

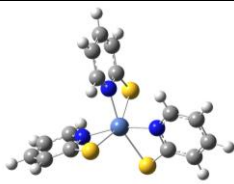

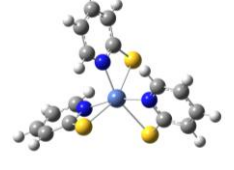
SUPPORTING INFORMATION
For Dalton Transactions

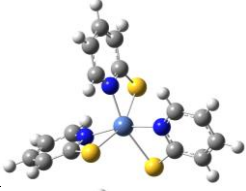
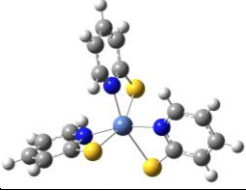
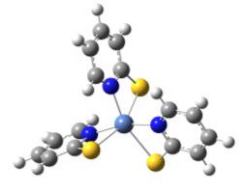
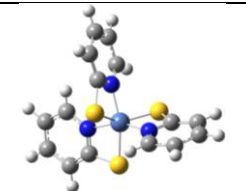
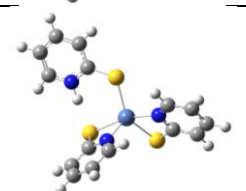
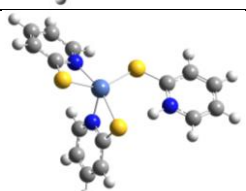
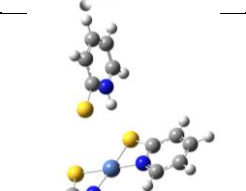
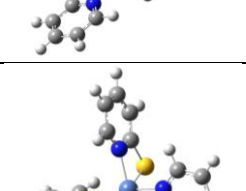
DFT analysis into the intermediates of nickel pyridine thiolate catalyzed proton reduction
Carolyn N. Virca and Theresa M. McCormick

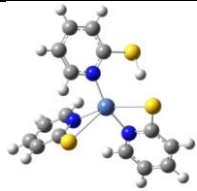
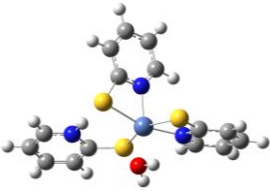
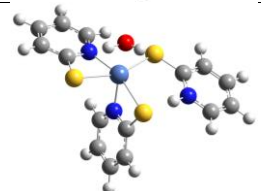
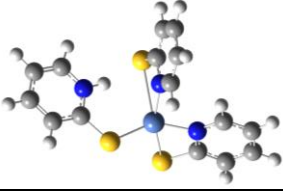
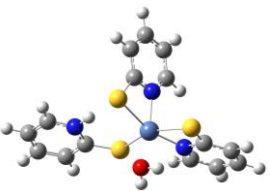
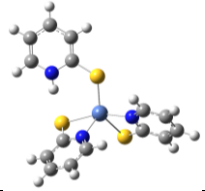
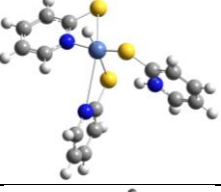
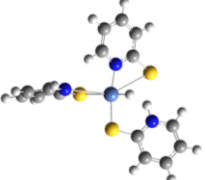
Table S1: Error in bond lengths of calculated vs experimental structures

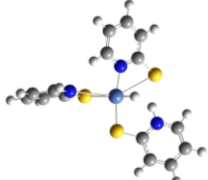
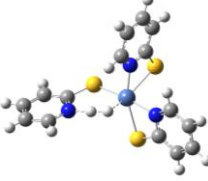
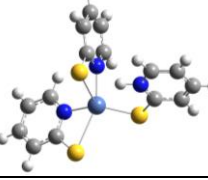

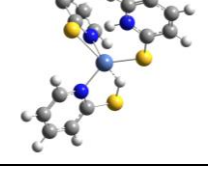
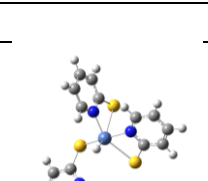
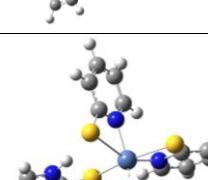
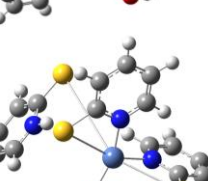
	B3LYP Ethanol CPCM	B3LYP gas	B3LYP Water CPCM	B3P86 Ethanol CPCM	B3P86 gas	B3P86 Water CPCM
Bond	%Error	%Error	%Error	%Error	%Error	%Error
Ni-N1	1.73	1.46	2.76	1.43	1.80	1.40
Ni-N2	2.98	2.95	1.18	0.01	0.15	0.16
Ni-N3	-0.86	-0.50	-0.53	-1.78	-2.07	-1.93
Ni-S1	0.95	2.69	2.45	0.33	0.50	0.32
Ni-S2	3.25	3.07	2.76	1.34	0.88	1.48
Ni-S3	3.52	1.81	3.79	1.07	-0.15	1.08
Energy Hartrees	3445.962706	-3445.882271	-3445.965484	-3449.714625	-3449.632615	-3449.717432

Table S2: Structure, energy, charge and spin state. B3P86 basis set unless indicated

Compound Name	Solvent	Structure	G in Hartrees	Charge	Spin State
1⁻	Gas B3LYP		-3445.882271	-1	3
1⁻	Water B3LYP		-3445.965484	-1	3
1⁻	Ethanol B3LYP		-3445.962706	-1	3

1 ⁻	gas		-3449.632615	-1	3
1 ⁻	water		-3449.717432	-1	3
1 ⁻	ethanol		-3449.714625	-1	3
1 ²⁻	water		-3449.831984	-2	2
2 _N	gas		-3450.134284	0	3
2 _N	water		-3450.157986	0	3
2 _N	water		-3450.146910	0	1
2 _s	water		-3450.143324	0	3

2s-	water		-3450.286344	-1	2
4	water		-3526.752702	0	3
4	gas		-3526.727817	0	3
2N ⁻	water		-3450.300346	-1	2
4 ⁻	water		-3526.849769	-1	2
2N ⁻	water		-3450.274555	-1	4
3	gas		-3450.789136	-1	1
3	water		-3450.789136	-1	1

3	water		-3450.887105	-1	3
TS	water		-3450.886085	-1	3
6	water		-3450.351589	-2	1
6	water		-3450.408214	-2	3
7	water		-3450.738376	0	2
Water	water		-76.604920	0	1
Hydrogen	water		-1.176915	0	1
8	water		-3450.418485	-2	3
5	water		-3526.285591	-1	3
5⁻	water		-3526.409986	-2	2

