H	-2.822958	-5.030362	2.353731
C	-2.367922	-3.550110	3.887855
H	-2.291642	-4.292072	4.698362
C	-2.167670	-2.183904	4.159004
H	-1.934197	-1.851182	5.182804
C	-2.257822	-1.236072	3.125383
H	-2.074294	-0.175548	3.354597
C	-3.743824	-1.080088	-0.769129
C	-3.481159	-1.109704	-2.153840
H	-2.502058	-0.765149	-2.521322
C	-4.462956	-1.564501	-3.052997
H	-4.244926	-1.587261	-4.132509
C	-5.716221	-1.987070	-2.575635
H	-6.484420	-2.343983	-3.279889
C	-5.988012	-1.951655	-1.194522
H	-6.969764	-2.276693	-0.815157
C	-5.007892	-1.502379	-0.293994
H	-5.227745	-1.484364	0.785569
C	2.429488	1.892570	-1.232717
H	3.158757	2.066977	-2.049472
H	1.953319	2.862530	-0.994539

C	3.055342	1.283953	-0.002344
H	2.296705	1.236340	0.801560
H	3.901818	1.895583	0.379091
C	4.601744	-0.185309	-1.283579
H	4.148614	0.132636	-2.242116
H	4.869965	-1.247046	-1.419414
C	5.861455	0.631051	-0.991988
H	6.578409	0.469978	-1.822868
H	5.660429	1.719735	-0.934936
H	6.364616	0.316056	-0.055516
C	3.928433	-0.670607	1.082587
H	4.802007	-0.086157	1.445166
H	3.093290	-0.459053	1.776481
C	4.249184	-2.158122	1.129916
H	4.580702	-2.376996	2.166435
H	5.120700	-2.404097	0.489035
C	3.064493	-3.082208	0.851574
H	2.232564	-2.833250	1.540104
H	3.368129	-4.134636	1.053649
C	3.522305	-3.513767	-1.532788
H	4.502706	-3.083181	-1.262759
H	3.620919	-4.614923	-1.398391
C	3.195205	-3.163206	-2.979510
H	3.974101	-3.588971	-3.644469
H	2.214334	-3.566417	-3.301435
H	3.172215	-2.063373	-3.124838
C	1.320848	-3.964096	-0.608252
H	1.512764	-4.834051	0.057646
H	1.258353	-4.352291	-1.642819
C	0.017967	-3.278371	-0.266810
H	-0.019767	-2.915093	0.777244
H	-0.838705	-3.962054	-0.430098
H	-1.485122	0.583746	-1.381625

2bd^{+} (acetone)

Ni	2.035846	-0.323054	-1.041883
Fe	-0.512366	0.066355	-0.315167
S	0.769543	1.287420	-1.909299
S	0.371424	-1.527167	-1.855175
P	-1.515267	1.783682	0.605267
P	-2.030615	-1.242466	0.545413
O	1.258014	-0.194067	2.027234
N	3.395944	1.039319	-0.484866
N	2.939421	-2.004336	-0.412036
C	0.657833	-0.099937	1.008966
C	-2.661560	1.124286	1.930905
H	-2.029338	0.937801	2.822775
H	-3.416484	1.887681	2.208023
C	-3.304158	-0.168637	1.426610
H	-4.073149	0.051259	0.655771
H	-3.788234	-0.746935	2.239787
C	-2.622677	2.819345	-0.458752
C	-2.630771	2.660793	-1.859524
H	-1.977111	1.899583	-2.314178
C	-3.469048	3.457458	-2.661118
H	-3.465361	3.323819	-3.754863
C	-4.309296	4.416207	-2.068167
H	-4.968846	5.037499	-2.695284
C	-4.304630	4.582279	-0.669694
H	-4.958640	5.334045	-0.199268
C	-3.463552	3.792435	0.131615
H	-3.454480	3.947513	1.222864
C	-0.508819	3.054106	1.499179
C	-0.295290	4.344000	0.961066
H	-0.806270	4.649346	0.034743
C	0.571145	5.248911	1.600032
H	0.729868	6.248193	1.163894
C	1.230266	4.881774	2.786572
H	1.910351	5.591059	3.284809
C	1.010954	3.605555	3.337846
H	1.516902	3.310798	4.271205
C	0.150385	2.697140	2.699370
H	0.008535	1.698205	3.136480
C	-3.116715	-2.259445	-0.552483
C	-3.028108	-2.162911	-1.956122
H	-2.267809	-1.503060	-2.401694
C	-3.905543	-2.896953	-2.775520
H	-3.823078	-2.816320	-3.871370
C	-4.883352	-3.726429	-2.198756
H	-5.570351	-4.300946	-2.840839
C	-4.985042	-3.818720	-0.797275
H	-5.753294	-4.462053	-0.338888
C	-4.107481	-3.090587	0.023170
H	-4.193808	-3.173700	1.118700
C	-1.459250	-2.456976	1.820433
C	-1.310103	-3.832682	1.530990
H	-1.648629	-4.235853	0.564209
C	-0.743229	-4.705452	2.476588
H	-0.632305	-5.774024	2.231562
C	-0.327695	-4.219457	3.729254
H	0.115445	-4.903845	4.470319
C	-0.488180	-2.854761	4.033054
H	-0.172760	-2.464859	5.014183
C	-1.043402	-1.978978	3.085298
H	-1.138572	-0.912005	3.335262
C	1.734512	2.730778	-1.278979
H	2.297878	3.137870	-2.143222
H	1.035878	3.515883	-0.933251
C	2.633573	2.292947	-0.146926
H	2.014310	2.059134	0.739943
H	3.339348	3.101722	0.145374
C	4.274286	1.214734	-1.700548
H	4.761077	0.238192	-1.881605
H	3.603795	1.377740	-2.565952
C	5.325169	2.324423	-1.630181
H	5.884829	2.333160	-2.588195
H	4.872300	3.328696	-1.502887
H	6.063568	2.167029	-0.818170
C	4.187541	0.676601	0.730594
H	4.960249	1.457587	0.896460
H	3.485786	0.730312	1.585191
C	4.830987	-0.705184	0.703721
H	5.473428	-0.779330	1.605959
H	5.518874	-0.825955	-0.158698
C	3.813920	-1.837987	0.789392
H	3.137296	-1.648788	1.644388
H	4.327558	-2.802434	0.990378
C	3.723495	-2.484295	-1.609928
H	4.483979	-1.708685	-1.817495
H	3.036325	-2.469002	-2.477199
C	4.391046	-3.855343	-1.487238
H	4.928739	-4.064242	-2.435090
H	5.137056	-3.899478	-0.668132
H	3.656134	-4.672181	-1.338009
C	1.842804	-2.963371	-0.026361

H	1.322559	-2.522844	0.845534
H	2.281834	-3.930913	0.303544
C	0.849082	-3.163699	-1.147109
H	-0.058338	-3.677147	-0.776420
H	1.258595	-3.766288	-1.983634
H	-1.681308	0.190594	-1.307961

2bdd^{+} (acetone)

Ni	2.224120	-1.039930	-0.532483
Fe	-0.470111	0.149358	-0.369539
S	1.467098	0.721610	-1.618586
S	0.303777	-1.898335	-1.177588
P	-1.280634	2.171584	-0.113583
P	-2.493361	-0.611153	-0.028877
O	0.465090	-0.195308	2.399928
N	3.644395	0.091486	0.327284
N	2.834299	-2.870537	0.122484
C	0.152935	-0.059034	1.270130
C	-3.115845	2.064365	-0.447388
H	-3.635784	3.001182	-0.159885
H	-3.199424	1.957968	-1.549464
C	-3.665190	0.829507	0.271808
H	-4.684254	0.558069	-0.070388
H	-3.707954	0.991695	1.367842
C	-0.702166	3.491659	-1.269451
C	-0.595495	3.160474	-2.640377
H	-0.861549	2.143632	-2.972261
C	-0.139762	4.112871	-3.566272
H	-0.060909	3.844064	-4.631978
C	0.226522	5.401568	-3.132506
H	0.595135	6.144753	-3.857728
C	0.121503	5.736589	-1.770781
H	0.402506	6.744635	-1.425488
C	-0.343382	4.788269	-0.840504
H	-0.423180	5.064814	0.222168
C	-1.154802	2.944979	1.561553
C	-2.277777	3.300859	2.340953
H	-3.299351	3.184291	1.950490
C	-2.107469	3.819142	3.638881
H	-2.994151	4.085711	4.236327
C	-0.818343	4.001690	4.168771
H	-0.689606	4.408741	5.184477
C	0.306792	3.663516	3.393119
H	1.322695	3.807461	3.794539
C	0.136380	3.132783	2.105287
H	1.018916	2.865280	1.507204
C	-2.716476	-1.702172	1.444212
C	-2.842072	-3.104889	1.331358
H	-2.919405	-3.576133	0.339422
C	-2.865243	-3.911446	2.483014
H	-2.964544	-5.003988	2.379270
C	-2.763166	-3.328560	3.759035
H	-2.783226	-3.961872	4.660455
C	-2.631211	-1.932111	3.878887
H	-2.544187	-1.467046	4.873996
C	-2.599960	-1.124349	2.730184
H	-2.464539	-0.035927	2.839100
C	-3.350889	-1.517955	-1.400392
C	-2.784475	-1.595435	-2.689156
H	-1.799537	-1.137131	-2.868826
C	-3.476592	-2.234249	-3.734610
H	-3.021192	-2.288147	-4.736568
C	-4.743206	-2.798352	-3.502348
H	-5.284484	-3.299720	-4.320823
C	-5.320986	-2.715833	-2.220798
H	-6.316615	-3.149096	-2.033132
C	-4.631498	-2.078410	-1.175998
H	-5.095481	-2.019057	-0.178045
C	2.528355	2.015179	-0.841639
H	3.321236	2.279587	-1.570661
H	1.915844	2.923040	-0.665050
C	3.077049	1.479853	0.458883
H	2.251300	1.394952	1.188364
H	3.837795	2.162799	0.897403
C	4.851608	0.065177	-0.571585
H	4.503964	0.384146	-1.573097
H	5.150570	-0.992490	-0.681739
C	6.053693	0.901135	-0.128950
H	6.856176	0.785823	-0.886498
H	5.819777	1.982835	-0.058604
H	6.467457	0.567149	0.844233
C	3.926312	-0.357667	1.727560
H	4.690098	0.317044	2.172593
H	2.985182	-0.196468	2.289787
C	4.352118	-1.808398	1.891670
H	4.598561	-1.950001	2.964887
H	5.293813	-2.022321	1.344862
C	3.256680	-2.817951	1.559376
H	2.347926	-2.576067	2.148292
H	3.590631	-3.837920	1.857867
C	3.962791	-3.381529	-0.732514
H	4.889215	-2.872665	-0.410692
H	4.102969	-4.462265	-0.500611
C	3.761921	-3.160485	-2.227757
H	4.623052	-3.590490	-2.779802
H	2.838675	-3.640618	-2.609344
H	3.699362	-2.077511	-2.463525
C	1.690781	-3.860175	0.019381
H	1.830395	-4.657006	0.782668
H	1.746981	-4.346175	-0.973593
C	0.346324	-3.180635	0.155226
H	0.201508	-2.695142	1.140020
H	-0.480025	-3.901500	-0.004897
H	-1.155041	0.388883	-1.735706

2c^{+} (acetone)

Ni	2.076740	-1.005565	-0.174260
Fe	-0.378576	0.034258	-0.205375
S	0.272533	-2.261452	-0.396548
S	1.004660	-0.418918	1.696360
P	-1.150409	2.020300	0.295471
P	-2.300238	-0.734182	0.717193
O	1.279945	1.334525	-2.216636
N	2.797674	-1.788980	-1.887401
N	3.608471	0.179222	0.341037
C	0.740162	0.744655	-1.338777
C	-2.371811	1.873018	1.699984
H	-1.782188	1.664904	2.616396
H	-2.913718	2.831573	1.838486
C	-3.310403	0.709522	1.370584
H	-4.007362	0.986039	0.550994
H	-3.918165	0.393500	2.242347
C	-2.175778	2.878664	-0.995783
C	-2.705846	2.154785	-2.083510
H	-2.445827	1.088963	-2.192304
C	-3.550874	2.784835	-3.015340

H	-3.957271	2.207076	-3.861090
C	-3.872078	4.145716	-2.867940
H	-4.530833	4.641313	-3.599170
C	-3.347842	4.874789	-1.782945
H	-3.595792	5.941745	-1.662415
C	-2.505676	4.246660	-0.850111
H	-2.100849	4.827312	-0.005266
C	0.012726	3.358253	0.805365
C	0.838805	3.941575	-0.185069
H	0.738400	3.633340	-1.236960
C	1.791116	4.912179	0.163389
H	2.430024	5.354044	-0.617869
C	1.929287	5.317817	1.504695
H	2.678247	6.077970	1.778507
C	1.100552	4.756012	2.491211
H	1.194739	5.075407	3.541419
C	0.145504	3.781095	2.146380
H	-0.487631	3.353013	2.938030
C	-3.493170	-1.626618	-0.372489
C	-3.207370	-1.844162	-1.735248
H	-2.251177	-1.478263	-2.142563
C	-4.134214	-2.508485	-2.559321
H	-3.898540	-2.675135	-3.622733
C	-5.355851	-2.956473	-2.026309
H	-6.082915	-3.476222	-2.670901
C	-5.648755	-2.740541	-0.665474
H	-6.604948	-3.089760	-0.243641
C	-4.722042	-2.082560	0.160030
H	-4.953257	-1.929060	1.226814
C	-2.130866	-1.886026	2.148073
C	-2.094759	-3.283758	1.934604
H	-2.281676	-3.692568	0.929542
C	-1.831639	-4.160132	3.002028
H	-1.812778	-5.247099	2.821473
C	-1.598171	-3.653799	4.293880
H	-1.394256	-4.341725	5.130106
C	-1.627919	-2.264012	4.512588
H	-1.447836	-1.858403	5.521257
C	-1.884785	-1.384187	3.446649
H	-1.890259	-0.300585	3.639455
C	0.538563	-2.856467	-2.124110
H	0.802584	-3.931543	-2.049267
H	-0.411799	-2.780963	-2.689368
C	1.619508	-2.035808	-2.792216
H	1.213868	-1.042292	-3.055442
H	1.961747	-2.515696	-3.735956
C	3.465487	-3.072283	-1.454976
H	4.277001	-2.784814	-0.760735
H	2.731831	-3.629424	-0.841981
C	4.013626	-3.968481	-2.567072
H	4.458898	-4.869415	-2.096805
H	3.220884	-4.316036	-3.260284
H	4.810772	-3.478929	-3.162155
C	3.734023	-0.900899	-2.642389
H	4.138882	-1.465671	-3.509321
H	3.118263	-0.077510	-3.052917
C	4.869000	-0.301594	-1.821958
H	5.538339	0.227169	-2.532129
H	5.497497	-1.082537	-1.345847
C	4.381730	0.731212	-0.812768
H	3.707073	1.445610	-1.324878
H	5.237651	1.319779	-0.417938
C	4.471979	-0.664277	1.246849
H	4.858326	-1.496887	0.629731
H	3.801079	-1.130541	1.993663
C	5.629211	0.052851	1.944427
H	6.169648	-0.687107	2.570103
H	6.362319	0.479186	1.230114
H	5.281786	0.863343	2.616732
C	3.006821	1.356396	1.058425
H	2.377156	1.884302	0.318231
H	3.807659	2.059594	1.377862
C	2.145236	0.934408	2.224997
H	1.550204	1.794089	2.588150
H	2.737457	0.546467	3.078863
H	-1.177891	-0.049448	-1.460721

$2c^{+}$ (acetonitrile)

Ni	2.056355	-1.028587	-0.173694
Fe	-0.386678	0.035104	-0.203613
S	0.240870	-2.265420	-0.419442
S	0.980282	-0.453568	1.698344
P	-1.139542	2.027497	0.297540
P	-2.320041	-0.717185	0.706758
O	1.306089	1.341198	-2.183320
N	2.775528	-1.796709	-1.893771
N	3.597277	0.134250	0.364081
C	0.750835	0.744356	-1.319773
C	-2.386667	1.893202	1.679400
H	-1.815862	1.680859	2.606496
H	-2.923558	2.855597	1.809512
C	-3.328905	0.737053	1.335567
H	-4.006215	1.016419	0.500626
H	-3.957754	0.429842	2.195529
C	-2.115821	2.913180	-1.013112
C	-2.511143	2.251805	-2.193228
H	-2.191527	1.208276	-2.351014
C	-3.300440	2.914450	-3.151506
H	-3.600722	2.386023	-4.070644
C	-3.701440	4.244703	-2.936292
H	-4.318158	4.765101	-3.686656
C	-3.310372	4.912067	-1.758860
H	-3.620300	5.955227	-1.585626
C	-2.521340	4.252264	-0.802097
H	-2.216082	4.785820	0.112997
C	0.033694	3.347904	0.832371
C	0.868959	3.938128	-0.146272
H	0.768621	3.647596	-1.203254
C	1.831955	4.891290	0.220892
H	2.479122	5.337533	-0.550970
C	1.970417	5.273760	1.569068
H	2.727820	6.019898	1.857669
C	1.131292	4.706471	2.543728
H	1.225311	5.007819	3.599243
C	0.166667	3.747806	2.180311
H	-0.474394	3.314471	2.962393
C	-3.508784	-1.613502	-0.384987
C	-3.227931	-1.813414	-1.751504
H	-2.277054	-1.434732	-2.159585
C	-4.152253	-2.478100	-2.578245
H	-3.919600	-2.631426	-3.644274
C	-5.366649	-2.944210	-2.044085
H	-6.091491	-3.464750	-2.690484
C	-5.654987	-2.745414	-0.679548
H	-6.605554	-3.108667	-0.256913

C	-4.730810	-2.086846	0.148472
H	-4.958611	-1.946364	1.217766
C	-2.166414	-1.859654	2.147090
C	-2.111394	-3.257555	1.937028
H	-2.275439	-3.669637	0.929406
C	-1.857083	-4.129722	3.010050
H	-1.823233	-5.216568	2.831281
C	-1.651478	-3.619018	4.305092
H	-1.454136	-4.303264	5.145826
C	-1.700774	-2.229230	4.520763
H	-1.542910	-1.820101	5.531697
C	-1.948852	-1.353452	3.449089
H	-1.969822	-0.270029	3.641344
C	0.505601	-2.837402	-2.155181
H	0.755947	-3.916753	-2.097747
H	-0.442455	-2.740075	-2.720784
C	1.598366	-2.018606	-2.806722
H	1.204109	-1.017250	-3.057562
H	1.940344	-2.488059	-3.755686
C	3.428249	-3.092719	-1.476146
H	4.235988	-2.824579	-0.769703
H	2.683695	-3.653432	-0.879917
C	3.978743	-3.975181	-2.597904
H	4.403649	-4.892048	-2.139773
H	3.190699	-4.296967	-3.308653
H	4.791670	-3.486197	-3.171678
C	3.724252	-0.909063	-2.633420
H	4.126114	-1.467447	-3.505688
H	3.119033	-0.074157	-3.035946
C	4.861891	-0.332984	-1.800538
H	5.539055	0.198640	-2.501038
H	5.480909	-1.126559	-1.333265
C	4.382696	0.691858	-0.779060
H	3.719626	1.422019	-1.283970
H	5.244118	1.263696	-0.372093
C	4.446764	-0.729397	1.264044
H	4.830792	-1.555928	0.637793
H	3.765921	-1.200647	1.998527
C	5.604272	-0.032660	1.981740
H	6.135877	-0.787544	2.596981
H	6.344829	0.401760	1.280059
H	5.258003	0.767290	2.667164
C	3.004705	1.308633	1.093910
H	2.385471	1.854571	0.358031
H	3.811626	1.998025	1.427660
C	2.133141	0.879678	2.250440
H	1.545711	1.740103	2.623849
H	2.717563	0.472959	3.100804
H	-1.187874	-0.034767	-1.458331
$2c^+$	(water)		
Ni	2.060009	-1.025179	-0.180080
Fe	-0.375298	0.037008	-0.200858
S	0.243379	-2.265999	-0.413055
S	0.996868	-0.456401	1.700694
P	-1.113939	2.031162	0.313693
P	-2.308140	-0.698641	0.720881
O	1.289490	1.343800	-2.198629
N	2.772082	-1.793870	-1.901910
N	3.600096	0.139950	0.347421
C	0.749366	0.742770	-1.325099
C	-2.313802	1.895579	1.736322
H	-1.714782	1.663566	2.640950
H	-2.832014	2.864301	1.891998
C	-3.281018	0.755681	1.405408
H	-3.983439	1.055852	0.599096
H	-3.881374	0.439150	2.281737
C	-2.153658	2.896062	-0.959451
C	-2.749074	2.165005	-2.008265
H	-2.528854	1.089112	-2.103113
C	-3.609030	2.801634	-2.921493
H	-4.066825	2.218754	-3.736458
C	-3.879966	4.175510	-2.794653
H	-4.549783	4.675870	-3.511931
C	-3.291946	4.910862	-1.747485
H	-3.501594	5.987265	-1.642336
C	-2.435458	4.276228	-0.832202
H	-1.982543	4.860329	-0.014872
C	0.080982	3.346546	0.799572
C	0.892846	3.923259	-0.206562
H	0.748466	3.639208	-1.259827
C	1.889615	4.851922	0.130473
H	2.519754	5.286533	-0.661389
C	2.085401	5.222750	1.474646
H	2.872030	5.946689	1.739451
C	1.265377	4.674214	2.475568
H	1.403044	4.968984	3.527776
C	0.265732	3.741102	2.142613
H	-0.359048	3.319310	2.943938
C	-3.522584	-1.550794	-0.374925
C	-3.233531	-1.784646	-1.734231
H	-2.264298	-1.450206	-2.137502
C	-4.175063	-2.424433	-2.560843
H	-3.937578	-2.604080	-3.621342
C	-5.413592	-2.831122	-2.033819
H	-6.151864	-3.331250	-2.680603
C	-5.709065	-2.598961	-0.676252
H	-6.678270	-2.915971	-0.259589
C	-4.767914	-1.965758	0.152121
H	-5.000214	-1.799077	1.216528
C	-2.156033	-1.873354	2.133069
C	-2.159108	-3.268289	1.900786
H	-2.366207	-3.657835	0.892056
C	-1.908996	-4.165019	2.954345
H	-1.920917	-5.249465	2.760490
C	-1.649444	-3.681306	4.249944
H	-1.456306	-4.384878	5.075192
C	-1.639269	-2.294081	4.486485
H	-1.437839	-1.906770	5.497933
C	-1.882808	-1.393876	3.434639
H	-1.856823	-0.312879	3.639881
C	0.505070	-2.842358	-2.147544
H	0.764887	-3.919033	-2.085152
H	-0.445022	-2.754701	-2.711226
C	1.589676	-2.019734	-2.806522
H	1.189565	-1.020814	-3.057357
H	1.925730	-2.489577	-3.757378
C	3.430065	-3.088210	-1.488508
H	4.252882	-2.818129	-0.800315
H	2.697177	-3.644571	-0.873840
C	3.955931	-3.977981	-2.615694
H	4.399612	-4.886478	-2.159573
H	3.150572	-4.311065	-3.301070
H	4.748840	-3.487674	-3.215347
C	3.714745	-0.906583	-2.649647

H	4.118024	-1.468795	-3.518837
H	3.104804	-0.077796	-3.056936
C	4.851698	-0.318187	-1.824934
H	5.518400	0.218503	-2.531193
H	5.481196	-1.104638	-1.359802
C	4.368747	0.703670	-0.803179
H	3.692538	1.424147	-1.304099
H	5.226717	1.286990	-0.405212
C	4.461080	-0.725049	1.233612
H	4.820672	-1.562936	0.607677
H	3.794075	-1.182319	1.989234
C	5.642237	-0.033610	1.915440
H	6.175714	-0.785456	2.532166
H	6.372273	0.378672	1.190248
H	5.319402	0.782786	2.592582
C	3.012880	1.310527	1.087959
H	2.386969	1.857811	0.359072
H	3.821393	2.000454	1.416605
C	2.154541	0.873099	2.250809
H	1.570791	1.729263	2.638399
H	2.749234	0.459455	3.090512
H	-1.173369	-0.024560	-1.458078

2cd^{+} (acetone)

Ni	-2.368474	-0.220770	0.342293
Fe	0.393297	-0.034491	-0.473807
S	-1.436404	1.497688	-0.664271
S	-0.589876	-0.100881	1.653408
P	2.325577	-1.067836	-0.386949
P	1.635220	1.847371	-0.108916
O	-0.745998	-2.541024	-1.441394
N	-3.636462	-0.410430	-1.223611
N	-3.219899	-1.555021	1.618455
C	-0.370961	-1.503137	-1.019871
C	3.659029	0.155140	-0.877167
H	4.660707	-0.301505	-0.739187
H	3.520035	0.391580	-1.952607
C	3.454561	1.404185	-0.015844
H	4.069016	2.262518	-0.355085
H	3.712396	1.196498	1.043166
C	2.515258	-2.496570	-1.533229
C	2.858210	-2.294121	-2.888094
H	3.093898	-1.285662	-3.262164
C	2.893085	-3.381500	-3.779703
H	3.169247	-3.212795	-4.833009
C	2.577978	-4.676929	-3.330642
H	2.607015	-5.527334	-4.030682
C	2.220323	-4.881457	-1.985051
H	1.964049	-5.891746	-1.627492
C	2.183632	-3.797802	-1.091847
H	1.893430	-3.967267	-0.042562
C	3.042645	-1.689318	1.210739
C	4.140828	-2.581803	1.227933
H	4.537182	-2.993262	0.286018
C	4.734246	-2.949362	2.447551
H	5.584866	-3.649985	2.449765
C	4.249455	-2.423676	3.661056
H	4.717910	-2.714759	4.615005
C	3.169918	-1.523385	3.649163
H	2.787309	-1.098589	4.591034
C	2.571450	-1.160389	2.428996
H	1.729773	-0.450551	2.416948
C	1.246955	2.791180	1.424921
C	0.212393	3.757370	1.405462
H	-0.258344	4.041071	0.452201
C	-0.221046	4.361332	2.597943
H	-1.025842	5.113373	2.564473
C	0.369945	4.011672	3.826195
H	0.029803	4.487083	4.760166
C	1.400448	3.054738	3.853398
H	1.874000	2.777092	4.808831
C	1.833598	2.444317	2.663259
H	2.633061	1.689746	2.714461
C	1.615304	3.131714	-1.440991
C	1.147380	2.805736	-2.730381
H	0.755629	1.790816	-2.909057
C	1.190035	3.756805	-3.765810
H	0.819611	3.489156	-4.768533
C	1.701263	5.043498	-3.519513
H	1.731926	5.791095	-4.328532
C	2.176586	5.374013	-2.235649
H	2.582192	6.379409	-2.038196
C	2.136530	4.424476	-1.200575
H	2.509989	4.693703	-0.199305
C	-2.270612	1.398461	-2.306234
H	-3.015294	2.219832	-2.344176
H	-1.526665	1.576401	-3.107651
C	-2.893246	0.029579	-2.459226
H	-2.091295	-0.712009	-2.625751
H	-3.570557	-0.013191	-3.340608
C	-4.815333	0.484444	-0.939025
H	-4.405242	1.491031	-0.729189
H	-5.259507	0.139710	0.011280
C	-5.895723	0.560918	-2.019131
H	-6.685488	1.258368	-1.671308
H	-5.510467	0.953016	-2.982243
H	-6.380052	-0.418827	-2.207084
C	-4.023948	-1.835469	-1.463253
H	-4.724399	-1.875137	-2.325909
H	-3.097700	-2.354827	-1.775296
C	-4.622131	-2.571244	-0.273226
H	-4.911455	-3.579979	-0.635887
H	-5.569137	-2.101261	0.063833
C	-3.652100	-2.789479	0.885972
H	-2.728125	-3.271259	0.505645
H	-4.114385	-3.482643	1.625273
C	-4.396322	-0.927307	2.317899
H	-5.246846	-0.924500	1.612501
H	-4.689114	-1.598321	3.157657
C	-4.147677	0.494209	2.810840
H	-5.052163	0.860148	3.339208
H	-3.292846	0.558876	3.513284
H	-3.935888	1.178563	1.962929
C	-2.221550	-1.976676	2.679842
H	-2.463502	-3.009401	3.013440
H	-2.351532	-1.311341	3.554716
C	-0.794805	-1.860556	2.192150
H	-0.570595	-2.534280	1.342416
H	-0.078338	-2.079535	3.010136
H	0.780686	0.161951	-1.922192

2cdd^{+} (acetone)

Ni	2.079309	-1.001246	-0.176530
Fe	-0.378834	0.032486	-0.207499
S	0.278720	-2.261175	-0.401799
S	1.004835	-0.419175	1.694092

P	-1.154622	2.016373	0.297002
P	-2.298215	-0.740843	0.716567
O	1.275828	1.337800	-2.218524
N	2.804032	-1.780408	-1.889307
N	3.608240	0.187345	0.342351
C	0.737688	0.746471	-1.340661
C	-2.371080	1.864082	1.705296
H	-1.778098	1.654892	2.619333
H	-2.914170	2.821423	1.847558
C	-3.308849	0.699773	1.376158
H	-4.009007	0.977025	0.559541
H	-3.913295	0.380859	2.249168
C	-2.188471	2.871651	-0.989564
C	-2.729358	2.143173	-2.068966
H	-2.471576	1.076580	-2.175321
C	-3.582163	2.769773	-2.995999
H	-3.997134	2.188359	-3.835062
C	-3.900212	4.131827	-2.852377
H	-4.564956	4.624752	-3.579992
C	-3.365181	4.865435	-1.775766
H	-3.610616	5.933311	-1.658153
C	-2.515483	4.240689	-0.847440
H	-2.102642	4.824886	-0.008962
C	0.005760	3.357804	0.804005
C	0.828656	3.942900	-0.188041
H	0.727290	3.634050	-1.239652
C	1.778976	4.916180	0.158412
H	2.415367	5.359434	-0.624123
C	1.918401	5.322701	1.499322
H	2.665876	6.084896	1.771552
C	1.092762	4.759184	2.487463
H	1.187883	5.079251	3.537391
C	0.139632	3.781693	2.144636
H	-0.491160	3.352436	2.937567
C	-3.492007	-1.632104	-0.372987
C	-3.206543	-1.849470	-1.735852
H	-2.250193	-1.484018	-2.143254
C	-4.134067	-2.512837	-2.559941
H	-3.898784	-2.679257	-3.623485
C	-5.355951	-2.960063	-2.026825
H	-6.083593	-3.478942	-2.671480
C	-5.648384	-2.744490	-0.665821
H	-6.604744	-3.093170	-0.243895
C	-4.721006	-2.087473	0.159709
H	-4.951856	-1.934158	1.226612
C	-2.124847	-1.895838	2.144387
C	-2.087187	-3.292981	1.927376
H	-2.275131	-3.699542	0.921575
C	-1.821243	-4.171624	2.992239
H	-1.801213	-5.258133	2.809010
C	-1.586445	-3.668123	4.284971
H	-1.380321	-4.357826	5.119202
C	-1.617780	-2.278917	4.507175
H	-1.436676	-1.875569	5.516577
C	-1.877553	-1.396813	3.443821
H	-1.884245	-0.313648	3.639203
C	0.546307	-2.853347	-2.130162
H	0.809059	-3.928854	-2.057248
H	-0.403393	-2.775859	-2.696315
C	1.628499	-2.032538	-2.796457
H	1.222228	-1.040188	-3.063236
H	1.973988	-2.514321	-3.738124
C	3.477618	-3.059902	-1.454702
H	4.262551	-2.772604	-0.730291
H	2.732609	-3.636116	-0.874097
C	4.076163	-3.930735	-2.560754
H	4.494404	-4.845219	-2.091791
H	3.317662	-4.257290	-3.301081
H	4.904022	-3.429810	-3.101978
C	3.735687	-0.886421	-2.642441
H	4.138854	-1.445198	-3.514122
H	3.116910	-0.062042	-3.046300
C	4.871140	-0.289734	-1.820826
H	5.540896	0.240730	-2.529320
H	5.498791	-1.072443	-1.346566
C	4.383420	0.741015	-0.809456
H	3.709781	1.456846	-1.320979
H	5.239175	1.328357	-0.412456
C	4.472038	-0.652756	1.251136
H	4.865909	-1.482102	0.634564
H	3.800284	-1.123954	1.994082
C	5.622291	0.069272	1.955209
H	6.164366	-0.669297	2.581127
H	6.355892	0.501575	1.244998
H	5.267503	0.875978	2.628233
C	3.001516	1.362877	1.058027
H	2.370973	1.888218	0.316740
H	3.799462	2.069042	1.378228
C	2.140021	0.938230	2.223767
H	1.541452	1.795819	2.585989
H	2.732611	0.552777	3.078509
H	-1.177436	-0.051362	-1.463440

$3a^{2+}$ (acetonitrile)

Ni	1.647539	-1.060766	-1.039016
Fe	-0.485102	-0.213134	0.212044
S	0.243373	0.421960	-1.898512
S	-0.236119	-2.197933	-0.903839
P	-0.339356	1.727937	1.275568
P	-2.679628	0.029185	0.288962
O	-0.554053	-1.477048	2.829712
N	3.168442	0.199057	-1.357857
N	2.604665	-2.588566	-0.173007
C	-0.549543	-0.972323	1.772502
C	-1.914671	1.878438	2.269483
H	-1.794611	1.185093	3.128093
H	-2.021904	2.907479	2.666868
C	-3.107455	1.488131	1.388534
H	-3.366326	2.320871	0.704911
H	-4.013143	1.261002	1.984998
C	-0.214486	3.301878	0.330815
C	-1.138777	3.555389	-0.712330
H	-1.911868	2.818239	-0.977350
C	-1.042275	4.733564	-1.470370
H	-1.766363	4.918270	-2.279379
C	-0.011815	5.657922	-1.214606
H	0.069776	6.575349	-1.818735
C	0.921267	5.399453	-0.195156
H	1.738108	6.111638	0.002144
C	0.822035	4.228718	0.578170
H	1.566360	4.036825	1.365443
C	1.021592	1.734605	2.501257
C	1.051591	2.625117	3.597334
H	0.257230	3.377089	3.726249
C	2.105920	2.550334	4.524089