Optimized Structure Coordinates

1- B3LYP gas:

Ni	0.08937700	-0.30871400	-0.13236700
C	2.98138100	0.55450800	0.86186000
C	3.93661500	-1.76154800	-0.25875500
C	4.34469300	0.29280800	0.95135500
H	2.54531000	1.45839300	1.28235100
C	4.81862200	-0.89888000	0.37170800
H	4.27601200	-2.68640800	-0.71497800
H	5.01014600	0.99100600	1.45049500
H	5.87889200	-1.14389500	0.41676700
C	-0.68502800	2.35289800	1.46742200
C	-0.48278600	3.72977900	-0.90073000
C	-0.92555700	3.72417100	1.47742700
H	-0.76222600	1.74234800	2.36469700
C	-0.81713700	4.41525700	0.25696700
H	-0.39634900	4.23817900	-1.85626300
H	-1.19226500	4.23105600	2.40023900
H	-0.99821200	5.48864700	0.21886400
C	-2.77947300	-0.88894200	-1.31271200
C	-4.07137600	-1.38128900	-1.15240300
H	-2.42919500	-0.46836300	-2.25260100
C	-3.49638500	-1.89985600	1.13948600
C	-4.42358700	-1.89539700	0.10827000
H	-4.77484200	-1.36397200	-1.97965700
H	-3.74151100	-2.29202700	2.12181900
H	-5.42426900	-2.29103300	0.27687700
N	2.12286500	-0.27406700	0.25672200
N	-0.35355200	1.68692200	0.35396200
N	-1.88093200	-0.89281400	-0.32077100
C	-2.19533500	-1.38450000	0.91124100
C	-0.24913200	2.33094500	-0.84402000
C	2.55651700	-1.43534100	-0.31517300
S	1.30495600	-2.36939100	-1.05299000
S	-0.90157700	-1.31214100	2.06297300
S	0.17256500	1.30478800	-2.17394500

1- B3LYP water

Ni	0.06598	-0.30522	-0.13197
C	2.9456	0.4957	0.88962
C	3.91666	-1.80139	-0.26253
C	4.30627	0.23021	0.98881
H	2.50595	1.39016	1.32331
C	4.79231	-0.9465	0.39563
H	4.26905	-2.71611	-0.72852

H	4.96356	0.91825	1.51015
H	5.85056	-1.18984	0.44968
C	-0.60164	2.37623	1.47025
C	-0.37498	3.73717	-0.90608
C	-0.79348	3.75354	1.47493
H	-0.68371	1.78058	2.37567
C	-0.67586	4.43901	0.25516
H	-0.27998	4.24501	-1.86071
H	-1.02743	4.27222	2.39886
H	-0.81956	5.51602	0.2164
C	-2.83925	-0.81095	-1.29443
C	-4.14022	-1.26832	-1.11735
H	-2.50027	-0.38608	-2.23557
C	-3.54191	-1.84447	1.15336
C	-4.48908	-1.79331	0.13747
H	-4.85662	-1.21492	-1.93054
H	-3.78839	-2.24515	2.13155
H	-5.49708	-2.15925	0.31666
N	2.09459	-0.3271	0.25396
N	-0.30857	1.69362	0.35104
N	-1.91992	-0.85948	-0.3162
C	-2.23748	-1.36612	0.90447
C	-0.19058	2.33911	-0.83864
C	2.54517	-1.47153	-0.32521
S	1.29194	-2.41091	-1.10384
S	-0.90884	-1.34822	2.04492
S	0.19344	1.2826	-2.18146

1⁻ B3LYP ethanol

Ni	0.06679	-0.30496	-0.13193
C	2.94851	0.49634	0.88763
C	3.91516	-1.80343	-0.26274
C	4.30895	0.22913	0.98587
H	2.51046	1.39196	1.32064
C	4.79257	-0.94915	0.3935
H	4.26551	-2.71926	-0.72812
H	4.96779	0.91687	1.50572
H	5.85057	-1.194	0.44677
C	-0.6034	2.37632	1.47007
C	-0.37733	3.73788	-0.90589
C	-0.79653	3.75351	1.47506
H	-0.68546	1.78005	2.37513
C	-0.6791	4.4392	0.25526
H	-0.28253	4.24573	-1.86054
H	-1.03141	4.2718	2.39901
H	-0.82379	5.51614	0.21657

C	-2.83641	-0.81446	-1.29547
C	-4.1368	-1.27404	-1.11949
H	-2.49668	-0.39036	-2.23672
C	-3.54025	-1.84597	1.15281
C	-4.48612	-1.79803	0.13571
H	-4.85223	-1.22325	-1.93373
H	-3.78689	-2.24602	2.13124
H	-5.49364	-2.16585	0.31413
N	2.09577	-0.32582	0.25394
N	-0.30929	1.69424	0.35101
N	-1.91847	-0.85983	-0.31606
C	-2.23615	-1.36537	0.90517
C	-0.19161	2.33963	-0.83898
C	2.54377	-1.47181	-0.32464
S	1.28865	-2.40927	-1.10044
S	-0.90938	-1.34396	2.04671
S	0.19327	1.28425	-2.18137

1⁻ B3P86 gas

Ni	0.09121	-0.31139	-0.12901
C	2.95371	0.58215	0.8469
C	3.90535	-1.7357	-0.25735
C	4.31517	0.32541	0.92954
H	2.51575	1.48778	1.26171
C	4.78648	-0.86694	0.35887
H	4.24297	-2.66369	-0.70808
H	4.98215	1.02913	1.41786
H	5.84726	-1.10899	0.39923
C	-0.69621	2.32111	1.45827
C	-0.48947	3.67496	-0.91567
C	-0.9418	3.68833	1.45526
H	-0.77393	1.71479	2.35886
C	-0.83089	4.36664	0.23247
H	-0.40055	4.17431	-1.87554
H	-1.21459	4.20244	2.37178
H	-1.01608	5.43856	0.18418
C	-2.75838	-0.8734	-1.30667
C	-4.04854	-1.3574	-1.13413
H	-2.41092	-0.45602	-2.24938
C	-3.45709	-1.87251	1.14871
C	-4.39058	-1.86529	0.1274
H	-4.75943	-1.33838	-1.95443
H	-3.69441	-2.26081	2.1343
H	-5.3914	-2.25525	0.30578
N	2.0977	-0.25172	0.25671
N	-0.35852	1.65093	0.35539