H	2.129947	3.243694	5.379721
C	3.126981	1.593740	4.362664
H	3.949301	1.539780	5.093828
C	3.096434	0.704500	3.272591
H	3.890182	-0.048498	3.145223
C	2.043832	0.773048	2.345516
H	1.995760	0.074860	1.489046
C	-3.550764	0.315536	-1.306541
C	-3.082499	-0.299797	-2.488352
H	-2.182798	-0.931229	-2.465794
C	-3.766406	-0.113432	-3.701546
H	-3.390409	-0.597091	-4.616836
C	-4.920127	0.689608	-3.745280
H	-5.451511	0.842317	-4.698038
C	-5.397924	1.293806	-2.567959
H	-6.306808	1.915726	-2.593138
C	-4.722231	1.107611	-1.349822
H	-5.124736	1.577397	-0.439712
C	-3.498846	-1.452945	1.007484
C	-3.761010	-2.568748	0.180278
H	-3.560641	-2.519924	-0.901524
C	-4.282197	-3.748539	0.736427
H	-4.489130	-4.612251	0.084864
C	-4.542531	-3.825139	2.117851
H	-4.952157	-4.751047	2.551871
C	-4.278804	-2.717024	2.943111
H	-4.479486	-2.771264	4.024905
C	-3.754276	-1.533781	2.394555
H	-3.535022	-0.684168	3.059129
C	1.422216	1.833453	-2.091191
H	1.667237	1.861532	-3.171523
H	0.925335	2.786019	-1.835646
C	2.631070	1.596832	-1.217003
H	3.431564	2.333999	-1.444689
H	2.356423	1.724872	-0.152965
C	3.554858	-0.137142	-2.782254
H	2.623064	-0.193245	-3.379113
H	3.962490	-1.164408	-2.760358
C	4.549270	0.809395	-3.455374
H	4.756403	0.421755	-4.473760
H	4.147365	1.836538	-3.566713
H	5.517120	0.864019	-2.917979
C	4.333844	0.076589	-0.428157
H	4.015063	0.513158	0.537043
H	5.155369	0.716258	-0.814437
C	4.835442	-1.342590	-0.195610
H	5.746545	-1.261768	0.432544
H	5.167457	-1.827515	-1.136546
C	3.845172	-2.207855	0.572729
H	4.340587	-3.137777	0.923145
H	3.509684	-1.663653	1.476411
C	2.894932	-3.529688	-1.321595
H	3.570926	-2.988846	-2.009553
H	1.948467	-3.672332	-1.879164
C	3.492364	-4.886638	-0.949169
H	3.655260	-5.458473	-1.885473
H	4.472985	-4.796016	-0.440758
H	2.815051	-5.486382	-0.308419
C	1.656461	-3.180441	0.834888
H	1.528724	-2.408803	1.615657
H	2.124527	-4.065669	1.317796
C	0.312038	-3.550106	0.234648
H	-0.451325	-3.693459	1.025010
H	0.350786	-4.474214	-0.375621

$3a^{2+}$ (water)

Ni	-1.750430	-1.055355	1.048393
Fe	0.567287	-0.194439	-0.221638
S	-0.351313	0.444020	1.920760
S	0.165055	-2.171373	0.947008
P	0.467433	1.740282	-1.298077
P	2.756917	0.035289	-0.220026
O	0.730444	-1.498894	-2.809217
N	-3.266130	0.217025	1.289989
N	-2.654755	-2.569471	0.119813
C	0.690345	-0.976794	-1.759140
C	2.089006	1.907043	-2.208133
H	2.016111	1.210751	-3.070083
H	2.211564	2.937908	-2.595275
C	3.233599	1.517858	-1.261580
H	3.434439	2.337329	-0.542709
H	4.178439	1.317785	-1.804358
C	0.255323	3.295244	-0.341546
C	1.117135	3.556282	0.751575
H	1.899106	2.838395	1.041653
C	0.945124	4.716841	1.522935
H	1.620481	4.909139	2.371005
C	-0.100190	5.613277	1.230785
H	-0.241843	6.515332	1.846350
C	-0.972023	5.345541	0.160892
H	-1.800233	6.035297	-0.064838
C	-0.796943	4.193226	-0.626265
H	-1.493180	3.991667	-1.454139
C	-0.856036	1.722492	-2.562375
C	-0.837044	2.574961	-3.687672
H	-0.015821	3.295639	-3.826525
C	-1.878747	2.504375	-4.628970
H	-1.865190	3.167534	-5.508081
C	-2.936308	1.592016	-4.450009
H	-3.750113	1.543229	-5.190572
C	-2.954395	0.740534	-3.329725
H	-3.778442	0.023718	-3.188198
C	-1.913397	0.800852	-2.389216
H	-1.909547	0.129002	-1.509040
C	3.558893	0.272470	1.417183
C	3.011433	-0.338614	2.566281
H	2.092915	-0.937890	2.489158
C	3.639756	-0.186312	3.813467
H	3.203976	-0.666088	4.703627
C	4.814604	0.578781	3.922554
H	5.302735	0.704270	4.901759
C	5.367973	1.181703	2.777948
H	6.292124	1.775494	2.856353
C	4.748251	1.030273	1.525896
H	5.205563	1.498482	0.640968
C	3.563193	-1.447806	-0.946912
C	3.624532	-2.630185	-0.173975
H	3.295629	-2.627240	0.877289
C	4.100883	-3.819534	-0.747723
H	4.148848	-4.736212	-0.139445
C	4.512909	-3.839495	-2.094027
H	4.884107	-4.773979	-2.543213
C	4.446965	-2.665379	-2.865179
H	4.765138	-2.676856	-3.919391
C	3.968679	-1.470470	-2.299051

H	3.901521	-0.567305	-2.924507
C	-1.531970	1.857660	2.054312
H	-1.815017	1.904866	3.124791
H	-1.026315	2.805677	1.799029
C	-2.711328	1.609460	1.144281
H	-3.515076	2.355427	1.329124
H	-2.397011	1.716186	0.089208
C	-3.713553	-0.090906	2.702822
H	-2.805748	-0.149511	3.335518
H	-4.133464	-1.114103	2.681111
C	-4.717348	0.881459	3.322477
H	-4.973631	0.510186	4.335462
H	-4.299818	1.901709	3.437839
H	-5.660487	0.947237	2.744152
C	-4.394566	0.093708	0.315779
H	-4.041050	0.534637	-0.635726
H	-5.232846	0.728979	0.671756
C	-4.880984	-1.325037	0.054233
H	-5.767458	-1.243018	-0.607625
H	-5.243741	-1.820750	0.977818
C	-3.854755	-2.174844	-0.681994
H	-4.330099	-3.096909	-1.078059
H	-3.472488	-1.611616	-1.555289
C	-3.002193	-3.525058	1.237578
H	-3.700014	-2.986737	1.906310
H	-2.080719	-3.686988	1.830343
C	-3.597458	-4.868479	0.818427
H	-3.791090	-5.459424	1.736529
H	-4.562188	-4.758339	0.284359
H	-2.905040	-5.456986	0.183642
C	-1.659607	-3.146072	-0.853436
H	-1.491096	-2.360611	-1.613581
H	-2.107190	-4.021207	-1.372938
C	-0.345655	-3.529202	-0.199966
H	0.447408	-3.678034	-0.959446
H	-0.418653	-4.449545	0.412661

3ad^{2+} (acetonitrile)

Ni	2.507454	0.481352	-1.556952
Fe	0.084094	1.231773	-0.121231
S	2.239486	2.395255	-0.462788
S	0.601477	1.162144	-2.438002
P	-0.318175	1.688548	2.011983
P	-1.716558	2.340545	-0.551815
O	-1.382043	-1.264683	-0.371080
N	4.125584	0.115366	-0.459349
N	2.424446	-1.160014	-2.709263
C	-0.606000	-0.372791	-0.118442
C	-2.178939	1.823620	2.152937
H	-2.576136	0.795284	2.016062
H	-2.470856	2.192795	3.157477
C	-2.651863	2.751362	1.030937
H	-2.403095	3.808333	1.263139
H	-3.745396	2.689591	0.860113
C	0.237094	3.338692	2.661685
C	0.524636	4.377261	1.750720
H	0.479585	4.174801	0.671286
C	0.876441	5.657323	2.213798
H	1.098145	6.456533	1.488454
C	0.947809	5.910943	3.595338
H	1.229574	6.911535	3.960807
C	0.658187	4.880982	4.510912
H	0.709928	5.074320	5.594561
C	0.301645	3.601812	4.049748
H	0.074219	2.805881	4.776608
C	0.169004	0.564406	3.394413
C	-0.779488	-0.165779	4.142085
H	-1.848765	-0.118272	3.894994
C	-0.367997	-0.964635	5.225248
H	-1.121052	-1.529588	5.797135
C	0.991740	-1.048917	5.570511
H	1.310345	-1.677282	6.417310
C	1.945562	-0.326337	4.826719
H	3.013753	-0.381595	5.089983
C	1.535810	0.474015	3.748834
H	2.284836	1.062433	3.200589
C	-1.676500	3.971403	-1.432299
C	-0.450435	4.534351	-1.839444
H	0.486129	3.984679	-1.657972
C	-0.420844	5.791737	-2.470552
H	0.543379	6.222122	-2.785302
C	-1.617887	6.493837	-2.697987
H	-1.595744	7.478555	-3.191919
C	-2.846822	5.935385	-2.294730
H	-3.787160	6.481731	-2.472673
C	-2.878420	4.678580	-1.667316
H	-3.844414	4.243143	-1.362926
C	-2.918720	1.386477	-1.582703
C	-2.861070	1.480052	-2.992093
H	-2.157080	2.180984	-3.468942
C	-3.696581	0.683058	-3.793544
H	-3.640576	0.765792	-4.890904
C	-4.606233	-0.209053	-3.195134
H	-5.269294	-0.827587	-3.821024
C	-4.666148	-0.307657	-1.793197
H	-5.375354	-1.002793	-1.320285
C	-3.817575	0.473145	-0.988407
H	-3.859713	0.356825	0.105435
C	3.441539	2.106149	0.905231
H	4.319648	2.761492	0.737811
H	2.970106	2.408170	1.862287
C	3.805364	0.636063	0.917083
H	4.652348	0.433645	1.610470
H	2.931808	0.046125	1.263534
C	5.243047	0.869810	-1.136091
H	4.893020	1.909644	-1.280036
H	5.336370	0.441668	-2.153159
C	6.595849	0.861520	-0.422536
H	7.302150	1.485010	-1.008401
H	6.535523	1.296735	0.595794
H	7.035744	-0.153269	-0.345628
C	4.448133	-1.333580	-0.304810
H	3.647227	-1.761784	0.331364
H	5.398548	-1.429253	0.262224
C	4.517772	-2.118214	-1.607491
H	4.958196	-3.109448	-1.376812
H	5.204023	-1.647208	-2.341165
C	3.135510	-2.367908	-2.190685
H	3.181146	-3.130178	-2.997087
H	2.489795	-2.783290	-1.393880
C	3.004787	-0.701214	-4.026468
H	4.069533	-0.468624	-3.828255
H	2.523238	0.263373	-4.279540
C	2.875966	-1.668342	-5.205106
H	3.356608	-1.201707	-6.089488

H	3.383654	-2.637578	-5.026443
H	1.818046	-1.868258	-5.470868
C	0.971274	-1.543655	-2.801894
H	0.675940	-1.855530	-1.782915
H	0.854211	-2.430686	-3.464022
C	0.083734	-0.407286	-3.265132
H	-0.973998	-0.610109	-3.004331
H	0.146357	-0.226557	-4.357054
H	0.565878	-0.641724	0.215096
C	-5.211745	-2.956029	0.521001
C	-4.934771	-2.225396	1.737240
C	-4.134412	-3.662597	-0.102340
C	-2.851786	-3.621727	0.436953
C	-2.559429	-2.882160	1.650906
C	-3.665333	-2.204801	2.270003
C	-0.133819	-4.068476	0.495187
C	-0.221901	-3.243712	1.684959
C	1.083941	-4.580715	0.049896
C	2.297698	-4.308958	0.760109
C	2.224760	-3.457247	1.924568
C	1.017007	-2.951335	2.351427
N	-1.349410	-2.737505	2.210713
H	-4.307576	-4.222275	-1.031427
H	-5.735589	-1.675673	2.247613
H	-3.453850	-1.645205	3.193615
H	1.100751	-5.211297	-0.849259
H	3.133950	-3.203664	2.484024
H	0.965651	-2.310546	3.242087
S	-1.580980	-4.495544	-0.401836
N	3.487062	-4.827584	0.348122
N	-6.456185	-2.947188	-0.029786
C	-6.722498	-3.682093	-1.266998
H	-6.512715	-4.765641	-1.141820
H	-7.785535	-3.562271	-1.537902
H	-6.100501	-3.298093	-2.104363
C	3.547349	-5.709931	-0.817433
H	2.997657	-6.659264	-0.634452
H	3.113012	-5.218983	-1.711978
H	4.602316	-5.950498	-1.034351
C	-7.539600	-2.170878	0.578262
H	-8.448140	-2.277926	-0.039379
H	-7.769612	-2.532216	1.602921
H	-7.279964	-1.092233	0.631822
C	4.700253	-4.642694	1.148090
H	4.915588	-3.568819	1.315135
H	4.609180	-5.141623	2.137130
H	5.556400	-5.083915	0.608990

$3b^{2+}$ (acetonitrile)

Ni	2.327234	-0.623912	-1.007795
Fe	-0.478518	0.082201	-0.173155
S	1.141762	1.129776	-1.602301
S	0.444492	-1.682945	-1.426542
P	-1.250102	1.948434	0.855392
P	-2.151257	-1.067568	0.838462
O	1.220068	-0.578123	2.102029
N	3.739940	0.590005	-0.247736
N	3.284795	-2.407469	-0.822952
C	0.590224	-0.279259	1.156615
C	-2.324109	1.359423	2.251895
H	-1.616234	1.068913	3.054661
H	-2.940213	2.192513	2.647141
C	-3.173859	0.168911	1.803751
H	-3.970886	0.499500	1.105654
H	-3.655030	-0.337789	2.664222
C	-2.302755	2.994392	-0.232649
C	-3.649463	3.288626	0.069504
H	-4.110618	2.938378	1.005014
C	-4.426331	4.040138	-0.832198
H	-5.478060	4.259187	-0.588545
C	-3.866893	4.508105	-2.033771
H	-4.479636	5.093346	-2.737689
C	-2.522107	4.221921	-2.337292
H	-2.076203	4.580357	-3.278401
C	-1.747328	3.463113	-1.446993
H	-0.705944	3.216615	-1.707237
C	-0.085117	3.124095	1.670916
C	0.046098	4.465024	1.243013
H	-0.578119	4.854109	0.425168
C	0.984402	5.314896	1.854732
H	1.078811	6.355806	1.506950
C	1.795299	4.841717	2.901160
H	2.533098	5.508599	3.374815
C	1.654059	3.514623	3.346463
H	2.277065	3.136546	4.172340
C	0.721494	2.659477	2.737054
H	0.631936	1.625951	3.102469
C	-1.669234	-2.373440	2.046621
C	-1.684792	-3.734400	1.666039
H	-2.035151	-4.025252	0.663845
C	-1.253281	-4.725803	2.563426
H	-1.270161	-5.782819	2.253801
C	-0.807457	-4.371067	3.849448
H	-0.470128	-5.149256	4.552471
C	-0.798735	-3.018452	4.236616
H	-0.457112	-2.732218	5.244087
C	-1.223183	-2.021846	3.341482
H	-1.197112	-0.970742	3.664606
C	-3.374628	-1.936700	-0.234637
C	-2.978599	-2.500530	-1.466671
H	-1.940578	-2.386488	-1.814984
C	-3.905539	-3.200431	-2.257960
H	-3.583034	-3.632310	-3.218589
C	-5.236327	-3.343587	-1.825991
H	-5.964401	-3.887998	-2.448254
C	-5.634471	-2.791835	-0.594538
H	-6.673411	-2.905960	-0.246389
C	-4.710376	-2.094008	0.202316
H	-5.040694	-1.684014	1.168755
C	2.180404	2.453828	-0.850119
H	2.768972	2.900414	-1.677118
H	1.533795	3.246106	-0.427536
C	3.041536	1.838449	0.225445
H	2.400758	1.544976	1.075773
H	3.786138	2.564563	0.617604
C	4.720374	0.893972	-1.353130
H	4.124106	1.201476	-2.233870
H	5.196684	-0.062130	-1.629153
C	5.794203	1.937440	-1.043353
H	6.468902	2.009164	-1.921077
H	5.371269	2.947037	-0.868301
H	6.416868	1.658892	-0.169212
C	4.384158	-0.008332	0.965351
H	5.149389	0.702272	1.345868
H	3.589055	-0.068727	1.733871

C	5.002204	-1.387363	0.783052
H	5.487203	-1.645843	1.747603
H	5.826493	-1.370671	0.040871
C	3.997307	-2.499421	0.493396
H	3.213926	-2.501267	1.278719
H	4.516548	-3.483341	0.532407
C	4.256278	-2.584768	-1.962729
H	5.163052	-1.999661	-1.729210
H	4.567263	-3.653679	-1.974510
C	3.709739	-2.151743	-3.318509
H	4.468345	-2.361619	-4.100215
H	2.779902	-2.688732	-3.594148
H	3.490735	-1.063604	-3.332675
C	2.285994	-3.547024	-0.891191
H	2.684138	-4.413166	-0.320316
H	2.199918	-3.863473	-1.948174
C	0.919865	-3.133856	-0.388501
H	0.922758	-2.850800	0.681248
H	0.175490	-3.941109	-0.536279
N	-1.704330	0.368118	-1.635593
C	-2.479890	0.555441	-2.488635
C	-3.473867	0.806582	-3.508073
H	-4.160091	-0.062898	-3.579932
H	-2.983585	0.969334	-4.489573
H	-4.052123	1.714116	-3.234983

$3b^{2+}$ (water)