N	-1.85576	-0.88057	-0.32554
C	-2.16031	-1.36517	0.9064
C	-0.25163	2.28209	-0.84383
C	2.52882	-1.41247	-0.30696
S	1.2748	-2.34119	-1.02354
S	-0.85624	-1.29009	2.03096
S	0.17816	1.24212	-2.14712

1⁻ B3P86 water

Ni	0.07036	-0.30713	-0.12697
C	2.93039	0.52492	0.86661
C	3.8824	-1.78499	-0.2617
C	4.28899	0.25999	0.95205
H	2.49538	1.42577	1.2922
C	4.76434	-0.92289	0.37152
H	4.22735	-2.70665	-0.71931
H	4.9539	0.95435	1.45438
H	5.82278	-1.16638	0.41543
C	-0.61535	2.34939	1.45932
C	-0.38971	3.68584	-0.92402
C	-0.81731	3.72209	1.44984
H	-0.69637	1.75945	2.36896
C	-0.70035	4.39406	0.22687
H	-0.29471	4.18433	-1.88346
H	-1.05911	4.24821	2.36715
H	-0.85262	5.4692	0.17701
C	-2.80897	-0.81149	-1.29459
C	-4.10556	-1.26882	-1.10958
H	-2.47097	-0.3951	-2.24031
C	-3.50046	-1.82006	1.16004
C	-4.44781	-1.78105	0.14816
H	-4.82468	-1.2254	-1.92054
H	-3.74219	-2.21187	2.14291
H	-5.45403	-2.148	0.33371
N	2.07496	-0.30395	0.25623
N	-0.31384	1.66191	0.3515
N	-1.89114	-0.84891	-0.32165
C	-2.20233	-1.34158	0.90136
C	-0.19566	2.29403	-0.84032
C	2.51497	-1.45333	-0.31078
S	1.25021	-2.38535	-1.05427
S	-0.87165	-1.30383	2.02168
S	0.19955	1.22492	-2.15518

1⁻ B3P86 ethanol

Ni	0.07114	-0.30714	-0.12686
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C	2.93274	0.52608	0.86484
C	3.8816	-1.78589	-0.26165
C	4.2912	0.26013	0.94942
H	2.49881	1.42779	1.28981
C	4.76479	-0.92403	0.36975
H	4.22497	-2.70846	-0.71863
H	4.95725	0.95451	1.45026
H	5.82308	-1.16855	0.413
C	-0.61728	2.34969	1.45918
C	-0.3919	3.68582	-0.92427
C	-0.82023	3.7223	1.4495
H	-0.69835	1.75956	2.36875
C	-0.70326	4.39402	0.22627
H	-0.29689	4.18395	-1.8839
H	-1.06286	4.24841	2.36664
H	-0.8562	5.4691	0.17606
C	-2.80647	-0.81437	-1.29552
C	-4.10276	-1.27304	-1.1114
H	-2.46764	-0.39877	-2.24132
C	-3.49929	-1.82099	1.15948
C	-4.44555	-1.78429	0.14666
H	-4.82105	-1.2315	-1.92323
H	-3.74125	-2.21215	2.14257
H	-5.45151	-2.1524	0.33162
N	2.07604	-0.30256	0.2564
N	-0.31493	1.66227	0.35179
N	-1.88983	-0.84955	-0.32166
C	-2.20118	-1.34122	0.90182
C	-0.19697	2.29382	-0.84056
C	2.51411	-1.45315	-0.31009
S	1.24836	-2.38383	-1.05137
S	-0.87223	-1.30097	2.02304
S	0.19908	1.22531	-2.15454

1²⁻B3P86 water

Ni	-0.00952	-0.35268	-0.0407
C	-2.90321	-0.1009	-0.78875
C	-4.18968	-0.56431	-1.03136
H	-2.62535	0.92799	-0.99778
C	-3.47055	-2.70759	-0.19652
C	-4.47382	-1.90392	-0.72259
H	-4.94283	0.10005	-1.4431
H	-3.66356	-3.74628	0.05238
H	-5.46784	-2.31127	-0.89144
C	0.25932	2.21995	-1.4411
C	-0.81794	3.956	0.34679

C	0.1626	3.55356	-1.81012
H	0.68696	1.49196	-2.12537
C	-0.39837	4.44329	-0.87985
H	-1.251	4.62204	1.08599
H	0.51166	3.88144	-2.78416
H	-0.50144	5.50048	-1.11361
C	2.30473	-0.89656	-1.67909
C	3.59287	-1.16865	-2.1136
H	1.4773	-0.87862	-2.3839
C	4.29207	-0.93414	0.17449
C	4.61376	-1.18315	-1.14925
H	3.78897	-1.36137	-3.16343
H	5.06043	-0.94266	0.94066
H	5.64315	-1.38906	-1.4333
N	1.97099	-0.64524	-0.39001
N	-0.15099	1.72317	-0.25149
N	-1.91825	-0.87217	-0.28214
S	-1.20929	1.9813	2.23383
S	-0.83936	-3.11308	0.6571
S	2.54215	-0.37578	2.23829
C	2.95102	-0.66633	0.56505
C	-2.17514	-2.18007	0.01973
C	-0.69072	2.57636	0.67192

2_N B3P86

Ni	-0.50033	-0.09989	-0.56222
C	-0.88623	1.98617	1.70151
C	0.78942	3.63051	0.27901
C	-0.6278	3.25576	2.19434
H	-1.54968	1.29267	2.21062
C	0.22611	4.08682	1.46059
H	1.44724	4.2543	-0.31686
H	-1.08698	3.58775	3.11934
H	0.44515	5.09162	1.81292
C	-2.54166	-1.73288	1.34009
C	-4.41147	-1.0918	-0.5666
C	-3.84849	-2.15932	1.52527
H	-1.75467	-1.96415	2.05436
C	-4.79204	-1.82531	0.54494
H	-5.12147	-0.82079	-1.34081
H	-4.11915	-2.7377	2.40219
H	-5.82601	-2.14351	0.6545
C	4.40115	-0.18005	-0.4781

C	5.33294	-1.06735	-0.00403
H	4.64655	0.74969	-0.98058
C	3.50992	-2.47184	0.74808
C	4.86063	-2.23929	0.62236
H	6.39154	-0.865	-0.11518
H	3.13238	-3.3696	1.22442
H	5.56869	-2.96763	1.00826
N	-0.33999	1.54339	0.56459
N	-2.16953	-1.02247	0.27076
N	3.08205	-0.42745	-0.33975
C	2.56416	-1.53755	0.25281
C	-3.06794	-0.69333	-0.69081
C	0.49049	2.33006	-0.15688
S	1.05877	1.5646	-1.61581
S	0.88052	-1.78114	0.38552
S	-2.34983	0.21772	-1.9795
H	2.40133	0.27247	-0.73891

2_N B3P86 water

Ni	-0.50276	0.10399	0.57869
C	-0.90759	-1.95936	-1.70899
C	0.76926	-3.62803	-0.31
C	-0.63616	-3.21619	-2.22792
H	-1.56469	-1.25728	-2.21384
C	0.2176	-4.05943	-1.5085
H	1.43436	-4.26159	0.2672
H	-1.08122	-3.52673	-3.16679
H	0.45056	-5.0514	-1.88557
C	-2.49539	1.75198	-1.3237
C	-4.42742	1.12084	0.52516
C	-3.79329	2.1897	-1.54461
H	-1.68993	1.97189	-2.01929
C	-4.76933	1.86372	-0.59642
H	-5.16665	0.85374	1.27308
H	-4.03256	2.76808	-2.43018
H	-5.79625	2.19036	-0.73635
C	4.44844	0.17084	0.49436
C	5.36974	1.06566	0.0099
H	4.70771	-0.75329	0.99779
C	3.53302	2.44928	-0.74382
C	4.89007	2.22743	-0.62027
H	6.42957	0.86999	0.11742
H	3.15311	3.34138	-1.22847
H	5.59042	2.9578	-1.01411
N	-0.37548	-1.54268	-0.55286
N	-2.16106	1.03741	-0.2421

N	3.12617	0.41144	0.35949
C	2.60578	1.51251	-0.23969
C	-3.09431	0.71267	0.68291
C	0.45413	-2.34299	0.15304
S	1.02068	-1.5934	1.62833
S	0.90418	1.74326	-0.37688
S	-2.42035	-0.2264	1.99103
H	2.45604	-0.28514	0.75578

2s B3P86 water

Ni	0.14077	-0.18099	-0.22973
C	3.02937	0.53222	0.79031
C	3.83297	-1.85773	-0.30404
C	4.36811	0.18031	0.87476
H	2.65176	1.46375	1.20258
C	4.7675	-1.03773	0.31351
H	4.11792	-2.80693	-0.74531
H	5.07727	0.83885	1.36405
H	5.80887	-1.34437	0.36007
C	-0.51638	2.28227	1.68887
C	-0.26629	3.82492	-0.57203
C	-0.6818	3.6548	1.80024
H	-0.60356	1.62273	2.54792
C	-0.55183	4.43128	0.64274
H	-0.16128	4.40543	-1.48266
H	-0.90513	4.10297	2.76218
H	-0.67464	5.50977	0.69296
C	-2.72327	-0.14765	-1.0895
C	-4.08678	-0.3973	-1.05873
H	-2.28488	0.56201	-1.78537
C	-3.67686	-1.96102	0.71171
C	-4.57285	-1.31602	-0.13064
H	-4.74672	0.12105	-1.74561
H	-4.01146	-2.7053	1.42616
H	-5.63364	-1.54049	-0.07283
N	2.12669	-0.25536	0.19273
N	-0.24057	1.69331	0.5185
N	-1.85055	-0.74523	-0.2591
C	-2.31778	-1.65311	0.61742
C	-0.11352	2.4299	-0.61004
C	2.49623	-1.43689	-0.35197
S	1.15365	-2.28543	-1.08128
S	-1.17673	-2.44997	1.71664
S	0.23707	1.44668	-2.00885
H	-0.17	-2.56071	0.78357

2s B3P86 water

Ni	0.14077	-0.18099	-0.22973
C	3.02937	0.53222	0.79031
C	3.83297	-1.85773	-0.30404
C	4.36811	0.18031	0.87476
H	2.65176	1.46375	1.20258
C	4.7675	-1.03773	0.31351
H	4.11792	-2.80693	-0.74531
H	5.07727	0.83885	1.36405
H	5.80887	-1.34437	0.36007
C	-0.51638	2.28227	1.68887
C	-0.26629	3.82492	-0.57203
C	-0.6818	3.6548	1.80024
H	-0.60356	1.62273	2.54792
C	-0.55183	4.43128	0.64274
H	-0.16128	4.40543	-1.48266
H	-0.90513	4.10297	2.76218
H	-0.67464	5.50977	0.69296
C	-2.72327	-0.14765	-1.0895
C	-4.08678	-0.3973	-1.05873
H	-2.28488	0.56201	-1.78537
C	-3.67686	-1.96102	0.71171
C	-4.57285	-1.31602	-0.13064
H	-4.74672	0.12105	-1.74561
H	-4.01146	-2.7053	1.42616
H	-5.63364	-1.54049	-0.07283
N	2.12669	-0.25536	0.19273
N	-0.24057	1.69331	0.5185
N	-1.85055	-0.74523	-0.2591
C	-2.31778	-1.65311	0.61742
C	-0.11352	2.4299	-0.61004
C	2.49623	-1.43689	-0.35197
S	1.15365	-2.28543	-1.08128
S	-1.17673	-2.44997	1.71664
S	0.23707	1.44668	-2.00885
H	-0.17	-2.56071	0.78357

4 B3P86 water

Ni	0.48818	-0.13499	0.59814
C	0.88626	1.96231	-1.71201
C	-0.77201	3.62811	-0.29311
C	0.61508	3.22265	-2.22455
H	1.53664	1.26047	-2.22685
C	-0.23024	4.06484	-1.49443
H	-1.43065	4.26068	0.29277
H	1.05326	3.53629	-3.16579

H	-0.46421	5.05928	-1.86459
C	2.3592	-1.84296	-1.33002
C	4.48483	-0.87967	0.10942
C	3.63879	-2.22008	-1.70721
H	1.48179	-2.19398	-1.86664
C	4.71724	-1.72274	-0.96644
H	5.30258	-0.47942	0.69975
H	3.78707	-2.88065	-2.55445
H	5.73521	-1.99511	-1.23201
C	-4.48927	-0.10233	0.56452
C	-5.44942	-0.90952	0.00866
H	-4.70549	0.74046	1.21097
C	-3.67873	-2.17843	-1.04681
C	-5.02217	-1.9679	-0.81448
H	-6.49869	-0.72608	0.20486
H	-3.34025	-2.9925	-1.67758
H	-5.7545	-2.62699	-1.2712
N	0.36563	1.53982	-0.55397
N	2.12793	-1.02862	-0.2907
N	-3.17972	-0.32871	0.31982
C	-2.707	-1.33405	-0.46335
C	3.16076	-0.5398	0.43659
C	-0.45455	2.34011	0.16145
S	-1.00955	1.58915	1.64121
S	-1.02296	-1.54261	-0.72428
S	2.65705	0.50019	1.74183
H	-2.47989	0.31045	0.75887
O	0.3679	-1.58821	2.16561
H	0.38544	-2.48561	1.79486
H	1.23747	-1.45024	2.58871