Ni	2.318784	-0.431531	-0.893729
Fe	-0.334000	-0.007940	0.013442
S	0.922531	1.097823	-1.621990
S	0.581039	-1.745786	-1.238183
P	-1.439077	1.709888	0.907353
P	-2.007019	-1.209270	0.852548
O	1.196520	-0.415932	2.409761
N	3.545334	1.018458	-0.242163
N	3.487553	-2.045301	-0.565457
C	0.595698	-0.238807	1.410645
C	-2.209579	1.092629	2.481432
H	-1.374513	1.121651	3.210336
H	-2.979161	1.810738	2.828267
C	-2.748742	-0.342380	2.341525
H	-3.848168	-0.360080	2.209909
H	-2.510658	-0.945517	3.238568
C	-2.787598	2.144692	-0.259283
C	-4.148557	1.966798	0.076312
H	-4.447703	1.648936	1.085502
C	-5.142409	2.180812	-0.893797
H	-6.199637	2.025135	-0.629225
C	-4.790589	2.581763	-2.194888
H	-5.573119	2.737056	-2.953767
C	-3.437289	2.773847	-2.528826
H	-3.154988	3.086902	-3.545925
C	-2.438618	2.545066	-1.570561
H	-1.380027	2.666733	-1.847723
C	-0.592169	3.266340	1.380396
C	-0.883217	4.499291	0.755280
H	-1.679490	4.568609	-0.000871
C	-0.144462	5.647077	1.091895
H	-0.373836	6.603681	0.597011
C	0.881532	5.574825	2.050710
H	1.463212	6.474586	2.305341
C	1.160708	4.351745	2.688538
H	1.959074	4.289226	3.444232
C	0.428843	3.200580	2.357882
H	0.667674	2.247463	2.855655
C	-1.671044	-2.935063	1.355019
C	-2.026562	-4.011706	0.513525
H	-2.597471	-3.830301	-0.410177
C	-1.638785	-5.319981	0.850670
H	-1.918348	-6.156687	0.191685
C	-0.893004	-5.558432	2.019222
H	-0.586173	-6.584104	2.277277
C	-0.538309	-4.485456	2.858528
H	0.047136	-4.668124	3.773032
C	-0.922713	-3.175496	2.530335
H	-0.618700	-2.339443	3.179711
C	-3.346549	-1.294037	-0.406601
C	-3.112167	-0.824002	-1.716520
H	-2.124699	-0.431203	-2.004101
C	-4.154020	-0.815331	-2.658632
H	-3.967485	-0.427687	-3.671723
C	-5.431018	-1.281122	-2.299389
H	-6.249953	-1.265377	-3.035521
C	-5.664810	-1.763394	-0.997683
H	-6.662969	-2.133230	-0.715490
C	-4.627669	-1.771746	-0.050802
H	-4.817549	-2.151452	0.966071
C	1.769362	2.622673	-1.024248
H	2.304662	3.061195	-1.889547
H	1.019389	3.355309	-0.669038
C	2.684012	2.207284	0.104282
H	2.067122	1.901159	0.967345
H	3.321375	3.053472	0.439131
C	4.517288	1.345169	-1.347671
H	3.910181	1.565801	-2.246804
H	5.071909	0.419969	-1.579785
C	5.500382	2.481832	-1.071152
H	6.154345	2.594726	-1.959615
H	4.994355	3.453978	-0.905839
H	6.154905	2.270892	-0.201793
C	4.204215	0.608663	1.040311
H	4.859437	1.439165	1.380467
H	3.388643	0.515232	1.782799
C	4.992526	-0.691829	1.002986
H	5.459581	-0.805983	2.003151
H	5.840194	-0.633250	0.290012
C	4.144738	-1.941696	0.778307
H	3.331917	-1.978448	1.532316
H	4.777466	-2.846642	0.917216
C	4.519367	-2.172048	-1.656601
H	5.337961	-1.463799	-1.439348
H	4.961649	-3.190473	-1.581003
C	3.970878	-1.908507	-3.054185
H	4.778586	-2.064479	-3.797528
H	3.131543	-2.583121	-3.315864
H	3.610651	-0.863005	-3.153927
C	2.655226	-3.314056	-0.588711
H	3.154459	-4.082248	0.040178
H	2.645955	-3.696733	-1.626816
C	1.234076	-3.080652	-0.132402
H	1.170835	-2.747432	0.919064
H	0.616597	-3.992061	-0.253518

$3c^{2+}$ (acetonitrile)

Ni	2.222558	-0.793299	-0.261804
Fe	-0.328092	0.006259	-0.174907

S	0.534721	-2.212289	-0.517403
S	1.131688	-0.416326	1.642743
P	-1.148430	1.968468	0.558429
P	-2.093609	-0.921462	1.081887
O	1.493843	1.525747	-1.898469
N	2.984461	-1.446272	-2.003744
N	3.704863	0.399745	0.362293
C	0.972838	0.808408	-1.118380
C	-1.924447	1.627352	2.217879
H	-1.091041	1.380526	2.909161
H	-2.436176	2.539840	2.586848
C	-2.894077	0.450307	2.074784
H	-3.801702	0.764690	1.520792
H	-3.225778	0.064414	3.058940
C	-2.537081	2.723962	-0.412320
C	-3.550216	1.895077	-0.950962
H	-3.505649	0.803308	-0.842534
C	-4.640046	2.452239	-1.640652
H	-5.415985	1.786562	-2.050622
C	-4.733666	3.845354	-1.808542
H	-5.583687	4.281917	-2.356712
C	-3.737494	4.677900	-1.268363
H	-3.805402	5.771227	-1.385778
C	-2.648403	4.124903	-0.571714
H	-1.887740	4.797752	-0.148685
C	0.016148	3.364382	0.828841
C	0.625854	3.968523	-0.297234
H	0.349893	3.650127	-1.312964
C	1.577694	4.985791	-0.128854
H	2.045842	5.444518	-1.014029
C	1.932487	5.414656	1.164028
H	2.686281	6.207018	1.296052
C	1.311362	4.838180	2.285347
H	1.570963	5.179504	3.299897
C	0.352399	3.821764	2.122694
H	-0.122433	3.392062	3.016805
C	-3.451925	-1.721074	0.129574
C	-3.130860	-2.491339	-1.011633
H	-2.081400	-2.610628	-1.316809
C	-4.146180	-3.106170	-1.763449
H	-3.880453	-3.702821	-2.650316
C	-5.492801	-2.953929	-1.386479
H	-6.290130	-3.428488	-1.980289
C	-5.818275	-2.197672	-0.245606
H	-6.870233	-2.082864	0.060692
C	-4.805404	-1.586057	0.513793
H	-5.082969	-1.008455	1.408757
C	-1.601668	-2.195371	2.316586
C	-1.556799	-3.560262	1.952490
H	-1.901791	-3.884819	0.958954
C	-1.083379	-4.519815	2.864306
H	-1.060139	-5.581631	2.571601
C	-0.647454	-4.128608	4.143538
H	-0.277516	-4.882583	4.856542
C	-0.688674	-2.771006	4.509807
H	-0.351001	-2.455774	5.509996
C	-1.157328	-1.806013	3.601672
H	-1.168538	-0.748242	3.905563
C	0.773710	-2.607149	-2.306564
H	1.068871	-3.675353	-2.345523
H	-0.194578	-2.502420	-2.836069
C	1.811464	-1.687815	-2.919676
H	1.357880	-0.701385	-3.125546
H	2.170691	-2.091313	-3.891290
C	3.707318	-2.728863	-1.653031
H	4.487671	-2.463128	-0.916078
H	2.988542	-3.369077	-1.108214
C	4.324207	-3.500469	-2.819576
H	4.785263	-4.423488	-2.412046
H	3.568305	-3.811372	-3.568767
H	5.122851	-2.932159	-3.336753
C	3.887701	-0.468534	-2.687348
H	4.318547	-0.959907	-3.584771
H	3.245670	0.355741	-3.050918
C	4.999349	0.109485	-1.818234
H	5.648104	0.712571	-2.486606
H	5.655705	-0.682941	-1.403488
C	4.488214	1.051373	-0.733444
H	3.822026	1.808577	-1.189709
H	5.334714	1.603665	-0.273799
C	4.567847	-0.511869	1.206919
H	4.966996	-1.285151	0.525369
H	3.897131	-1.045248	1.907201
C	5.708600	0.156873	1.973222
H	6.255513	-0.631387	2.530054
H	6.438003	0.657971	1.305704
H	5.343510	0.894464	2.715939
C	3.074073	1.500850	1.174382
H	2.470775	2.112872	0.478360
H	3.863339	2.164080	1.589782
C	2.188276	0.958944	2.273451
H	1.545669	1.757967	2.688145
H	2.764336	0.519302	3.113072
C	-1.867653	-0.136813	-2.790157
N	-1.305814	-0.068064	-1.765679
C	-2.636225	-0.243380	-4.012006
H	-3.220086	-1.187750	-3.994733
H	-1.966096	-0.242503	-4.895916
H	-3.337962	0.614039	-4.084213

$3c^{2+}$ (water)

Ni	2.180397	-0.874325	-0.216766
Fe	-0.416041	0.056068	-0.175429
S	0.427984	-2.227782	-0.548295
S	0.981247	-0.385705	1.581048
P	-1.292220	1.985954	0.461586
P	-2.278874	-0.840338	0.891323
O	1.378263	1.578738	-1.931987
N	2.950452	-1.496525	-1.950960
N	3.617197	0.371910	0.410545
C	0.812377	0.883445	-1.167662
C	-2.284491	1.717383	2.008621
H	-1.558950	1.500368	2.820861
H	-2.838177	2.642561	2.269531
C	-3.220142	0.527863	1.758232
H	-4.046242	0.811744	1.073713
H	-3.668082	0.142526	2.695294
C	-2.525485	2.499029	-0.802347
C	-2.644272	1.739084	-1.985930
H	-1.966993	0.886739	-2.164999
C	-3.627418	2.062007	-2.936742
H	-3.719310	1.460566	-3.854474
C	-4.489656	3.149298	-2.708546
H	-5.262359	3.403319	-3.451183
C	-4.366999	3.915789	-1.532589

H	-5.041487	4.768666	-1.357581
C	-3.388197	3.594334	-0.577793
H	-3.296219	4.193554	0.342537
C	-0.233652	3.453301	0.735398
C	0.316387	4.102591	-0.394460
H	0.034600	3.778941	-1.408283
C	1.223993	5.159529	-0.225335
H	1.651122	5.657667	-1.109708
C	1.586628	5.579329	1.068658
H	2.304124	6.404544	1.199306
C	1.022377	4.952189	2.193522
H	1.290427	5.287647	3.207502
C	0.111492	3.892912	2.032539
H	-0.322090	3.414939	2.923820
C	-3.439339	-1.600429	-0.300637
C	-3.054642	-1.722293	-1.653340
H	-2.061011	-1.370455	-1.975441
C	-3.939618	-2.288695	-2.586773
H	-3.636196	-2.381099	-3.641174
C	-5.207026	-2.734642	-2.170516
H	-5.900645	-3.179338	-2.901424
C	-5.591731	-2.615563	-0.820585
H	-6.583830	-2.966777	-0.495966
C	-4.711564	-2.050676	0.116937
H	-5.009961	-1.962557	1.174010
C	-1.935742	-2.119095	2.152182
C	-1.902190	-3.483323	1.785705
H	-2.187825	-3.790090	0.767528
C	-1.511358	-4.452160	2.726045
H	-1.494769	-5.514901	2.437542
C	-1.145273	-4.067646	4.029293
H	-0.838902	-4.829257	4.763527
C	-1.171963	-2.708662	4.393749
H	-0.886304	-2.402446	5.412382
C	-1.560011	-1.733688	3.459382
H	-1.563629	-0.672984	3.754349
C	0.740398	-2.640367	-2.321702
H	1.046566	-3.706235	-2.340421
H	-0.206281	-2.547689	-2.890426
C	1.795757	-1.718784	-2.894590
H	1.351970	-0.725113	-3.089584
H	2.174466	-2.106643	-3.865458
C	3.658350	-2.781290	-1.585982
H	4.422920	-2.518708	-0.830000
H	2.925052	-3.420283	-1.058524
C	4.296653	-3.554420	-2.739322
H	4.743593	-4.480629	-2.324283
H	3.554151	-3.857935	-3.504621
H	5.108510	-2.988034	-3.237332
C	3.868499	-0.521366	-2.616690
H	4.306755	-1.009601	-3.512434
H	3.232992	0.309232	-2.979152
C	4.968186	0.047092	-1.729466
H	5.641313	0.635687	-2.386039
H	5.602134	-0.748639	-1.287244
C	4.430489	1.004746	-0.674445
H	3.773074	1.748467	-1.164811
H	5.261721	1.569974	-0.202940
C	4.459919	-0.502815	1.312267
H	4.881825	-1.299026	0.670051
H	3.772354	-1.015644	2.012368
C	5.572390	0.198479	2.090518
H	6.098244	-0.564353	2.699885
H	6.325083	0.671355	1.428623
H	5.179882	0.966812	2.786735
C	2.946957	1.498572	1.157407
H	2.375709	2.087302	0.415074
H	3.715567	2.176147	1.587765
C	2.009201	0.995573	2.229004
H	1.347492	1.805461	2.590484
H	2.536912	0.571728	3.108288

4a^{2+} (water)

Ni	-1.760706	-1.382297	0.540044
Fe	0.342295	0.023477	-0.444963
S	-0.373639	-0.174930	1.847653
S	0.154864	-2.333530	0.026630
P	0.657736	2.205822	-0.692388
P	2.582062	-0.113803	0.054113
O	0.840794	-0.440178	-3.273177
N	-3.310212	-0.296277	1.185912
N	-2.673577	-2.551775	-0.807615
C	0.673725	-0.242445	-2.133642
C	2.448404	2.428974	-1.156413
H	2.484431	2.134213	-2.226544
H	2.724334	3.499599	-1.079378
C	3.359501	1.550545	-0.299704
H	3.534076	2.028271	0.683409
H	4.351151	1.402100	-0.771281
C	0.308928	3.248430	0.779183
C	1.114800	3.140846	1.937804
H	1.977792	2.460144	1.970256
C	0.798505	3.884668	3.086264
H	1.434429	3.795922	3.980643
C	-0.332127	4.723140	3.100654
H	-0.582384	5.296511	4.006824
C	-1.147563	4.816009	1.959009
H	-2.040494	5.460252	1.966068
C	-0.831078	4.084007	0.800960
H	-1.482150	4.160104	-0.083022
C	-0.243191	3.038809	-2.064358
C	0.147994	4.348746	-2.431711
H	0.964763	4.857815	-1.896578
C	-0.517567	5.016594	-3.471688
H	-0.206808	6.035634	-3.750386
C	-1.578828	4.389345	-4.151427
H	-2.099783	4.916401	-4.966076
C	-1.973963	3.091014	-3.786934
H	-2.804603	2.594579	-4.312205
C	-1.309399	2.416047	-2.747450
H	-1.633533	1.399002	-2.479148
C	3.176982	-0.570590	1.740153
C	2.551381	-1.614554	2.460665
H	1.695883	-2.154045	2.030735
C	3.018927	-1.982594	3.733255
H	2.518166	-2.798033	4.278129
C	4.113200	-1.312117	4.306455
H	4.475665	-1.597158	5.306599
C	4.746231	-0.278436	3.593694
H	5.610711	0.246904	4.029040
C	4.286125	0.091007	2.318037
H	4.813239	0.892691	1.780887
C	3.398610	-1.323307	-1.069786
C	3.482912	-2.687955	-0.710777
H	3.176854	-3.024826	0.290729

C	3.971872	-3.629810	-1.632306
H	4.034450	-4.690229	-1.341818
C	4.384861	-3.220810	-2.913161
H	4.768671	-3.960851	-3.632803
C	4.310252	-1.862302	-3.270275
H	4.635295	-1.533150	-4.269736
C	3.815493	-0.915434	-2.357413
H	3.742401	0.138644	-2.666454
C	-1.618919	1.043483	2.442535
H	-1.899881	0.708398	3.461304
H	-1.150888	2.038993	2.538893
C	-2.790792	1.082836	1.497814
H	-3.611357	1.713843	1.903082
H	-2.476675	1.532750	0.533627
C	-3.765016	-1.042722	2.418092
H	-2.867939	-1.225474	3.040732
H	-4.099229	-2.039880	2.074368
C	-4.857355	-0.373947	3.251507
H	-5.080508	-1.030911	4.116609
H	-4.537965	0.608527	3.653819
H	-5.801227	-0.236467	2.687166
C	-4.416531	-0.109495	0.197776
H	-4.022398	0.573897	-0.581930
H	-5.250968	0.421775	0.702431
C	-4.916095	-1.381277	-0.470185
H	-5.808930	-1.105826	-1.068057
H	-5.267405	-2.133935	0.264837
C	-3.890529	-1.951048	-1.437056
H	-4.354912	-2.713883	-2.096715
H	-3.526675	-1.134684	-2.093071
C	-2.986845	-3.816115	-0.043499
H	-3.619279	-3.517970	0.814859
H	-2.036248	-4.172855	0.396478
C	-3.658072	-4.937577	-0.834943
H	-3.776265	-5.810226	-0.160970
H	-4.667288	-4.658475	-1.197580
H	-3.047806	-5.265921	-1.700344
C	-1.698866	-2.773184	-1.936798
H	-1.566428	-1.787001	-2.422722
H	-2.144119	-3.457617	-2.690951
C	-0.360226	-3.287669	-1.460655
H	0.414570	-3.173446	-2.244896
H	-0.387110	-4.352752	-1.153933
H	-1.291534	-0.205447	-0.693437
H	-1.044852	0.684201	-0.822812

$4b^{2+}$ (water)