4 B3P86

Ni	0.55643	-0.14112	0.6769
C	0.39909	1.68475	-1.86528
C	-1.10587	3.41254	-0.35736
C	0.00749	2.88867	-2.43095
H	1.0055	0.96317	-2.40609
C	-0.75565	3.76472	-1.65206
H	-1.68918	4.07391	0.27469
H	0.29933	3.13817	-3.44557
H	-1.07099	4.72284	-2.05762
C	2.4008	-1.90435	-1.21115
C	4.51304	-0.43101	-0.26768
C	3.66913	-2.17988	-1.69781
H	1.52463	-2.45373	-1.5467
C	4.73962	-1.41969	-1.20989

H	5.32133	0.17346	0.13022
H	3.81604	-2.96381	-2.43317
H	5.7491	-1.60536	-1.56888
C	-4.35878	-0.0403	0.34336
C	-5.29539	-0.82826	-0.27269
H	-4.58603	0.89339	0.84711
C	-3.5163	-2.36368	-0.8578
C	-4.84716	-2.01919	-0.88433
H	-6.33904	-0.53746	-0.28242
H	-3.15845	-3.27465	-1.32414
H	-5.56014	-2.67075	-1.38239
N	0.06185	1.34263	-0.61843
N	2.17597	-0.94869	-0.30166
N	-3.05705	-0.39826	0.35772
C	-2.55987	-1.5316	-0.21503
C	3.20023	-0.20779	0.18877
C	-0.68303	2.17206	0.14484
S	-1.01619	1.53689	1.73675
S	-0.90781	-1.92001	-0.1321
S	2.70614	0.97515	1.35948
H	-2.37781	0.23135	0.8569
O	0.97673	-1.29685	2.45047
H	0.29701	-1.06114	3.09984
H	1.75108	-0.72738	2.66213

2N⁻ B3P86 water doublet

Ni	-0.52611	-0.53489	-0.22818
C	-3.25975	0.81998	-0.59163
C	-4.49428	-1.41973	0.37287
C	-4.64501	0.81263	-0.51697
H	-2.71773	1.6862	-0.9631
C	-5.26868	-0.33883	-0.02293
H	-4.95236	-2.32304	0.76317
H	-5.21597	1.67899	-0.83422
H	-6.35192	-0.3882	0.0534
C	0.01834	2.13636	-1.51611
C	0.67046	3.38178	0.81641
C	0.28677	3.49574	-1.55356
H	-0.24576	1.59005	-2.41883
C	0.61575	4.12842	-0.34973
H	0.93273	3.84292	1.76318
H	0.23721	4.03956	-2.4911
H	0.83181	5.19343	-0.3264
C	3.98648	-0.15432	1.13068
C	5.17949	-0.57459	0.60196
H	3.89804	0.46186	2.0185

C	3.93238	-1.71206	-1.13362
C	5.13806	-1.37353	-0.55958
H	6.11527	-0.29484	1.07028
H	3.8906	-2.32447	-2.02753
H	6.06335	-1.72496	-1.00693
N	-2.50115	-0.22168	-0.21667
N	0.05769	1.40429	-0.38972
N	2.81548	-0.50044	0.54979
C	2.70954	-1.26907	-0.57106
C	0.39038	1.99978	0.78347
C	-3.0919	-1.34535	0.27226
S	-1.97583	-2.59784	0.72672
S	1.17533	-1.66679	-1.22264
S	0.46887	0.97733	2.19601
H	1.93953	-0.16242	1.0086

4- B3P86 water

Ni	0.48561	-0.13627	0.59705
C	0.89716	1.96326	-1.70856
C	-0.76007	3.63194	-0.29192
C	0.63099	3.22504	-2.22016
H	1.54705	1.26029	-2.22249
C	-0.21377	4.06873	-1.49113
H	-1.41824	4.26567	0.29322
H	1.07266	3.53869	-3.15977
H	-0.44364	5.06445	-1.86046
C	2.35769	-1.84262	-1.33196
C	4.4818	-0.88816	0.11549
C	3.63747	-2.22002	-1.70821
H	1.48083	-2.19029	-1.87169
C	4.71516	-1.72719	-0.9633
H	5.29894	-0.49133	0.70894
H	3.78644	-2.8773	-2.55791
H	5.73329	-1.99984	-1.22804
C	-4.4899	-0.09956	0.56636
C	-5.45112	-0.90628	0.01159
H	-4.70489	0.74195	1.21487
C	-3.68249	-2.17234	-1.05077
C	-5.02546	-1.9629	-0.81461
H	-6.49995	-0.72378	0.21096
H	-3.34527	-2.9851	-1.68388
H	-5.75863	-2.62154	-1.27065
N	0.37223	1.54072	-0.55254
N	2.12548	-1.03214	-0.28984
N	-3.18091	-0.32484	0.3179
C	-2.7097	-1.3287	-0.46808

C	3.15756	-0.54759	0.44145
C	-0.4477	2.34234	0.16161
S	-1.009	1.59085	1.63872
S	-1.02616	-1.53584	-0.73336
S	2.65298	0.4886	1.74935
H	-2.48021	0.31409	0.75605
O	0.35585	-1.59214	2.16077
H	0.37555	-2.48906	1.78903
H	1.22369	-1.45378	2.58753

2_N B3P86 water quartet

Ni	-0.40281	0.12983	0.49192
C	-1.32134	-2.01648	-1.55623
C	0.2295	-3.81823	-0.18083
C	-1.29109	-3.33249	-1.99095
H	-1.91979	-1.25944	-2.05532
C	-0.49868	-4.24367	-1.28205
H	0.85031	-4.50494	0.38516
H	-1.87098	-3.63661	-2.85547
H	-0.45313	-5.28415	-1.59214
C	-2.361	1.86638	-1.36203
C	-4.22221	1.54575	0.63124
C	-3.61553	2.43509	-1.52923
H	-1.5821	1.96134	-2.11408
C	-4.55673	2.26528	-0.5071
H	-4.93469	1.40002	1.43661
H	-3.8491	2.9927	-2.42967
H	-5.55008	2.69559	-0.60295
C	4.58624	-0.16081	0.12526
C	5.51407	0.83057	-0.0479
H	4.83448	-1.18353	0.38482
C	3.70375	2.39794	-0.48083
C	5.10472	2.144	-0.38075
H	6.56578	0.58959	0.08259
H	3.34214	3.39958	-0.69623
H	5.82457	2.94488	-0.51155
N	-0.61816	-1.60367	-0.49395
N	-2.03394	1.17254	-0.26486
N	3.22718	0.09236	-0.0863
C	2.77854	1.39641	-0.31234
C	-2.93188	1.00024	0.73318
C	0.15642	-2.46858	0.20208
S	0.97758	-1.71709	1.54256
S	1.04332	1.65799	-0.47186
S	-2.28361	0.06761	2.05622
H	2.55017	-0.56347	0.31042

3 B3P86 singlet

C	1.64865	2.15366	-0.701
C	-0.03023	4.15449	0.05887
C	2.08897	3.45915	-0.82683
H	2.26967	1.30152	-0.96787
C	1.21725	4.48237	-0.43152
H	-0.73002	4.91895	0.37992
H	3.08399	3.6635	-1.20972
H	1.51781	5.52625	-0.50465
C	3.91306	-1.49044	-1.40952
C	3.85823	-1.84724	1.27621
C	4.98306	-2.15766	-0.82413
H	3.8958	-1.32539	-2.48828
C	4.94026	-2.3293	0.56664
H	3.78913	-1.97254	2.35284
H	5.81042	-2.52496	-1.42515
H	5.74818	-2.84256	1.08613
C	-4.46882	-0.14728	-0.04536
C	-5.41322	-1.13352	-0.17164
H	-4.69437	0.90647	0.08784
C	-3.60647	-2.73752	-0.33889
C	-4.95185	-2.46422	-0.31639
H	-6.46968	-0.89186	-0.14985
H	-3.2364	-3.75114	-0.4523
H	-5.66752	-3.27746	-0.41268
N	0.42964	1.83005	-0.23345
N	2.85979	-1.00877	-0.74501
N	-3.15307	-0.43434	-0.07412
C	-2.64362	-1.69373	-0.22912
C	2.80267	-1.18154	0.59651
C	-0.44253	2.80107	0.16164
S	-1.99502	2.39793	0.79813
S	-0.97089	-1.97102	-0.26358
S	1.44385	-0.58272	1.4958
H	-2.48548	0.37143	0.07078
Ni	-0.06632	0.00491	-0.15713
H	-0.94845	0.33484	-1.27749

3 B3P86 water singlet

C	1.64865	2.15366	-0.701
C	-0.03023	4.15449	0.05887
C	2.08897	3.45915	-0.82683
H	2.26967	1.30152	-0.96787
C	1.21725	4.48237	-0.43152
H	-0.73002	4.91895	0.37992

H	3.08399	3.6635	-1.20972
H	1.51781	5.52625	-0.50465
C	3.91306	-1.49044	-1.40952
C	3.85823	-1.84724	1.27621
C	4.98306	-2.15766	-0.82413
H	3.8958	-1.32539	-2.48828
C	4.94026	-2.3293	0.56664
H	3.78913	-1.97254	2.35284
H	5.81042	-2.52496	-1.42515
H	5.74818	-2.84256	1.08613
C	-4.46882	-0.14728	-0.04536
C	-5.41322	-1.13352	-0.17164
H	-4.69437	0.90647	0.08784
C	-3.60647	-2.73752	-0.33889
C	-4.95185	-2.46422	-0.31639
H	-6.46968	-0.89186	-0.14985
H	-3.2364	-3.75114	-0.4523
H	-5.66752	-3.27746	-0.41268
N	0.42964	1.83005	-0.23345
N	2.85979	-1.00877	-0.74501
N	-3.15307	-0.43434	-0.07412
C	-2.64362	-1.69373	-0.22912
C	2.80267	-1.18154	0.59651
C	-0.44253	2.80107	0.16164
S	-1.99502	2.39793	0.79813
S	-0.97089	-1.97102	-0.26358
S	1.44385	-0.58272	1.4958
H	-2.48548	0.37143	0.07078
Ni	-0.06632	0.00491	-0.15713
H	-0.94845	0.33484	-1.27749

3 B3P86 water triplet

-1 3

C	3.03190100	0.80216600	-1.08984800
C	2.85934400	3.31781200	-0.02177400
C	4.08060400	1.68390700	-1.30766200
H	3.04427200	-0.20968400	-1.48807000
C	3.98139800	2.96807700	-0.75716000
H	2.75896400	4.30670900	0.41437400
H	4.94518000	1.37821700	-1.88729300
H	4.78013800	3.69042000	-0.90513400
C	0.64696900	-2.36027500	-1.58362500
C	1.90446300	-3.56840300	0.52332300
C	1.13604200	-3.64538600	-1.75994700
H	0.13727000	-1.82691300	-2.38264100
C	1.77802800	-4.25414300	-0.67344600

H	2.39774400	-4.01903500	1.37876100
H	1.01988400	-4.15315700	-2.71150100
H	2.17645800	-5.26131200	-0.76660700
C	-3.96535100	1.07339900	-1.67845500
C	-5.28528600	0.94448000	-1.32112300
H	-3.63225400	1.53373500	-2.60233500
C	-4.55906600	-0.13903500	0.72030700
C	-5.57501000	0.32137500	-0.09155600
H	-6.06845700	1.31333400	-1.97235800
H	-4.77265400	-0.61923000	1.66891700
H	-6.60809600	0.20177200	0.22196200
N	1.94694000	1.13458800	-0.38116900
N	0.76573200	-1.69262000	-0.42858700
N	-2.99119100	0.61694600	-0.86617900
C	-3.20727400	0.00863600	0.32980100
C	1.38334400	-2.26156700	0.63554900
C	1.83295300	2.37043400	0.16025100
S	0.35449200	2.61393600	1.04191800
S	-1.86659500	-0.52677600	1.26309300
S	1.45536800	-1.27368800	2.06119300
H	-1.96511800	0.69170600	-1.14483900
Ni	0.17583400	0.19139300	0.10188300
H	-0.53765600	0.61762000	-1.31147200