Ni	2.188311	-0.750229	-0.947044
Fe	-0.552873	0.110800	-0.350503
S	1.146894	0.985573	-1.801555
S	0.306999	-1.788569	-1.452608
P	-1.242197	2.013905	0.646756
P	-2.349409	-0.907456	0.572380
O	0.972809	-0.532228	2.048217
N	3.599774	0.476998	-0.206931
N	3.060658	-2.530491	-0.531651
C	0.437388	-0.259122	1.041341
C	-2.323581	1.476244	2.056593
H	-1.630763	1.107365	2.840103
H	-2.868257	2.342977	2.481850
C	-3.270254	0.372150	1.584423
H	-4.045049	0.786172	0.905588
H	-3.778889	-0.126098	2.433402
C	-2.273264	3.071541	-0.450269
C	-3.459858	3.684893	0.007264
H	-3.812380	3.535483	1.038585
C	-4.206442	4.501465	-0.860376
H	-5.135068	4.970053	-0.498618
C	-3.771095	4.721144	-2.179518
H	-4.358902	5.362915	-2.854440
C	-2.584397	4.118474	-2.636000
H	-2.235773	4.288107	-3.666623
C	-1.841019	3.291764	-1.778303
H	-0.916066	2.817393	-2.143937
C	-0.038325	3.177891	1.412890
C	0.188875	4.458251	0.858867
H	-0.387431	4.798133	-0.014821
C	1.164852	5.304111	1.413617
H	1.337405	6.296443	0.968609
C	1.916367	4.886321	2.525812
H	2.684279	5.549054	2.954587
C	1.678947	3.621487	3.093900
H	2.257436	3.289066	3.969801
C	0.709169	2.768694	2.542619
H	0.552554	1.778536	2.994614
C	-2.028801	-2.322443	1.700091
C	-2.237849	-3.647368	1.256705
H	-2.646690	-3.839326	0.252799
C	-1.909731	-4.728639	2.091424
H	-2.071905	-5.758046	1.735512
C	-1.375864	-4.497935	3.371842
H	-1.116312	-5.347309	4.023059
C	-1.179514	-3.179117	3.821822
H	-0.770065	-2.991735	4.826784
C	-1.501985	-2.092782	2.991812
H	-1.335083	-1.067987	3.354835
C	-3.610881	-1.574332	-0.590100
C	-3.278100	-1.934432	-1.912617
H	-2.251819	-1.796127	-2.284349
C	-4.255425	-2.484027	-2.761270
H	-3.985583	-2.761847	-3.792077
C	-5.567586	-2.676276	-2.295537
H	-6.332881	-3.103700	-2.962343
C	-5.901898	-2.324577	-0.974178
H	-6.927420	-2.477229	-0.602899
C	-4.929562	-1.779938	-0.119982
H	-5.201883	-1.523954	0.915669
C	2.182385	2.338459	-1.104640
H	2.847097	2.677955	-1.924412
H	1.539122	3.189905	-0.813013
C	2.931877	1.796166	0.086596
H	2.218576	1.613184	0.908867
H	3.679047	2.526569	0.465043
C	4.666165	0.624453	-1.263284
H	4.150310	0.919116	-2.197427
H	5.078188	-0.380534	-1.456246
C	5.802598	1.597628	-0.952277
H	6.506061	1.588442	-1.809612
H	5.449440	2.640493	-0.825229
H	6.376293	1.305488	-0.049945
C	4.124620	-0.013202	1.107980
H	4.900106	0.697775	1.464888
H	3.278945	0.052563	1.817966
C	4.675016	-1.430778	1.123769
H	5.055058	-1.609328	2.151053

H	5.561328	-1.530207	0.464383
C	3.639852	-2.519851	0.851347
H	2.787372	-2.407293	1.551697
H	4.100671	-3.516269	1.034584
C	4.129623	-2.836433	-1.550914
H	5.033782	-2.263875	-1.278761
H	4.397904	-3.910789	-1.440289
C	3.727490	-2.510563	-2.984609
H	4.551222	-2.800024	-3.668042
H	2.814197	-3.051710	-3.303077
H	3.539194	-1.424004	-3.110109
C	2.038675	-3.648830	-0.608059
H	2.354298	-4.473600	0.066064
H	2.048292	-4.049673	-1.639405
C	0.641733	-3.177594	-0.275738
H	0.543237	-2.827874	0.768911
H	-0.101319	-3.979531	-0.450963
H	-1.244779	0.320058	-1.897831
H	-1.839977	0.536524	-1.368829

4c^{2+} (water)

Ni	2.123160	-0.831460	-0.267773
Fe	-0.406776	0.005200	-0.348411
S	0.425704	-2.208773	-0.679935
S	0.910628	-0.475140	1.561471
P	-1.240692	1.968691	0.337690
P	-2.249179	-0.917382	0.735743
O	1.530388	1.554819	-1.922084
N	3.000294	-1.461974	-1.958165
N	3.570357	0.338153	0.477291
C	0.940216	0.825246	-1.207850
C	-2.188617	1.622345	1.900177
H	-1.445978	1.355796	2.680946
H	-2.725562	2.540028	2.216375
C	-3.147515	0.460736	1.624965
H	-3.967363	0.776215	0.946241
H	-3.607383	0.072379	2.554917
C	-2.512528	2.767243	-0.746627
C	-3.276129	2.021566	-1.671129
H	-3.098238	0.944652	-1.817730
C	-4.294029	2.640595	-2.417630
H	-4.879395	2.043858	-3.134409
C	-4.559612	4.010634	-2.249906
H	-5.353263	4.496095	-2.839273
C	-3.808404	4.759196	-1.325123
H	-4.012725	5.832272	-1.184527
C	-2.792761	4.143833	-0.575205
H	-2.216130	4.741046	0.148210
C	-0.089005	3.343954	0.720529
C	0.571723	3.986024	-0.353746
H	0.333428	3.709845	-1.391741
C	1.529629	4.979186	-0.100864
H	2.043348	5.467312	-0.943607
C	1.832932	5.347422	1.223720
H	2.592244	6.120174	1.421309
C	1.152122	4.739422	2.292216
H	1.368269	5.038273	3.329687
C	0.188122	3.745107	2.045787
H	-0.336934	3.288296	2.897478
C	-3.519932	-1.716072	-0.324496
C	-3.229642	-2.100208	-1.650580
H	-2.231909	-1.922955	-2.077103
C	-4.217893	-2.718830	-2.437407
H	-3.982560	-3.015481	-3.471421
C	-5.497603	-2.954819	-1.906021
H	-6.271659	-3.435375	-2.524817
C	-5.788499	-2.579494	-0.580398
H	-6.788799	-2.766233	-0.159147
C	-4.804115	-1.967475	0.212078
H	-5.037037	-1.688331	1.251989
C	-1.886267	-2.191501	2.003307
C	-1.801732	-3.548568	1.617552
H	-2.036712	-3.846769	0.583970
C	-1.428930	-4.524522	2.557338
H	-1.371383	-5.580854	2.251146
C	-1.136489	-4.154847	3.883190
H	-0.846209	-4.921842	4.618348
C	-1.218837	-2.804349	4.269178
H	-0.993415	-2.510039	5.306200
C	-1.585724	-1.821593	3.333888
H	-1.633424	-0.768362	3.650654
C	0.808374	-2.592437	-2.447961
H	1.103413	-3.661272	-2.464871
H	-0.113387	-2.482048	-3.053042
C	1.897810	-1.675755	-2.964291
H	1.472707	-0.680761	-3.189812
H	2.326026	-2.067856	-3.912312
C	3.679477	-2.758051	-1.571261
H	4.411084	-2.512584	-0.779281
H	2.916877	-3.392765	-1.081945
C	4.361490	-3.527495	-2.701100
H	4.786655	-4.457624	-2.272272
H	3.651481	-3.824163	-3.499127
H	5.196126	-2.962074	-3.161066
C	3.958297	-0.484079	-2.563488
H	4.447011	-0.969060	-3.434288
H	3.348582	0.349652	-2.959736
C	5.010350	0.076603	-1.614369
H	5.700917	0.689544	-2.229362
H	5.638450	-0.723572	-1.172002
C	4.428435	1.003168	-0.552765
H	3.795035	1.767568	-1.042046
H	5.242707	1.546107	-0.028548
C	4.372772	-0.589106	1.363560
H	4.825650	-1.345997	0.697582
H	3.656777	-1.141298	2.001633
C	5.451556	0.065962	2.224856
H	5.960166	-0.733498	2.801016
H	6.224134	0.583543	1.622036
H	5.030616	0.785394	2.955591
C	2.891994	1.430371	1.262961
H	2.341893	2.059273	0.538499
H	3.654489	2.080897	1.742886
C	1.934028	0.873454	2.290695
H	1.273216	1.667170	2.685640
H	2.451141	0.406548	3.153630
H	-0.788946	-0.064638	-1.880841
H	-1.547628	0.063185	-1.441300

TS-2a2b^{+} (acetone)

Ni	2.168904	-0.509960	-0.864956
Fe	-0.277608	-0.016342	0.056246
S	0.580347	0.315195	-2.166181
S	0.639185	-2.108538	-0.677859
P	-1.414754	1.623258	0.950090
P	-2.142233	-1.155130	0.431282

O	1.667405	0.734068	2.128334
N	3.281387	1.125161	-1.215554
N	3.460876	-1.592348	0.220013
C	0.982590	0.391935	1.216602
C	-2.556032	0.927683	2.253738
H	-1.918417	0.541311	3.074996
H	-3.223049	1.718824	2.655225
C	-3.328386	-0.199782	1.558804
H	-4.126809	0.213709	0.907314
H	-3.800176	-0.893776	2.282540
C	-2.655354	2.504613	-0.124945
C	-2.981925	2.026555	-1.409936
H	-2.457137	1.145527	-1.814068
C	-3.976926	2.661461	-2.175750
H	-4.222833	2.274549	-3.177568
C	-4.653438	3.780827	-1.660766
H	-5.432465	4.280133	-2.259021
C	-4.332522	4.263780	-0.376905
H	-4.857610	5.142743	0.030389
C	-3.341077	3.629229	0.389531
H	-3.095084	4.017362	1.391439
C	-0.508199	3.035861	1.700152
C	0.064222	3.996045	0.834851
H	-0.105682	3.927746	-0.252108
C	0.846206	5.039743	1.354892
H	1.288672	5.783078	0.672534
C	1.060037	5.135865	2.743637
H	1.673496	5.954736	3.152403
C	0.485124	4.186592	3.607735
H	0.645536	4.260679	4.695349
C	-0.294848	3.135870	3.090558
H	-0.728001	2.394669	3.779398
C	-3.246720	-1.748046	-0.928946
C	-2.795095	-1.612124	-2.257994
H	-1.797685	-1.179876	-2.442323
C	-3.613887	-2.008971	-3.330821
H	-3.252955	-1.898941	-4.366145
C	-4.892729	-2.538880	-3.079843
H	-5.537945	-2.844866	-3.919156
C	-5.349221	-2.677653	-1.754394
H	-6.350662	-3.092921	-1.556156
C	-4.529460	-2.288021	-0.681105
H	-4.889012	-2.409742	0.353638
C	-1.812232	-2.689904	1.416624
C	-2.014620	-3.988525	0.903559
H	-2.449948	-4.126167	-0.098522
C	-1.653350	-5.116308	1.666226
H	-1.809874	-6.125305	1.251591
C	-1.096847	-4.958906	2.947726
H	-0.816818	-5.842996	3.542599
C	-0.887253	-3.663881	3.462418
H	-0.439393	-3.530481	4.460376
C	-1.229943	-2.536909	2.696980
H	-1.018332	-1.527671	3.086385
C	1.238259	2.040798	-2.338457
H	1.618297	2.139095	-3.375375
H	0.404067	2.759193	-2.207714
C	2.303219	2.265395	-1.288426
H	1.819207	2.316816	-0.293642
H	2.840063	3.225494	-1.455478
C	3.988456	0.880015	-2.524511
H	4.642172	0.001301	-2.369495
H	3.221804	0.552251	-3.251943
C	4.798334	2.047136	-3.091489
H	5.244549	1.724883	-4.054924
H	4.169781	2.936771	-3.299763
H	5.631916	2.353357	-2.427581
C	4.237336	1.449707	-0.114430
H	4.827600	2.344710	-0.406767
H	3.618944	1.740800	0.758006
C	5.164330	0.309697	0.291647
H	5.911490	0.731260	0.995919
H	5.750559	-0.076931	-0.567590
C	4.433125	-0.800806	1.035283
H	3.847517	-0.348389	1.858333
H	5.160270	-1.501020	1.499128
C	4.153031	-2.453357	-0.810169
H	4.660541	-1.762884	-1.510096
H	3.359885	-2.950192	-1.401011
C	5.146664	-3.490734	-0.282967
H	5.553774	-4.050461	-1.150226
H	6.006140	-3.032547	0.246945
H	4.670582	-4.230416	0.392430
C	2.655434	-2.408921	1.196847
H	2.224212	-1.694821	1.921545
H	3.327316	-3.091755	1.762709
C	1.540051	-3.178646	0.532083
H	0.822757	-3.552666	1.287893
H	1.902868	-4.050099	-0.051041
H	-0.796547	1.016447	-0.877058

TS-2a2c^{+} (acetone)

Ni	-2.555342	-0.289476	-0.082452
Fe	0.199128	0.122384	-0.105084
S	-1.162960	-1.462572	-1.309706
S	-1.539552	1.283829	-1.220162
P	1.615063	1.717384	-0.594227
P	2.023494	-1.160301	-0.574098
O	-0.206873	0.972997	2.659852
N	-3.156295	-1.958997	0.848005
N	-3.704570	1.075841	0.833908
C	-0.070531	0.554661	1.542981
C	2.754662	1.151031	-1.965700
H	2.128745	0.977241	-2.865048
H	3.520335	1.919810	-2.199979
C	3.370540	-0.149315	-1.445587
H	4.159376	0.072593	-0.698030
H	3.820741	-0.763770	-2.249752
C	2.901406	2.136466	0.688538
C	3.053077	1.347547	1.846211
H	2.344913	0.531025	2.045039
C	4.110122	1.588194	2.743303
H	4.216652	0.956324	3.639594
C	5.024944	2.624983	2.491967
H	5.853298	2.815295	3.193351
C	4.880394	3.420423	1.338102
H	5.594110	4.235175	1.135099
C	3.829147	3.175816	0.439284
H	3.730002	3.801017	-0.463097
C	0.998244	3.375084	-1.101361
C	0.822111	4.398116	-0.141254
H	1.138221	4.236300	0.901544
C	0.239805	5.624050	-0.509304
H	0.111759	6.415408	0.246485
C	-0.187069	5.833876	-1.833575

H	-0.648926	6.792182	-2.120364
C	-0.023951	4.814974	-2.790697
H	-0.357228	4.973386	-3.828910
C	0.564876	3.590477	-2.429508
H	0.677712	2.799048	-3.186838
C	2.885991	-1.948035	0.862390
C	2.131382	-2.329965	1.991892
H	1.046217	-2.138952	2.011371
C	2.753785	-2.939238	3.095209
H	2.151304	-3.228767	3.971130
C	4.141508	-3.169110	3.082284
H	4.633277	-3.636632	3.950376
C	4.899107	-2.802927	1.954379
H	5.985287	-2.987178	1.934267
C	4.276042	-2.202596	0.846237
H	4.884756	-1.939707	-0.032796
C	1.840869	-2.586549	-1.742854
C	2.030344	-3.929897	-1.354736
H	2.338527	-4.171612	-0.325483
C	1.827881	-4.969444	-2.282453
H	1.979071	-6.014968	-1.968788
C	1.438847	-4.676680	-3.601470
H	1.281731	-5.492000	-4.325773
C	1.250617	-3.337166	-3.994165
H	0.945321	-3.100293	-5.026096
C	1.440279	-2.298186	-3.068782
H	1.273143	-1.252310	-3.375316
C	-1.287749	-3.069933	-0.404313
H	-1.859941	-3.762004	-1.054856
H	-0.272939	-3.494180	-0.271889
C	-1.943546	-2.842800	0.937968
H	-1.232334	-2.313241	1.604039
H	-2.204852	-3.807361	1.427097
C	-4.230965	-2.539955	-0.037336
H	-5.049353	-1.795927	-0.067942
H	-3.819008	-2.575433	-1.063959
C	-4.779138	-3.912211	0.359364
H	-5.536739	-4.213393	-0.393304
H	-3.993821	-4.695262	0.368133
H	-5.281423	-3.906602	1.347802
C	-3.632140	-1.750108	2.248656
H	-3.996868	-2.718956	2.652913
H	-2.736250	-1.470434	2.839823
C	-4.688667	-0.666426	2.417316
H	-5.061380	-0.729177	3.460844
H	-5.573582	-0.845328	1.772131
C	-4.113237	0.730824	2.229659
H	-3.198026	0.822696	2.848661
H	-4.828338	1.499453	2.593953
C	-4.892766	1.227023	-0.084384
H	-5.400146	0.243963	-0.109445
H	-4.493948	1.386791	-1.104873
C	-5.897134	2.327284	0.266170
H	-6.707222	2.310848	-0.491932
H	-6.370519	2.177504	1.257587
H	-5.443645	3.338979	0.242211
C	-2.892167	2.338512	0.935165
H	-2.078653	2.124837	1.651500
H	-3.512462	3.155774	1.366507
C	-2.291872	2.751826	-0.387040
H	-1.513481	3.523528	-0.233700
H	-3.038251	3.160450	-1.098887
H	-0.100334	-0.734816	1.231672

TS-2b2c^{+} (acetone)

Ni	-2.076460	-1.281298	-0.113831
Fe	0.337938	0.140340	0.321656
S	-1.280246	-0.672564	1.849896
S	-0.022151	-2.030096	-0.402528
P	1.121345	2.172598	0.364755
P	2.463901	-0.466614	0.659100
O	-1.162905	1.313112	-1.918088
N	-3.687858	-0.101449	0.195698
N	-2.687965	-2.268883	-1.768642
C	-0.646543	0.778054	-0.990438
C	2.672426	2.214680	1.401854
H	3.172097	3.198690	1.293630
H	2.378336	2.079261	2.462508
C	3.546828	1.053184	0.918915
H	4.361475	0.816238	1.632532
H	4.014433	1.303227	-0.055448
C	-0.063037	3.390001	1.075091
C	-0.177384	3.549955	2.474309
H	0.518391	3.035816	3.155989
C	-1.198625	4.351793	3.013523
H	-1.275818	4.472643	4.105927
C	-2.122707	4.989031	2.164843
H	-2.927285	5.609910	2.590236
C	-2.013560	4.831664	0.770522
H	-2.732694	5.327802	0.099225
C	-0.987859	4.040386	0.225900
H	-0.914350	3.918895	-0.866098
C	1.703270	2.974508	-1.202888
C	2.084058	4.335878	-1.215043
H	1.961164	4.954363	-0.310665
C	2.616620	4.907588	-2.383062
H	2.910835	5.969488	-2.386911
C	2.774658	4.126201	-3.544494
H	3.194248	4.576938	-4.458308
C	2.394449	2.772217	-3.536611
H	2.514807	2.156082	-4.442104
C	1.857952	2.199383	-2.369381
H	1.556458	1.140047	-2.352605
C	3.237014	-1.379047	-0.756239
C	3.168890	-2.792966	-0.792072
H	2.794475	-3.350245	0.080386
C	3.574679	-3.498139	-1.938632
H	3.511273	-4.598244	-1.950332
C	4.062067	-2.805866	-3.062544
H	4.378896	-3.359599	-3.960875
C	4.149339	-1.401750	-3.028208
H	4.539132	-0.848631	-3.897968
C	3.736672	-0.693419	-1.886184
H	3.800661	0.405099	-1.890983
C	2.906605	-1.555241	2.094999
C	1.905125	-1.948117	3.004348
H	0.868073	-1.613735	2.841649
C	2.227180	-2.759657	4.108962
H	1.435626	-3.064090	4.812677
C	3.553170	-3.180762	4.310627
H	3.806588	-3.815897	5.174798
C	4.559212	-2.791349	3.403699
H	5.599479	-3.121149	3.557463
C	4.238806	-1.985624	2.298824
H	5.028064	-1.696631	1.585188

C	-2.487859	0.667962	2.261394
H	-3.169177	0.264449	3.038237
H	-1.943354	1.533403	2.687888
C	-3.205641	1.080881	0.996740
H	-2.494000	1.630757	0.353235
H	-4.054368	1.766158	1.213679
C	-4.699175	-0.916904	0.957697
H	-4.162883	-1.368512	1.814553
H	-4.988344	-1.761160	0.306834
C	-5.950145	-0.180616	1.440850
H	-6.605463	-0.911505	1.958146
H	-5.716716	0.624449	2.166675
H	-6.537680	0.256968	0.608180
C	-4.226803	0.453830	-1.085100
H	-5.122879	1.071713	-0.858454
H	-3.450753	1.141919	-1.470567
C	-4.562800	-0.565051	-2.166517
H	-4.991959	0.006470	-3.016309
H	-5.371656	-1.252222	-1.842672
C	-3.362753	-1.330288	-2.723795
H	-2.589930	-0.609506	-3.059468
H	-3.686093	-1.918209	-3.612893
C	-3.624819	-3.382574	-1.379626
H	-4.612019	-2.934633	-1.169395
H	-3.760406	-4.037582	-2.270445
C	-3.170811	-4.188215	-0.167395
H	-3.892094	-5.011615	0.014065
H	-2.167728	-4.638792	-0.306477
H	-3.129987	-3.551466	0.740619
C	-1.500914	-2.893438	-2.480373
H	-1.734106	-2.981661	-3.564034
H	-1.373863	-3.920999	-2.088783
C	-0.221561	-2.120110	-2.243521
H	-0.249383	-1.096279	-2.661854
H	0.658213	-2.650149	-2.664288
H	0.524281	0.731059	1.701572

TS-HD-a^{2+} (water)

Ni	-1.973296	-1.304154	-0.014289
Fe	0.494950	-0.021136	-0.282616
S	-0.705927	-0.617547	1.681128
S	-0.075640	-2.257895	-0.566310
P	0.811309	2.202125	-0.025473
P	2.517504	-0.356506	0.582481
O	1.669714	0.072483	-2.943660
N	-3.548092	-0.384938	0.792848
N	-2.762897	-1.986758	-1.719800
C	1.192944	0.063422	-1.873318
C	2.636093	2.423523	0.300627
H	3.096054	2.432444	-0.709836
H	2.816244	3.410741	0.771490
C	3.192119	1.280248	1.150145
H	2.862466	1.367068	2.205365
H	4.300435	1.262530	1.144948
C	-0.067760	3.084654	1.325913
C	0.457132	3.139816	2.636674
H	1.432825	2.691726	2.873960
C	-0.275177	3.764460	3.661587
H	0.143013	3.805776	4.679317
C	-1.537403	4.324548	3.391552
H	-2.112049	4.804678	4.198890
C	-2.061495	4.273513	2.086626
H	-3.046484	4.713978	1.867068
C	-1.329215	3.662522	1.055411
H	-1.742366	3.635676	0.034667
C	0.533396	3.329563	-1.462707
C	0.908858	4.686962	-1.318281
H	1.319103	5.051182	-0.362859
C	0.753607	5.579886	-2.390134
H	1.050783	6.633422	-2.268787
C	0.217604	5.131009	-3.612332
H	0.093904	5.833817	-4.451287
C	-0.162763	3.785973	-3.757264
H	-0.587729	3.428752	-4.708329
C	-0.006559	2.886576	-2.686835
H	-0.320107	1.841998	-2.811378
C	2.755996	-1.483660	2.026145
C	1.970228	-2.643719	2.198247
H	1.165405	-2.879494	1.488076
C	2.213354	-3.513102	3.274768
H	1.590226	-4.413077	3.394977
C	3.240750	-3.232828	4.192367
H	3.427434	-3.911888	5.039074
C	4.031975	-2.082626	4.022402
H	4.844132	-1.858300	4.731576
C	3.796956	-1.210462	2.945640
H	4.442084	-0.327051	2.831578
C	3.675744	-1.026747	-0.681447
C	3.503000	-2.364894	-1.105619
H	2.748801	-3.009035	-0.626483
C	4.289095	-2.881100	-2.147142
H	4.149337	-3.925060	-2.468551
C	5.248487	-2.066727	-2.778490
H	5.861981	-2.471211	-3.598775
C	5.420458	-0.735672	-2.360120
H	6.169605	-0.093805	-2.849656
C	4.636674	-0.211247	-1.316602
H	4.780547	0.837009	-1.015675
C	-1.920340	0.522379	2.478331
H	-2.270591	-0.015042	3.382399
H	-1.412141	1.444832	2.812417
C	-3.037505	0.834082	1.510804
H	-3.874564	1.350787	2.029508
H	-2.666162	1.518043	0.726595
C	-4.082940	-1.445461	1.729057
H	-3.231034	-1.811719	2.334767
H	-4.391257	-2.297931	1.093732
C	-5.228785	-1.019565	2.646127
H	-5.505104	-1.887537	3.278567
H	-4.938086	-0.192119	3.324189
H	-6.134338	-0.715817	2.084041
C	-4.592524	0.094733	-0.164904
H	-4.173110	0.989441	-0.663844
H	-5.472207	0.436055	0.420374
C	-5.018333	-0.910395	-1.225831
H	-5.864893	-0.456414	-1.780552
H	-5.419463	-1.842426	-0.777438
C	-3.919376	-1.194740	-2.241399
H	-4.335875	-1.723305	-3.124793
H	-3.506189	-0.234317	-2.609346
C	-3.163706	-3.411981	-1.407338
H	-3.961223	-3.350618	-0.642758
H	-2.304734	-3.897811	-0.905357
C	-3.625067	-4.258247	-2.593013
H	-3.891239	-5.265620	-2.213452

H	-4.523825	-3.842135	-3.090232
H	-2.828522	-4.388613	-3.352844
C	-1.670503	-1.901439	-2.755510
H	-1.433005	-0.825776	-2.873547
H	-2.048036	-2.272310	-3.733442
C	-0.421984	-2.651557	-2.338662
H	0.447795	-2.359552	-2.958844
H	-0.534066	-3.752445	-2.395416
H	-2.036056	0.954149	-1.647543
H	-1.720265	1.256757	-1.005583

TS-HD-b^{2+} (water)

Ni	2.170551	-0.775367	-0.947770
Fe	-0.503582	0.118469	-0.322449
S	1.149733	0.982709	-1.775427
S	0.274454	-1.758374	-1.478221
P	-1.188230	2.036312	0.665488
P	-2.341242	-0.847554	0.601491
O	0.976468	-0.538666	2.057793
N	3.602944	0.421197	-0.201522
N	2.995776	-2.578919	-0.548671
C	0.437778	-0.263941	1.047408
C	-2.269618	1.534786	2.086885
H	-1.577349	1.168622	2.872111
H	-2.797924	2.418143	2.498999
C	-3.233040	0.436622	1.634353
H	-4.021671	0.856771	0.976704
H	-3.725350	-0.061034	2.493110
C	-2.227376	3.042258	-0.470739
C	-3.483576	3.555538	-0.079650
H	-3.882857	3.368894	0.928392
C	-4.241730	4.319295	-0.985018
H	-5.223682	4.709602	-0.674838
C	-3.750534	4.584981	-2.275492
H	-4.348172	5.183645	-2.980728
C	-2.494909	4.082431	-2.665178
H	-2.102815	4.287701	-3.673474
C	-1.740011	3.308211	-1.770742
H	-0.765474	2.903589	-2.086433
C	0.012795	3.217506	1.404193
C	0.215690	4.502708	0.852741
H	-0.379601	4.840406	-0.008868
C	1.192026	5.356061	1.395223
H	1.345874	6.352886	0.953357
C	1.967747	4.940038	2.491477
H	2.736038	5.608792	2.910119
C	1.754813	3.669383	3.056505
H	2.353436	3.338415	3.919328
C	0.784181	2.809350	2.518175
H	0.645068	1.813839	2.965170
C	-2.047155	-2.269257	1.732605
C	-2.294510	-3.592654	1.305387
H	-2.718639	-3.785175	0.308132
C	-1.987990	-4.673695	2.148828
H	-2.181146	-5.701919	1.805088
C	-1.438288	-4.444794	3.422833
H	-1.196201	-5.294087	4.080849
C	-1.204278	-3.127116	3.857429
H	-0.782069	-2.939778	4.857142
C	-1.504812	-2.041398	3.018429
H	-1.307224	-1.018121	3.370151
C	-3.614685	-1.497411	-0.559970
C	-3.245993	-2.022300	-1.816502
H	-2.192609	-2.003250	-2.134750
C	-4.219076	-2.579070	-2.663784
H	-3.919060	-2.985454	-3.642263
C	-5.566310	-2.614809	-2.263277
H	-6.329342	-3.047055	-2.929543
C	-5.937465	-2.100732	-1.007162
H	-6.989895	-2.132691	-0.684418
C	-4.968559	-1.547827	-0.153219
H	-5.275868	-1.168920	0.833303
C	2.217212	2.317155	-1.088766
H	2.883975	2.646006	-1.910845
H	1.592631	3.179012	-0.786876
C	2.961311	1.752045	0.097079
H	2.246512	1.579809	0.919878
H	3.723629	2.466506	0.475142
C	4.672608	0.551252	-1.256369
H	4.161668	0.844488	-2.193861
H	5.075391	-0.459330	-1.439975
C	5.817842	1.515379	-0.949587
H	6.528701	1.484923	-1.800271
H	5.475915	2.564059	-0.841299
H	6.379728	1.229774	-0.037774
C	4.115914	-0.089392	1.110535
H	4.912273	0.597503	1.468794
H	3.273690	-0.003565	1.822073
C	4.626524	-1.522346	1.119198
H	4.998206	-1.716000	2.146843
H	5.512641	-1.641686	0.463008
C	3.565407	-2.584882	0.838307
H	2.710971	-2.452386	1.532658
H	4.000709	-3.592452	1.022694
C	4.064205	-2.898741	-1.564323
H	4.978806	-2.348561	-1.281678
H	4.308591	-3.979560	-1.462516
C	3.677314	-2.549146	-2.996628
H	4.502133	-2.841025	-3.677610
H	2.758861	-3.072576	-3.329261
H	3.506048	-1.458253	-3.109467
C	1.950359	-3.675725	-0.641591
H	2.240350	-4.507995	0.034615
H	1.965111	-4.073978	-1.673707
C	0.558427	-3.178276	-0.325655
H	0.452363	-2.836699	0.720631
H	-0.202076	-3.958453	-0.523373
H	-2.164115	0.533619	-2.032096
H	-1.449595	0.396767	-2.322075

TS-HD-c^{2+} (water)

Ni	2.297709	-0.754410	-0.218167
Fe	-0.462087	0.026774	-0.379257
S	0.694350	-2.239059	-0.649805
S	0.940572	-0.342512	1.485823
P	-1.462348	1.906597	0.317699
P	-2.226585	-1.052579	0.765447
O	1.407569	1.620698	-1.996087
N	3.228621	-1.320276	-1.898519
N	3.585555	0.607635	0.487885
C	0.789930	0.924916	-1.278046
C	-2.313419	1.493350	1.922593
H	-1.516437	1.301678	2.671813
H	-2.910879	2.366025	2.256995
C	-3.185967	0.253000	1.702700
H	-4.065842	0.502969	1.074573

H	-3.562034	-0.162639	2.658174
C	-2.833279	2.586154	-0.727065
C	-3.645034	1.729139	-1.504618
H	-3.451186	0.645230	-1.540166
C	-4.730070	2.244247	-2.234130
H	-5.352970	1.561918	-2.833228
C	-5.015385	3.620501	-2.198061
H	-5.861730	4.024812	-2.775263
C	-4.216950	4.478675	-1.420304
H	-4.436581	5.557282	-1.383001
C	-3.133922	3.967694	-0.685132
H	-2.522790	4.651904	-0.076741
C	-0.397715	3.363402	0.651697
C	0.226173	4.004372	-0.444818
H	0.006668	3.678246	-1.472355
C	1.122566	5.061501	-0.228672
H	1.607487	5.548691	-1.088846
C	1.402717	5.493284	1.081706
H	2.115402	6.315564	1.251081
C	0.759152	4.883143	2.171845
H	0.958160	5.229095	3.198057
C	-0.144710	3.825912	1.961795
H	-0.640914	3.367284	2.829654
C	-3.457410	-1.933540	-0.277983
C	-3.056458	-2.503815	-1.506146
H	-2.014727	-2.408530	-1.845072
C	-3.986561	-3.199455	-2.298030
H	-3.664404	-3.641680	-3.253723
C	-5.321027	-3.325187	-1.872826
H	-6.050923	-3.863848	-2.497431
C	-5.722593	-2.764021	-0.646195
H	-6.765506	-2.864216	-0.306704
C	-4.795874	-2.075005	0.154062
H	-5.122622	-1.652000	1.116552
C	-1.718528	-2.306614	2.007251
C	-1.557993	-3.654355	1.613719
H	-1.818341	-3.970236	0.591728
C	-1.074573	-4.602655	2.531484
H	-0.959384	-5.652261	2.218368
C	-0.743931	-4.214931	3.842963
H	-0.365912	-4.960197	4.560410
C	-0.899699	-2.873221	4.236586
H	-0.643759	-2.563225	5.261939
C	-1.378998	-1.918491	3.323423
H	-1.481027	-0.871042	3.645908
C	1.144014	-2.634114	-2.396611
H	1.539890	-3.670386	-2.385891
H	0.229806	-2.623718	-3.023059
C	2.152308	-1.627899	-2.908615
H	1.643058	-0.671991	-3.130878
H	2.617183	-1.980223	-3.855254
C	4.012261	-2.550786	-1.499942
H	4.757567	-2.222729	-0.751060
H	3.317753	-3.221179	-0.958358
C	4.700264	-3.311505	-2.632910
H	5.232266	-4.177804	-2.189807
H	3.977950	-3.709509	-3.373689
H	5.452741	-2.697311	-3.166450
C	4.105217	-0.274116	-2.512471
H	4.645329	-0.728910	-3.369305
H	3.427460	0.495800	-2.928454
C	5.089050	0.394818	-1.561501
H	5.748230	1.037947	-2.180058
H	5.761812	-0.339934	-1.073342
C	4.402161	1.305915	-0.552837
H	3.708971	1.982350	-1.089273
H	5.147906	1.948624	-0.039242
C	4.443335	-0.199855	1.436009
H	4.948169	-0.970840	0.824998
H	3.760235	-0.751445	2.110497
C	5.470443	0.581284	2.254735
H	6.012213	-0.138573	2.901344
H	6.223596	1.090345	1.620849
H	4.997918	1.333233	2.918180
C	2.791515	1.673950	1.199207
H	2.221353	2.223671	0.427466
H	3.480721	2.403659	1.676174
C	1.838319	1.088686	2.212906
H	1.109624	1.844549	2.559740
H	2.351175	0.680895	3.108266
H	-0.973437	-0.379073	-2.226987
H	-1.641357	0.020586	-1.986708

TS-HT-a^{2+} (acetonitrile)

Ni	-0.656235	-1.849255	-1.830361
Fe	1.175564	-0.475540	-0.183864
S	1.141383	-2.733435	-0.925406
S	0.853106	-0.392858	-2.473805
P	1.643623	-0.864198	1.979554
P	3.127854	0.511244	-0.250283
O	0.285920	2.267771	-0.407734
N	-1.745007	-3.342846	-1.058654
N	-2.058986	-0.773911	-2.743548
C	0.374895	1.138167	0.021434
C	2.687777	0.595962	2.503799
H	2.031048	1.489895	2.465214
H	3.058257	0.461461	3.540601
C	3.825452	0.708926	1.485465
H	4.557941	-0.114791	1.615916
H	4.379529	1.664111	1.573607
C	2.782401	-2.273494	2.384752
C	3.590549	-2.843806	1.377668
H	3.491151	-2.504681	0.337093
C	4.523039	-3.848172	1.691661
H	5.143243	-4.281818	0.891061
C	4.659190	-4.293283	3.018215
H	5.385208	-5.084270	3.265410
C	3.865596	-3.721628	4.031031
H	3.971095	-4.060666	5.074095
C	2.935950	-2.714836	3.720055
H	2.327372	-2.272997	4.524614
C	0.335808	-1.026026	3.269641
C	-0.053115	0.071755	4.068020
H	0.427370	1.051419	3.946311
C	-1.061532	-0.077238	5.037132
H	-1.353759	0.789127	5.651368
C	-1.695567	-1.318824	5.218179
H	-2.488592	-1.430479	5.974475
C	-1.310600	-2.419863	4.429252
H	-1.794833	-3.399393	4.567793
C	-0.302067	-2.275038	3.462895
H	0.010328	-3.151679	2.876637
C	4.513800	-0.289933	-1.179933
C	4.301504	-1.411386	-2.005802
H	3.290510	-1.830376	-2.111609