TS B3P86 water

Ni	0.19286	0.18448	0.25059
S	-1.87364	-0.40664	1.36582
N	1.94214	1.06072	-0.41411
S	1.45572	-1.26444	2.01079
N	0.62719	-1.70186	-0.41642
S	0.50747	2.57956	1.12046
C	-3.15746	0.13749	0.32429
C	2.96122	0.68932	-1.19699
C	1.9149	2.29563	0.13987
C	1.27828	-2.28744	0.61734
C	0.41741	-2.37177	-1.5563
C	-4.52325	0.01631	0.66716
N	-2.84473	0.69653	-0.86219
C	4.02748	1.5305	-1.48007
C	2.96455	3.20198	-0.10357
C	1.73851	-3.61379	0.49759
C	0.8431	-3.67855	-1.74113
C	-5.49463	0.46604	-0.20857
C	-3.77787	1.13335	-1.71849
C	4.0188	2.81228	-0.91541
C	1.51701	-4.30354	-0.68384

C	-5.12732	1.04098	-1.43558
H	2.90571	-0.319	-1.60005
H	-0.11118	-1.8274	-2.33518
H	-4.79056	-0.43033	1.6195
H	-1.53032	0.72748	-1.08798
H	4.83753	1.19559	-2.11913
H	2.93572	4.18973	0.34543
H	0.65514	-4.19072	-2.67866
H	-6.5444	0.37303	0.05646
H	-3.4053	1.56365	-2.64516
H	4.83563	3.50202	-1.11193
H	1.86661	-5.32756	-0.78749
H	-5.86704	1.40251	-2.14116
H	2.25881	-4.07657	1.33015
H	-0.55563	0.71595	-1.20353

6 B3P86 water singlet

Ni	-0.52611	-0.53489	-0.22818
C	-3.25975	0.81998	-0.59163
C	-4.49428	-1.41973	0.37287
C	-4.64501	0.81263	-0.51697
H	-2.71773	1.6862	-0.9631
C	-5.26868	-0.33883	-0.02293
H	-4.95236	-2.32304	0.76317
H	-5.21597	1.67899	-0.83422
H	-6.35192	-0.3882	0.0534
C	0.01834	2.13636	-1.51611
C	0.67046	3.38178	0.81641
C	0.28677	3.49574	-1.55356
H	-0.24576	1.59005	-2.41883
C	0.61575	4.12842	-0.34973
H	0.93273	3.84292	1.76318
H	0.23721	4.03956	-2.4911
H	0.83181	5.19343	-0.3264
C	3.98648	-0.15432	1.13068
C	5.17949	-0.57459	0.60196
H	3.89804	0.46186	2.0185
C	3.93238	-1.71206	-1.13362
C	5.13806	-1.37353	-0.55958
H	6.11527	-0.29484	1.07028
H	3.8906	-2.32447	-2.02753
H	6.06335	-1.72496	-1.00693
N	-2.50115	-0.22168	-0.21667
N	0.05769	1.40429	-0.38972
N	2.81548	-0.50044	0.54979
C	2.70954	-1.26907	-0.57106

C	0.39038	1.99978	0.78347
C	-3.0919	-1.34535	0.27226
S	-1.97583	-2.59784	0.72672
S	1.17533	-1.66679	-1.22264
S	0.46887	0.97733	2.19601
H	1.93953	-0.16242	1.0086

6 B3P86 water triplet

-2 3

Ni	-0.64466300	-0.66252700	-0.07288300
C	-2.93904000	1.28364800	-0.39843800
C	-4.77254000	-0.70413300	-0.02880900
C	-4.28469400	1.61306200	-0.45305500
H	-2.16649500	2.03534100	-0.53661900
C	-5.21861600	0.58775900	-0.26362400
H	-5.47437500	-1.51801100	0.12346200
H	-4.59079600	2.63766100	-0.63709300
H	-6.28445300	0.79892900	-0.29816200
C	0.50250000	1.56410500	-1.58021400
C	1.20512600	3.18848600	0.47789700
C	1.03486800	2.80580100	-1.88574800
H	0.20069100	0.87566600	-2.36701400
C	1.38873300	3.63881600	-0.81805200
H	1.47529400	3.81049700	1.32534800
H	1.16390100	3.10968900	-2.91937200
H	1.80623300	4.62608800	-0.99962900
C	4.05233700	0.01302200	0.90294600
C	5.08453800	-0.33211900	0.07030600
H	4.12045200	0.77559800	1.67050000
C	3.60737600	-1.92237400	-1.03459600
C	4.90605000	-1.33889000	-0.90793400
H	6.03430300	0.18665600	0.17216500
H	3.40845700	-2.65369500	-1.81324800
H	5.70817800	-1.61771700	-1.58353400
N	-2.49435300	0.03511700	-0.17506400
N	0.31022700	1.11596400	-0.32539200
N	2.83539700	-0.66743300	0.83622200
C	2.57602600	-1.57906700	-0.19176700
C	0.66328600	1.90463000	0.72421600
C	-3.38993500	-0.97338600	0.01553600
S	-2.69148400	-2.53755000	0.30534000
S	0.95571000	-2.26554700	-0.24640000
S	0.45837100	1.29489100	2.34458400
H	2.03263800	-0.26635300	1.32519400

7 B3P86 water

Ni	-0.25695	-0.4206	-0.09203
C	-2.47622	-0.56909	1.87457
C	-4.36489	-1.55984	0.16676
C	-3.74389	-0.83153	2.36918
H	-1.6884	-0.15969	2.49987
C	-4.70587	-1.33589	1.49297
H	-5.08902	-1.95191	-0.53947
H	-3.96901	-0.64122	3.41284
H	-5.7122	-1.55248	1.83915
C	-0.87199	2.06612	-1.75117
C	0.04599	3.66576	0.26508
C	-0.89682	3.43951	-1.93733
H	-1.22747	1.38386	-2.51869
C	-0.42734	4.25115	-0.89958
H	0.4194	4.2698	1.08549
H	-1.27391	3.85907	-2.86379
H	-0.43066	5.33295	-1.00269
C	4.24437	0.09301	1.1826
C	5.40839	-0.54141	0.82505
H	4.18596	0.87981	1.92608
C	4.12446	-1.87353	-0.73414
C	5.3348	-1.54591	-0.15629
H	6.34619	-0.26678	1.29229
H	4.05614	-2.64647	-1.49134
H	6.23516	-2.06965	-0.46337
N	-2.12823	-0.78157	0.59103
N	-0.41859	1.49274	-0.62531
N	3.07337	-0.24654	0.60187
C	2.94281	-1.20589	-0.34883
C	0.0466	2.26461	0.38802
C	-3.06153	-1.27201	-0.25253
S	-2.57571	-1.54142	-1.92199
S	1.40656	-1.56895	-1.05188
S	0.61395	1.4034	1.79909
H	2.20966	0.25993	0.91735
H	-1.26301	-1.13157	-1.59979

Water:

O	-1.76084	-0.07227	0.
H	-0.80084	-0.07227	0.
H	-2.0813	0.83266	0.