C	5.380580	-2.005683	-2.685756
H	5.202427	-2.883833	-3.326748
C	6.677511	-1.482118	-2.544680
H	7.523041	-1.949167	-3.074610
C	6.894038	-0.356644	-1.725737
H	7.907904	0.060394	-1.615221
C	5.818621	0.240955	-1.048095
H	5.996908	1.127900	-0.418722
C	3.128227	2.206477	-0.975437
C	3.130314	2.342224	-2.381305
H	3.233956	1.450947	-3.021584
C	2.996308	3.611364	-2.969349
H	3.000254	3.707778	-4.066912
C	2.859043	4.754242	-2.158306
H	2.752041	5.749313	-2.619096
C	2.856334	4.621751	-0.758079
H	2.737487	5.510389	-0.118301
C	2.983105	3.353289	-0.166632
H	2.936807	3.265073	0.929871
C	0.339601	-3.951807	0.204278
H	0.527046	-4.962253	-0.210894
H	0.824264	-3.897746	1.199269
C	-1.135285	-3.615631	0.291567
H	-1.699496	-4.423166	0.809366
H	-1.266437	-2.680513	0.873872
C	-1.570797	-4.477330	-2.040380
H	-0.494558	-4.538899	-2.293055
H	-2.085063	-4.160245	-2.968412
C	-2.079501	-5.847284	-1.588676
H	-1.894061	-6.572462	-2.407484
H	-1.545255	-6.217814	-0.690464
H	-3.168120	-5.855752	-1.379573
C	-3.190291	-3.049888	-0.821202
H	-3.229005	-2.406554	0.076078
H	-3.708027	-3.997360	-0.561417
C	-3.915134	-2.331351	-1.950234
H	-4.981521	-2.263191	-1.651008
H	-3.900394	-2.906265	-2.899001
C	-3.412185	-0.905918	-2.129380
H	-4.133932	-0.303840	-2.721828
H	-3.337821	-0.426973	-1.136442
C	-2.028759	-1.247788	-4.175166
H	-2.238996	-2.334677	-4.150119
H	-0.984292	-1.151634	-4.529095
C	-2.981108	-0.541181	-5.140222
H	-2.823125	-0.961293	-6.154702
H	-4.047121	-0.697076	-4.879036
H	-2.788328	0.549366	-5.198882
C	-1.663168	0.672019	-2.591411
H	-1.724548	0.889974	-1.507410
H	-2.405259	1.323504	-3.102995
C	-0.259401	0.948871	-3.086718
H	0.111121	1.918839	-2.703375
H	-0.177351	0.949921	-4.191800
H	-0.495831	0.898199	0.905490
C	-0.696244	5.674508	0.967988
C	0.063870	4.863673	1.885085
C	-1.844616	5.084045	0.353402
C	-2.195958	3.757015	0.614236
C	-1.424148	2.931112	1.504609
C	-0.294424	3.552387	2.125037
C	-3.842291	1.548721	0.572415
C	-2.815628	0.986736	1.399114
C	-5.034222	0.862212	0.305986
C	-5.254678	-0.449105	0.826954
C	-4.239906	-1.002997	1.681777
C	-3.067674	-0.309241	1.932536
N	-1.630709	1.601043	1.746483
H	-2.472531	5.674715	-0.327850
H	0.952232	5.271382	2.383955
H	0.315092	2.932936	2.799277
H	-5.786094	1.336763	-0.339384
H	-4.373061	-1.992714	2.136523
H	-2.294062	-0.754739	2.571068
S	-3.616142	3.115419	-0.215150
N	-6.372395	-1.169523	0.500084
N	-0.332548	6.963805	0.702223
C	-1.063321	7.748982	-0.289776
H	-2.108742	7.949871	0.034119
H	-0.552231	8.717252	-0.434681
H	-1.097013	7.225484	-1.269051
C	-7.347799	-0.623708	-0.437750
H	-7.808790	0.311868	-0.051343
H	-6.882032	-0.397968	-1.423006
H	-8.152871	-1.362412	-0.598238
C	0.772611	7.590116	1.426574
H	0.842525	8.651204	1.129235
H	0.611620	7.548783	2.525017
H	1.744719	7.101523	1.198098
C	-6.560825	-2.518350	1.028457
H	-5.745661	-3.202645	0.705393
H	-6.596274	-2.521170	2.139503
H	-7.518334	-2.922273	0.654944

TS-HT-b^{2+} (acetonitrile)

Ni	-2.738935	0.712646	0.538210
Fe	-0.238909	-0.872182	0.107044
S	-1.926821	-0.096782	-1.321470
S	-0.636405	1.257286	0.879514
P	0.236692	-2.663831	-1.124725
P	1.580802	-1.359865	1.323090
O	-1.904594	-2.162056	2.147739
N	-4.443868	-0.312685	0.229714
N	-3.291344	1.805132	2.162400
C	-1.264978	-1.663316	1.291570
C	1.427060	-3.723116	-0.161898
H	0.789395	-4.277543	0.556509
H	1.905313	-4.482575	-0.812152
C	2.445604	-2.834753	0.552494
H	3.175960	-2.413675	-0.168815
H	3.007867	-3.394632	1.326626
C	1.039961	-2.376473	-2.760521
C	2.190918	-3.079224	-3.183520
H	2.647044	-3.851608	-2.546622
C	2.784076	-2.784994	-4.424361
H	3.687819	-3.331809	-4.737252
C	2.230783	-1.796774	-5.258821
H	2.701381	-1.565095	-6.227701
C	1.075402	-1.105489	-4.850595
H	0.635010	-0.329118	-5.496242
C	0.488989	-1.390005	-3.607531
H	-0.400217	-0.832087	-3.278844
C	-1.114861	-3.861149	-1.533367
C	-1.433592	-4.218717	-2.862603
H	-0.842656	-3.820706	-3.701453

C	-2.521659	-5.071002	-3.125465
H	-2.764916	-5.335310	-4.167026
C	-3.296585	-5.579245	-2.067971
H	-4.153203	-6.239654	-2.277196
C	-2.969360	-5.245254	-0.739978
H	-3.565114	-5.645782	0.095684
C	-1.886237	-4.392008	-0.473531
H	-1.649304	-4.132867	0.569091
C	1.186821	-1.946650	3.050660
C	1.168632	-1.034038	4.129454
H	1.466399	0.013559	3.974053
C	0.784846	-1.451582	5.415800
H	0.778340	-0.723370	6.242807
C	0.422258	-2.790513	5.648551
H	0.125394	-3.118530	6.657603
C	0.447954	-3.708649	4.583536
H	0.171873	-4.761987	4.752210
C	0.820890	-3.290311	3.294466
H	0.812710	-4.028323	2.479464
C	2.952325	-0.192047	1.748969
C	2.664287	1.163274	2.001550
H	1.681980	1.571485	1.724258
C	3.628486	2.004978	2.582877
H	3.381444	3.060529	2.776214
C	4.903300	1.504729	2.893023
H	5.658662	2.161529	3.352723
C	5.217344	0.163632	2.599834
H	6.224142	-0.228508	2.813695
C	4.247890	-0.683938	2.039619
H	4.507378	-1.735609	1.848146
C	-3.277318	-1.273159	-1.771403
H	-3.864446	-0.780595	-2.572949
H	-2.848366	-2.203978	-2.185863
C	-4.090399	-1.564287	-0.533762
H	-3.494588	-2.196741	0.148207
H	-5.016148	-2.129069	-0.779437
C	-5.356055	0.582594	-0.567721
H	-4.780520	0.912409	-1.454431
H	-5.522675	1.491683	0.036226
C	-6.699328	-0.012084	-0.992173
H	-7.258403	0.762341	-1.556712
H	-6.586220	-0.890283	-1.659424
H	-7.325299	-0.306171	-0.125445
C	-5.040450	-0.775996	1.521808
H	-5.961242	-1.358817	1.301007
H	-4.305823	-1.482022	1.957718
C	-5.342256	0.312553	2.541023
H	-5.858617	-0.180518	3.391052
H	-6.069011	1.052782	2.147844
C	-4.100882	0.984604	3.120287
H	-3.420123	0.206459	3.522513
H	-4.397212	1.642920	3.968002
C	-4.064691	3.019995	1.721251
H	-5.089874	2.694678	1.467459
H	-4.156994	3.698236	2.600044
C	-3.450222	3.744216	0.528666
H	-4.050653	4.646858	0.296431
H	-2.408545	4.069809	0.718301
H	-3.433357	3.094142	-0.370606
C	-2.059185	2.280116	2.903662
H	-2.309240	2.412594	3.978553
H	-1.779528	3.274934	2.507164
C	-0.897990	1.331111	2.711172
H	-1.102039	0.313252	3.095229
H	0.018126	1.716338	3.202119
H	0.780784	-0.031969	-1.012924
C	-1.052359	4.431762	-1.882904
C	-1.302212	3.282461	-2.709120
C	0.190717	4.482269	-1.178014
C	1.076233	3.402094	-1.210143
C	0.761341	2.185656	-1.916265
C	-0.428379	2.210405	-2.707768
C	3.483062	2.126210	-0.842450
C	2.803971	1.029315	-1.465487
C	4.834006	2.047437	-0.490369
C	5.564393	0.834079	-0.662019
C	4.887412	-0.268985	-1.291884
C	3.566689	-0.154912	-1.681826
N	1.493113	1.024560	-1.884026
H	0.473801	5.385575	-0.620030
H	-2.197366	3.233384	-3.342038
H	-0.627334	1.341750	-3.347132
H	5.308545	2.915593	-0.014812
H	5.413631	-1.214121	-1.476768
H	3.062569	-0.997099	-2.173229
S	2.627481	3.603926	-0.400379
N	6.855648	0.715331	-0.230076
N	-1.958062	5.450340	-1.797777
C	-1.704182	6.591261	-0.923652
H	-0.836394	7.193779	-1.273033
H	-2.595117	7.243696	-0.908952
H	-1.501551	6.259941	0.117525
C	7.550903	1.866322	0.336498
H	7.574864	2.715593	-0.380573
H	7.063860	2.216667	1.272732
H	8.592327	1.584378	0.572059
C	-3.182937	5.421333	-2.594214
H	-2.961980	5.436637	-3.683873
H	-3.789700	4.517450	-2.373897
H	-3.791378	6.310617	-2.352574
C	7.543515	-0.571218	-0.302382
H	6.962233	-1.367346	0.210566
H	7.718558	-0.888655	-1.354077
H	8.523718	-0.485638	0.199222

TS-HT-c^{2+} (acetonitrile)

Ni	-0.291277	-1.129773	2.374457
Fe	0.228119	-0.900767	-0.279286
S	1.716221	-0.627298	1.548340
S	-0.026541	-2.875526	1.051992
P	-0.934556	-1.602959	-2.020725
P	2.028663	-1.960966	-1.403131
O	-2.031709	0.686548	0.668447
N	-0.198301	0.505977	3.545814
N	-2.073047	-1.863156	2.948775
C	-1.105405	-0.004756	0.396828
C	-0.144851	-3.165429	-2.662358
H	-0.300596	-3.949304	-1.892410
H	-0.645568	-3.482730	-3.600298
C	1.338405	-2.863720	-2.889692
H	1.449128	-2.190112	-3.763225
H	1.933193	-3.774264	-3.102034
C	-0.872121	-0.556553	-3.547507
C	0.272569	0.240558	-3.774746
H	1.074800	0.272738	-3.022279

C	0.369585	1.027916	-4.933758
H	1.264947	1.648611	-5.096663
C	-0.681991	1.037302	-5.868399
H	-0.614791	1.668057	-6.769236
C	-1.822642	0.241239	-5.649765
H	-2.647274	0.244578	-6.380523
C	-1.916647	-0.560498	-4.498675
H	-2.814283	-1.176911	-4.332991
C	-2.721063	-2.018114	-1.837140
C	-3.622268	-0.987857	-1.482225
H	-3.262091	0.041960	-1.365862
C	-4.982521	-1.266190	-1.277787
H	-5.667380	-0.448217	-1.001914
C	-5.463255	-2.581509	-1.419084
H	-6.529122	-2.803754	-1.251005
C	-4.576547	-3.610096	-1.783350
H	-4.945087	-4.641095	-1.905458
C	-3.213331	-3.333395	-1.997528
H	-2.545403	-4.158099	-2.286055
C	3.487504	-1.019623	-2.039667
C	4.212923	-0.199045	-1.144111
H	3.850477	-0.048399	-0.115456
C	5.390892	0.444164	-1.560230
H	5.959523	1.053625	-0.840303
C	5.834493	0.320141	-2.888569
H	6.751978	0.834073	-3.216565
C	5.097037	-0.460981	-3.796284
H	5.430794	-0.558999	-4.841690
C	3.939026	-1.138184	-3.374417
H	3.400334	-1.764454	-4.100421
C	2.846651	-3.322502	-0.432584
C	3.901408	-3.050042	0.468082
H	4.325853	-2.040179	0.546762
C	4.438726	-4.069531	1.273993
H	5.264447	-3.833878	1.964461
C	3.932055	-5.378819	1.196663
H	4.354282	-6.176747	1.828243
C	2.884908	-5.661253	0.301720
H	2.479770	-6.683108	0.225919
C	2.342830	-4.643099	-0.501514
H	1.515864	-4.900992	-1.178423
C	1.901305	1.049674	2.289785
H	2.639924	0.947730	3.111016
H	2.330292	1.734001	1.535355
C	0.559030	1.546646	2.768180
H	-0.070379	1.793766	1.895323
H	0.664350	2.475993	3.370311
C	0.551733	0.044560	4.772912
H	-0.079967	-0.721101	5.261263
H	1.454225	-0.491590	4.420736
C	0.940456	1.128694	5.779070
H	1.473066	0.643035	6.622444
H	1.627671	1.882073	5.343736
H	0.061989	1.656176	6.202424
C	-1.520395	1.115433	3.890764
H	-1.349932	1.945282	4.609452
H	-1.902858	1.571175	2.957131
C	-2.568027	0.150982	4.433552
H	-3.440299	0.764099	4.742043
H	-2.226210	-0.363071	5.355455
C	-3.066554	-0.832943	3.382402
H	-3.352677	-0.273036	2.471342
H	-3.979274	-1.353856	3.742695
C	-1.735664	-2.824313	4.064223
H	-1.276144	-2.220768	4.868746
H	-0.932043	-3.488014	3.691932
C	-2.892129	-3.654926	4.621570
H	-2.490246	-4.316569	5.416304
H	-3.686212	-3.031847	5.080098
H	-3.354451	-4.305540	3.851859
C	-2.668118	-2.559397	1.753031
H	-2.874291	-1.777701	0.998544
H	-3.642813	-3.019190	2.027871
C	-1.725270	-3.583575	1.164859
H	-2.064932	-3.891112	0.157357
H	-1.641169	-4.498261	1.786843
H	0.172140	0.776669	-0.904617
C	-3.978669	3.408621	-1.046484
C	-3.477692	2.539093	-2.078636
C	-3.026664	3.964757	-0.136705
C	-1.677338	3.610915	-0.203046
C	-1.186893	2.668430	-1.175035
C	-2.141742	2.190752	-2.121017
C	0.993133	3.896221	0.353056
C	1.135391	2.866365	-0.634051
C	2.103447	4.540624	0.911735
C	3.429160	4.182454	0.520781
C	3.572019	3.149652	-0.472052
C	2.463977	2.522987	-1.012531
N	0.103806	2.198507	-1.263593
H	-3.344253	4.695651	0.619673
H	-4.152582	2.125996	-2.838961
H	-1.784240	1.511170	-2.902441
H	1.937906	5.332910	1.654658
H	4.567423	2.842066	-0.812546
H	2.588566	1.730992	-1.765825
S	-0.594694	4.385499	0.950653
N	4.524081	4.793115	1.064913
N	-5.307303	3.704142	-0.955378
C	-5.799285	4.568741	0.114781
H	-5.389476	5.599060	0.027395
H	-6.900312	4.627337	0.057888
H	-5.523167	4.168035	1.113955
C	4.358331	5.819286	2.090319
H	3.784068	6.690444	1.705166
H	3.826594	5.419979	2.981844
H	5.352407	6.176123	2.412174
C	-6.257533	3.159640	-1.925048
H	-6.010363	3.479233	-2.960162
H	-6.274070	2.048358	-1.897208
H	-7.270165	3.527724	-1.683560
C	5.871198	4.414534	0.641657
H	6.081153	3.344364	0.859156
H	6.019795	4.584117	-0.446693
H	6.608025	5.028699	1.188871

TS-PTa^{+} (water)

Ni	-1.389627	-1.683375	0.769501
Fe	0.592844	0.072295	-0.549952
S	0.102162	-0.358084	1.742989
S	0.389365	-2.259957	-0.406277
P	0.875602	2.273551	-0.426829
P	2.873451	-0.031576	-0.340040
O	0.918356	0.022029	-3.439000
N	-2.793908	-0.974421	2.015473