Hydrogen:

H	0.	0.	0.37139
H	0.	0.	-0.37139

5-

Charge = -2 Multiplicity = 2

Ni	0.70373	-0.03528	0.94575
C	1.57219	1.94187	-1.03698
C	-0.29573	3.78832	-0.31736
C	1.56047	3.15683	-1.70223
H	2.29676	1.16961	-1.27783
C	0.60014	4.10248	-1.32882
H	-1.0549	4.49828	-0.00525
H	2.283	3.35517	-2.48722
H	0.55222	5.06997	-1.8218
C	1.61107	-1.82081	-1.16373
C	4.25562	-2.04251	-0.61653
C	2.36777	-2.66227	-1.96116
H	0.5449	-1.69424	-1.34321
C	3.73318	-2.77038	-1.66949
H	5.31057	-2.10604	-0.36924
H	1.90739	-3.21013	-2.77682
H	4.37779	-3.41611	-2.26092
C	-3.70513	-0.91083	1.43591
C	-4.60689	-1.93532	1.30535
H	-3.36432	-0.52003	2.38834
C	-4.39857	-1.71494	-1.09663
C	-4.95312	-2.33834	-0.00005
H	-5.02938	-2.40943	2.1828
H	-4.66128	-2.01945	-2.10335
H	-5.66358	-3.1473	-0.14495
N	0.71024	1.62382	-0.04937
N	2.10308	-1.1054	-0.13384
N	-3.17365	-0.31629	0.34473
C	-3.46751	-0.65342	-0.94849
C	3.42853	-1.19561	0.16429
C	-0.23467	2.5353	0.32092
S	-1.32344	2.06793	1.6015
S	-2.73454	0.17806	-2.24396
S	4.09322	-0.27545	1.48601
H	-2.50108	0.45837	0.52232
O	0.20598	-1.3454	2.23858
H	0.80416	-2.10345	2.17004

5

Charge = -1 Multiplicity = 3

Ni	0.48818	-0.13499	0.59814
C	0.88626	1.96231	-1.71201

C	-0.77201	3.62811	-0.29311
C	0.61508	3.22265	-2.22455
H	1.53664	1.26047	-2.22685
C	-0.23024	4.06484	-1.49443
H	-1.43065	4.26068	0.29277
H	1.05326	3.53629	-3.16579
H	-0.46421	5.05928	-1.86459
C	2.3592	-1.84296	-1.33002
C	4.48483	-0.87967	0.10942
C	3.63879	-2.22008	-1.70721
H	1.48179	-2.19398	-1.86664
C	4.71724	-1.72274	-0.96644
H	5.30258	-0.47942	0.69975
H	3.78707	-2.88065	-2.55445
H	5.73521	-1.99511	-1.23201
C	-4.48927	-0.10233	0.56452
C	-5.44942	-0.90952	0.00866
H	-4.70549	0.74046	1.21097
C	-3.67873	-2.17843	-1.04681
C	-5.02217	-1.9679	-0.81448
H	-6.49869	-0.72608	0.20486
H	-3.34025	-2.9925	-1.67758
H	-5.7545	-2.62699	-1.2712
N	0.36563	1.53982	-0.55397
N	2.12793	-1.02862	-0.2907
N	-3.17972	-0.32871	0.31982
C	-2.707	-1.33405	-0.46335
C	3.16076	-0.5398	0.43659
C	-0.45455	2.34011	0.16145
S	-1.00955	1.58915	1.64121
S	-1.02296	-1.54261	-0.72428
S	2.65705	0.50019	1.74183
H	-2.47989	0.31045	0.75887
O	0.3679	-1.58821	2.16561
H	1.23747	-1.45024	2.58871

8

Charge = -2 Multiplicity = 3

C	3.0319	0.80217	-1.08985
C	2.85934	3.31781	-0.02177
C	4.0806	1.68391	-1.30766
H	3.04427	-0.20968	-1.48807
C	3.9814	2.96808	-0.75716
H	2.75896	4.30671	0.41437
H	4.94518	1.37822	-1.88729

H	4.78014	3.69042	-0.90513
C	0.64697	-2.36028	-1.58363
C	1.90446	-3.5684	0.52332
C	1.13604	-3.64539	-1.75995
H	0.13727	-1.82691	-2.38264
C	1.77803	-4.25414	-0.67345
H	2.39774	-4.01903	1.37876
H	1.01988	-4.15316	-2.7115
H	2.17646	-5.26131	-0.76661
C	-3.96535	1.0734	-1.67846
C	-5.28529	0.94448	-1.32112
H	-3.63225	1.53374	-2.60234
C	-4.55907	-0.13904	0.72031
C	-5.57501	0.32138	-0.09156
H	-6.06846	1.31333	-1.97236
H	-4.77265	-0.61923	1.66892
H	-6.6081	0.20177	0.22196
N	1.94694	1.13459	-0.38117
N	0.76573	-1.69262	-0.42859
N	-2.99119	0.61695	-0.86618
C	-3.20727	0.00864	0.3298
C	1.38334	-2.26157	0.63555
C	1.83295	2.37043	0.16025
S	0.35449	2.61394	1.04192
S	-1.8666	-0.52678	1.26309
S	1.45537	-1.27369	2.06119
Ni	0.17583	0.19139	0.10188
H	-0.53766	0.61762	-1.31147

Corrected pKa referenced to experimental conditions to calculate ΔG

$$\Delta G = G_{\text{products}} - G_{\text{reactants}}$$

$$\ln(10)RT = 1.364247$$

$$\text{pKa}_{\text{calculated}} = \frac{\Delta G}{\ln(10)RT}$$

$$\text{pKa}_{\text{corrected}} = \text{pKa}_{\text{calculated}} - \text{pH}_{\text{experimental}}$$

$$\Delta G_{\text{corrected}} = \text{pKa}_{\text{corrected}} * \ln(10)RT$$

Example:



$$\Delta G = -2173599.531 - (-2173321.982 - 264) = -13.549 \text{ kcal/mol}$$

$$\ln(10) RT = 1.364247$$

$$\text{pKa}_{\text{calculated}} = -\frac{13.549}{1.364247} = 9.9315$$

$$\text{pKa}_{\text{corrected}} = 9.9315 - 12 = -2.0685$$

$$\Delta G_{\text{corrected}} = -2.0685 * 1.364247 = 2.821942 \text{ kcal/mol}$$