N	-2.479710	-2.897918	-0.365917
C	0.812993	0.060543	-2.273603
C	2.496871	2.597265	-1.281663
H	2.360698	2.339375	-2.352426
H	2.765876	3.669939	-1.204444
C	3.550412	1.698228	-0.618942
H	3.811930	2.102047	0.379891
H	4.487869	1.649259	-1.207021
C	1.118831	3.093659	1.211164
C	1.837304	2.423375	2.228300
H	2.195377	1.394050	2.080488
C	2.076275	3.049857	3.461916
H	2.633338	2.510451	4.243685
C	1.597213	4.351131	3.697314
H	1.775712	4.838961	4.668487
C	0.887922	5.026654	2.688036
H	0.512558	6.047186	2.863120
C	0.651723	4.406076	1.448801
H	0.098733	4.950267	0.668259
C	-0.434905	3.231369	-1.262726
C	-0.270642	3.769717	-2.556243
H	0.698308	3.706762	-3.074087
C	-1.360489	4.387347	-3.196754
H	-1.230846	4.803470	-4.208186
C	-2.609146	4.468346	-2.554744
H	-3.462315	4.940074	-3.066720
C	-2.773269	3.932102	-1.263920
H	-3.755753	3.941773	-0.767855
C	-1.692878	3.309692	-0.622580
H	-1.830698	2.868297	0.377158
C	3.653500	-0.635294	1.217084
C	3.097465	-1.754233	1.879071
H	2.209637	-2.257989	1.468743
C	3.675914	-2.238199	3.064500
H	3.231020	-3.110806	3.567824
C	4.809066	-1.606732	3.606301
H	5.257403	-1.980982	4.540053
C	5.370870	-0.496672	2.949573
H	6.263333	-0.001494	3.363345
C	4.801579	-0.012826	1.759248
H	5.266182	0.850287	1.259696
C	3.626157	-1.083732	-1.653264
C	3.755870	-2.477866	-1.458693
H	3.506437	-2.934768	-0.489675
C	4.217396	-3.296050	-2.504034
H	4.318821	-4.380312	-2.339279
C	4.552365	-2.734700	-3.749665
H	4.914634	-3.378109	-4.566840
C	4.425642	-1.347817	-3.946461
H	4.687101	-0.899368	-4.917843
C	3.961557	-0.523693	-2.906872
H	3.850345	0.556198	-3.088797
C	-1.090769	0.795313	2.560028
H	-0.946152	0.642620	3.648579
H	-0.820822	1.842642	2.325478
C	-2.504140	0.499231	2.106731
H	-3.240347	0.992253	2.780207
H	-2.664670	0.896532	1.086504
C	-2.541749	-1.726771	3.302922
H	-1.448971	-1.741848	3.477400
H	-2.831435	-2.777160	3.101969
C	-3.250204	-1.195982	4.550405
H	-2.971779	-1.843169	5.407037
H	-2.937098	-0.161905	4.799529
H	-4.355002	-1.216687	4.465399
C	-4.232776	-1.105310	1.613769
H	-4.458604	-0.271569	0.925178
H	-4.859605	-0.943302	2.515387
C	-4.600613	-2.421662	0.944846
H	-5.698278	-2.408760	0.783048
H	-4.402033	-3.292184	1.603877
C	-3.938174	-2.574789	-0.417438
H	-4.449294	-3.357249	-1.017427
H	-4.027611	-1.619897	-0.970486
C	-2.238091	-4.277211	0.200202
H	-2.586441	-4.248043	1.251230
H	-1.143205	-4.425583	0.255234
C	-2.886167	-5.440005	-0.551195
H	-2.578015	-6.384928	-0.059011
H	-3.993537	-5.400843	-0.530366
H	-2.554633	-5.492250	-1.608131
C	-1.948571	-2.721675	-1.764939
H	-2.132957	-1.664059	-2.035452
H	-2.523565	-3.359770	-2.472486
C	-0.464807	-3.012754	-1.862159
H	-0.040414	-2.588358	-2.792741
H	-0.231977	-4.096326	-1.837704
H	-1.012835	0.226833	-0.446952
C	-4.172425	1.468005	-3.191581
H	-4.873188	2.121652	-2.636450
H	-3.704328	2.025253	-4.024886
H	-4.759129	0.625275	-3.617111
C	-3.127036	0.889285	-2.246580
O	-3.477306	0.627943	-1.050977
O	-1.959995	0.648271	-2.704115
H	-0.999425	0.331388	-1.344602
O	-5.166997	2.160539	0.305649
H	-6.011029	2.081249	-0.180626
H	-4.551498	1.594288	-0.257124

TS-PTb^{+} (water)

Ni	2.077231	-0.984250	-1.161331
Fe	-0.368970	0.128298	-0.040124
S	1.067889	0.849771	-1.814686
S	0.042397	-1.814977	-1.291850
P	-0.647426	2.106375	1.003349
P	-2.026084	-0.700124	1.213767
O	1.514282	-0.814055	1.985988
N	3.716211	0.091053	-0.695726
N	2.828578	-2.849927	-0.921666
C	0.835127	-0.401006	1.119812
C	-1.884677	1.858906	2.386916
H	-1.285687	1.617908	3.287287
H	-2.408063	2.813805	2.591583
C	-2.873257	0.738891	2.058020
H	-3.629865	1.078305	1.323179
H	-3.397677	0.374104	2.964091
C	-1.264605	3.529214	0.004694
C	-1.796643	4.669875	0.649433
H	-1.859987	4.714177	1.748284
C	-2.232943	5.768959	-0.108891
H	-2.648279	6.652029	0.401755
C	-2.136926	5.743185	-1.513108
H	-2.481477	6.605781	-2.105117
C	-1.599028	4.614975	-2.156802

H	-1.521974	4.584689	-3.254879
C	-1.164313	3.512727	-1.401301
H	-0.758767	2.627609	-1.912728
C	0.824694	2.817328	1.864197
C	1.474474	3.971010	1.371053
H	1.047387	4.529121	0.523956
C	2.675378	4.412497	1.953444
H	3.175600	5.307533	1.551690
C	3.233819	3.716772	3.039788
H	4.177937	4.060489	3.490685
C	2.575159	2.585474	3.556120
H	2.996924	2.042663	4.416454
C	1.378651	2.136614	2.974440
H	0.889579	1.241493	3.385916
C	-1.540822	-1.855668	2.562464
C	-1.647700	-3.252690	2.380347
H	-2.091771	-3.657121	1.457913
C	-1.188723	-4.133454	3.374297
H	-1.277161	-5.220324	3.219807
C	-0.622536	-3.630095	4.559510
H	-0.263129	-4.321651	5.337708
C	-0.519726	-2.239713	4.748769
H	-0.081249	-1.836991	5.675253
C	-0.971908	-1.355052	3.755518
H	-0.869305	-0.271864	3.916469
C	-3.410644	-1.590700	0.387178
C	-3.417333	-1.865875	-0.994764
H	-2.591691	-1.542904	-1.644797
C	-4.510341	-2.537869	-1.569840
H	-4.508283	-2.748984	-2.650361
C	-5.603238	-2.929915	-0.778579
H	-6.457566	-3.452912	-1.236339
C	-5.603193	-2.649833	0.600791
H	-6.456478	-2.951581	1.228425
C	-4.510791	-1.987690	1.183893
H	-4.512262	-1.785920	2.267012
C	2.344709	2.083484	-1.329574
H	2.886807	2.363447	-2.255374
H	1.845284	2.991417	-0.942590
C	3.240789	1.462592	-0.285086
H	2.676115	1.335777	0.656934
H	4.111796	2.113340	-0.055173
C	4.583254	0.160341	-1.928756
H	3.930637	0.488098	-2.760699
H	4.884130	-0.872271	-2.175048
C	5.821628	1.051718	-1.838979
H	6.371356	0.975525	-2.799192
H	5.567823	2.119816	-1.686263
H	6.514682	0.734294	-1.033983
C	4.427589	-0.474298	0.494784
H	5.327348	0.145941	0.696642
H	3.744819	-0.335254	1.353687
C	4.823614	-1.941227	0.402828
H	5.370787	-2.178160	1.339014
H	5.556557	-2.111304	-0.412124
C	3.656194	-2.923632	0.326028
H	2.965771	-2.749647	1.175251
H	4.047698	-3.962009	0.414588
C	3.650804	-3.237268	-2.124228
H	4.644033	-2.764777	-2.027372
H	3.823741	-4.335574	-2.071030
C	3.025109	-2.840025	-3.456322
H	3.667353	-3.205244	-4.283290
H	2.012867	-3.269469	-3.595690
H	2.940203	-1.737016	-3.544756
C	1.703552	-3.861546	-0.806753
H	2.057569	-4.729721	-0.210039
H	1.477324	-4.234797	-1.823681
C	0.449152	-3.260959	-0.214084
H	0.585100	-2.931828	0.832272
H	-0.395542	-3.976904	-0.252822
H	-1.330919	0.367939	-1.323309
C	-5.087493	0.693424	-2.714244
H	-5.742881	0.451023	-1.856553
H	-5.514768	1.559879	-3.262731
H	-5.052886	-0.161303	-3.419010
C	-3.672021	1.038162	-2.268779
O	-2.744645	1.026412	-3.140183
O	-3.476026	1.322308	-1.033914
H	-1.973972	0.782026	-0.851264
O	-2.435095	-1.378724	-4.309438
H	-3.292562	-1.817721	-4.149758
H	-2.594834	-0.463400	-3.934858

TS-PTc^{+} (water)

Ni	-2.314095	-0.818637	0.448563
Fe	0.168445	-0.012735	-0.070132
S	-0.544793	-2.133917	0.723772
S	-1.490203	-0.727825	-1.618604
P	0.860003	1.850577	-1.056127
P	1.798827	-1.032564	-1.376412
O	-1.519736	1.765442	1.547632
N	-2.815323	-1.181755	2.360739
N	-3.908840	0.230593	-0.161263
C	-1.018130	0.923907	0.885376
C	1.511913	1.383614	-2.735864
H	0.643994	1.053961	-3.344234
H	1.972089	2.269354	-3.219805
C	2.518792	0.248072	-2.533370
H	3.437182	0.629114	-2.039604
H	2.819021	-0.224287	-3.489406
C	2.316636	2.705629	-0.297478
C	3.248763	1.990503	0.485995
H	3.094331	0.928978	0.731336
C	4.403421	2.626706	0.975000
H	5.103931	2.035960	1.584622
C	4.636513	3.983877	0.693803
H	5.537163	4.482719	1.085350
C	3.714752	4.702618	-0.089803
H	3.890915	5.765679	-0.318303
C	2.564076	4.068239	-0.587495
H	1.855501	4.640662	-1.206276
C	-0.348169	3.202975	-1.338054
C	-0.755029	3.990133	-0.234800
H	-0.280132	3.847104	0.747308
C	-1.761910	4.955348	-0.388014
H	-2.074504	5.558206	0.478917
C	-2.370176	5.149596	-1.642780
H	-3.167185	5.900654	-1.759571
C	-1.945701	4.394470	-2.749740
H	-2.401648	4.555897	-3.739024
C	-0.933428	3.429000	-2.603033
H	-0.609067	2.856471	-3.484414
C	3.242853	-1.805268	-0.537049
C	3.067172	-2.428890	0.716697

H	2.089355	-2.388942	1.215594
C	4.137951	-3.094655	1.335651
H	3.987476	-3.568020	2.318028
C	5.395907	-3.138530	0.710918
H	6.238563	-3.651635	1.200032
C	5.580575	-2.511093	-0.535190
H	6.565704	-2.536724	-1.026930
C	4.509903	-1.850827	-1.162924
H	4.669779	-1.381630	-2.145774
C	1.192499	-2.396455	-2.456841
C	1.116360	-3.710653	-1.942315
H	1.509071	-3.939870	-0.939888
C	0.547903	-4.740309	-2.711970
H	0.499421	-5.761448	-2.301981
C	0.049807	-4.470322	-3.999735
H	-0.393588	-5.278819	-4.602098
C	0.122888	-3.163807	-4.515712
H	-0.263596	-2.943725	-5.523375
C	0.683867	-2.128384	-3.748244
H	0.714634	-1.111744	-4.168072
C	-0.518349	-2.192094	2.571963
H	-0.728430	-3.244387	2.850807
H	0.500880	-1.928517	2.921381
C	-1.528340	-1.216941	3.143981
H	-1.104309	-0.196962	3.117789
H	-1.743911	-1.452864	4.208934
C	-3.502273	-2.527507	2.323741
H	-4.379729	-2.417163	1.659211
H	-2.821190	-3.227631	1.804652
C	-3.928030	-3.107878	3.671504
H	-4.377683	-4.105026	3.488531
H	-3.069825	-3.251721	4.358517
H	-4.691482	-2.488674	4.183186
C	-3.680971	-0.133945	2.984938
H	-3.972303	-0.478979	3.999342
H	-3.045155	0.760788	3.121535
C	-4.917488	0.253124	2.181694
H	-5.516727	0.932590	2.822123
H	-5.571709	-0.619638	1.979055
C	-4.585247	1.025469	0.909888
H	-3.903650	1.860519	1.159086
H	-5.504423	1.478144	0.482084
C	-4.826219	-0.820367	-0.744538
H	-5.090114	-1.504227	0.083563
H	-4.227256	-1.425383	-1.451208
C	-6.091961	-0.308997	-1.431760
H	-6.645571	-1.185591	-1.825479
H	-6.770257	0.227312	-0.738588
H	-5.866112	0.354304	-2.290893
C	-3.422747	1.207797	-1.201007
H	-2.761849	1.929496	-0.685374
H	-4.281070	1.785821	-1.607194
C	-2.660731	0.518938	-2.310813
H	-2.096205	1.254233	-2.913843
H	-3.323381	-0.044995	-2.998436
H	1.373579	-0.100474	0.900117
C	2.948125	1.703127	4.249827
H	3.496434	2.406248	3.586977
H	2.268579	2.304998	4.884780
H	3.684127	1.163635	4.875410
C	2.162365	0.744416	3.367064
O	2.645143	-0.399302	3.103137
O	1.051604	1.171981	2.883230
H	0.867685	0.421977	1.505854
O	5.239976	-0.235452	2.322818
H	4.302722	-0.321144	2.663085
H	5.116925	-0.380994	1.363686
CH3COOH_H2O			
C	-0.319885	1.355116	0.036930
H	-0.599668	1.829579	-0.926675
H	-0.857467	1.897896	0.840050
H	0.772983	1.410757	0.182862
C	-0.742471	-0.085975	0.015341
O	0.023186	-1.053247	0.040499
O	-2.082081	-0.240440	-0.048294
H	-2.275010	-1.207441	-0.075560
O	2.668188	-0.109180	0.061894
H	2.683684	0.218833	-0.859398
H	1.775264	-0.541528	0.092303
CH3COO_H2O			
C	0.357596	1.321237	-0.000746
H	0.178993	1.635408	1.051128
H	1.113076	2.003746	-0.437838
H	-0.610790	1.410164	-0.531314
C	0.851520	-0.136903	-0.000916
O	-0.046959	-1.054970	0.078530
O	2.094995	-0.354518	-0.046294
O	-2.524767	-0.108172	-0.117871
H	-2.532483	0.486705	0.657418
H	-1.589641	-0.500739	-0.044340
H2			
H	0.000000	0.000000	0.383859
H	0.000000	0.000000	-0.383859
H2O			
O	0.000000	-0.000000	0.123841
H	0.000000	0.756806	-0.495363
H	-0.000000	-0.756806	-0.495363
MBH (acetonitrile)			
C	-3.752436	-0.053209	0.216629
C	-3.609085	1.364847	0.283251
C	-2.592285	-0.802464	-0.146806
C	-1.372608	-0.165700	-0.430813
C	-1.230451	1.242201	-0.338329
C	-2.373940	1.981666	0.033459
C	1.376779	-0.163751	-0.460634
C	1.233987	1.243548	-0.361215
C	2.601643	-0.799515	-0.196545
C	3.770810	-0.048295	0.131423
C	3.619695	1.366849	0.232155
C	2.379714	1.982532	0.004743
N	-0.000880	1.868700	-0.608097
H	-2.635640	-1.897780	-0.223684
H	-4.462851	2.002397	0.549988
H	-2.291552	3.078424	0.117384
H	2.642746	-1.895245	-0.268237
H	4.472904	2.003461	0.502874
H	2.293324	3.077188	0.109365
S	-0.003153	-1.154565	-1.036215
N	4.993408	-0.672001	0.344651
N	-4.958881	-0.681326	0.492679
C	-5.085910	-2.117046	0.305011
H	-4.368144	-2.682623	0.941553
H	-6.105714	-2.434906	0.591174
H	-4.913323	-2.429959	-0.753146

C	5.063799	-2.123588	0.384861
H	4.719055	-2.578254	-0.570781
H	6.113776	-2.434880	0.539118
H	4.449337	-2.564601	1.207191
C	-6.147397	0.117970	0.741569
H	-6.017173	0.790413	1.619582
H	-6.427078	0.756695	-0.130809
H	-6.999604	-0.552176	0.960259
C	6.121318	0.106810	0.830122
H	6.382378	0.931716	0.130162
H	5.932769	0.563841	1.832015
H	7.008103	-0.548693	0.915685
H	-0.000188	2.883293	-0.468156

MB (acetonitrile)

C	-3.822505	-0.004499	0.000019
C	-3.637542	1.430432	-0.000110
C	-2.654073	-0.834021	0.000169
C	-1.380941	-0.269366	0.000235
C	-1.184583	1.169309	0.000148
C	-2.374549	1.976586	-0.000042
C	1.380939	-0.269357	0.000200
C	1.184545	1.169332	0.000237
C	2.654087	-0.833968	-0.000000
C	3.822512	-0.004439	-0.000106
C	3.637517	1.430503	0.000057
C	2.374508	1.976616	0.000198
N	-0.000019	1.803623	0.000216
H	-2.754145	-1.928069	0.000269
H	-4.507682	2.099165	-0.000245
H	-2.232582	3.068379	-0.000133
H	2.754153	-1.928010	-0.000033
H	4.507551	2.099379	0.000096
H	2.232510	3.068405	0.000285
S	0.000030	-1.358963	0.000662
N	5.068792	-0.545261	-0.000267
N	-5.068795	-0.545285	-0.000062
C	-5.249718	-1.997880	-0.000247
H	-4.792008	-2.458918	0.900928
H	-6.329118	-2.228098	0.000296
H	-4.792963	-2.458600	-0.902088
C	5.249675	-1.997890	-0.000343
H	4.792521	-2.458765	0.901179
H	4.792422	-2.458725	-0.901865
H	6.329083	-2.228100	-0.000531
C	-6.257524	0.311311	-0.000613
H	-6.287709	0.958953	0.901083
H	-6.287433	0.958209	-0.902860
H	-7.157860	-0.326818	-0.000476
C	6.257618	0.311231	-0.000486
H	6.287496	0.958384	-0.902536
H	6.287734	0.958655	0.901380
H	7.157892	-0.326962	-0.000451

MeCN (acetonitrile)

C	-0.274598	0.000083	0.000025
N	-1.446994	-0.000025	-0.000010
C	1.181571	0.000029	0.000006
H	1.562639	1.014033	-0.239298
H	1.562136	-0.714501	-0.758596
H	1.562339	-0.300030	0.997776