Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary Information

Water-Assisted Proton Delivery and Removal in bio-inspired Hydrogen Production Catalysts

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Computational analysis of the early deprotonation steps

In dry acetonitrile, both endo and exo deprotonation (protonation) start with the binding of the aniline (anilinium) to form a hydrogen-bonded complex. Because of steric hindrance, the association of both aniline and anilinium to the endo position is disfavored with respect to the more accessible exo position, *i.e.* $\Delta G°$(**ee**$^{2+}$•**B**) > $\Delta G°$(**ex**$^{2+}$•**B**) and $\Delta G°$(**eNiH**$^{2+}$•**B**) > $\Delta G°$(**ex'**$^{2+}$•**B**) (see Figure 5, steps 1 and 2 of panels a and c). The steric penalty arises from the displacement of the endo protonated pendant amine and the cyclohexyl substituent on the opposite ligand.[1,2]

We assume that isomerization in the presence of water starts with the association of water to the protonated pendant amine via hydrogen bonding, which in turn helps shuttle protons between the catalyst and the base. Binding water to the catalyst is slightly favored over aniline due to the higher steric accessibility of water. The energy necessary to distort the catalysts to accommodate aniline and water in the endo position is ΔE_{dis} = 9.2 kcal/mol for aniline and 7.4 kcal/mol for water (see computational details),[18] which results in a binding free energy of formation of $\Delta G°$ = 7.9 kcal/mol (**ee**$^{2+}$**:B**, Figure 5a, step 1) and 5.6 kcal/mol (**ee**$^{2+}$**:H$_2$O**, Figure 5b, step 1).

The calculated binding of aniline to the exo position is $\Delta G°$ = 4.8 kcal/mol (Figure 5c, step 1), where that of water is $\Delta G°$ = 3.0 kcal/mol (Figure 5d, step 1). Once aniline or water binds to the endo protonated pendant amine, an intramolecular proton transfer occurs, leading to the formation of **eNiH**$^{2+}$**·B** or **eNiH**$^{2+}$**·H$_2$O**, where the N-H or O-H hydrogen interact with the hydridic Ni-H hydrogen. In the case of binding of water, a second O-H bond points outward, providing a binding site for the base (Figure 6). However, the realization of a ternary complex where water bridges the catalyst and the base (Figure 5b, step 3) is unfavorable because of loss of solvation energy of each individual species, and in particular of water, which is not counterbalanced by the formation of hydrogen bonds between the three species. The ternary complex is about 7-8 kcal/mol higher in free energy than the binary association complexes between the catalyst and either water or aniline.

(1) O'Hagan, M.; Ho, M.-H.; Yang, J. Y.; Appel, A. M.; DuBois, M. R.; Raugei, S.; Shaw, W. J.; DuBois, D. L.; Bullock, R. M. *J. Am. Chem. Soc.* **2012**, *134* (47), 19409.

(2) Lense, S.; Ho, M.-H.; Chen, S.; Jain, A.; Raugei, S.; Linehan, J. C.; Roberts, J. A. S.; Appel, A. M.; Shaw, W. *Organometallics* **2012**, *31* (19), 6719.

Table S1. Relative free energies (in kcal/mol vs $\mathbf{ex}^{2+}$) and distribution of three isomers (values in parenthesis) at 298.15 K as obtained from QM calculations on $[Ni(P^{Cy}_2N^{Me}_2(H)_2)_2]^{2+}$ (Theory) and NMR measurements on $[Ni(P^{Cy}_2N^{Bz}_2(H)_2)_2]^{2+}$ (Exp.).

	$\mathbf{ee}^{2+}$	$\mathbf{ex}^{2+}$	$\mathbf{xx}^{2+}$
Acetonitrile (Theory)	1.6 (4 %)	0.0 (62%)	0.4 (34%)
Water (Theory)	2.1 (1%)	0.0 (48%)	0.0 (51%)
Acetonitrile (Exp.)	0.3 (30 %)	0.0 (55 %)	0.7 (15 %)
1 M Water in acetonitrile	0.3 (32 %)	0.0 (52 %)	0.7 (15 %)

Table S2. Decomposition of the free energy change ($\Delta G°_{total}$, see Figure 5) for the transfer of a proton from a given intermediate to the aniline (**B**) in its electronic (ΔE_{el}), thermal ($\Delta G°_{thermal}$), and solvation ($\Delta G°_{sol}$) contributions. The prime on the $\mathbf{NiH}^+$ ($\mathbf{NiH}^{+\prime}$) species in the last reaction indicates that water or the base is bound to the exo site.

Reaction	ΔE_{el}	$\Delta G°_{thermal}$	$\Delta G°_{sol}$	$\Delta G°_{total}$
$\mathbf{eNiH}^{2+}\cdot\mathbf{B} \rightarrow \mathbf{NiH}^{+}\cdot\mathbf{BH}^{+}$	-3.2	-0.1	+9.3	+6.0
$\mathbf{eNiH}^{2+}\cdot\mathbf{H_2O}\cdot\mathbf{B} \rightarrow \mathbf{NiH}^{+}\cdot\mathbf{H_2O}\cdot\mathbf{BH}^{+}$	+0.2	-1.2	+3.7	+2.7
$\mathbf{ex'}^{2+}\cdot\mathbf{B} \rightarrow \mathbf{NiH}^{+\prime}\cdot\mathbf{BH}^{+}$	-3.7	+0.6	+8.6	+5.5
$\mathbf{ex'}^{2+}\cdot\mathbf{H_2O}\cdot\mathbf{B} \rightarrow \mathbf{NiH}^{+\prime}\cdot\mathbf{H_2O}\cdot\mathbf{BH}^{+}$	+0.6	-0.8	+2.3	+2.5

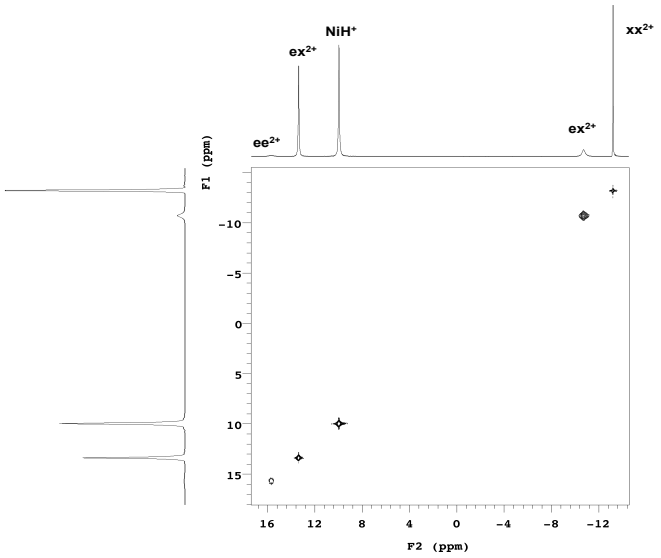

Figure S1: Representative ^{31}P EXSY spectrum of 23 mM $[Ni(P^{Cy}_2N^{Bz}_2)_2]^{2+}$ with 10 eq. of aniline and 1 eq. of water, 25 ºC, 0 ms mixing time; showing no exchange.

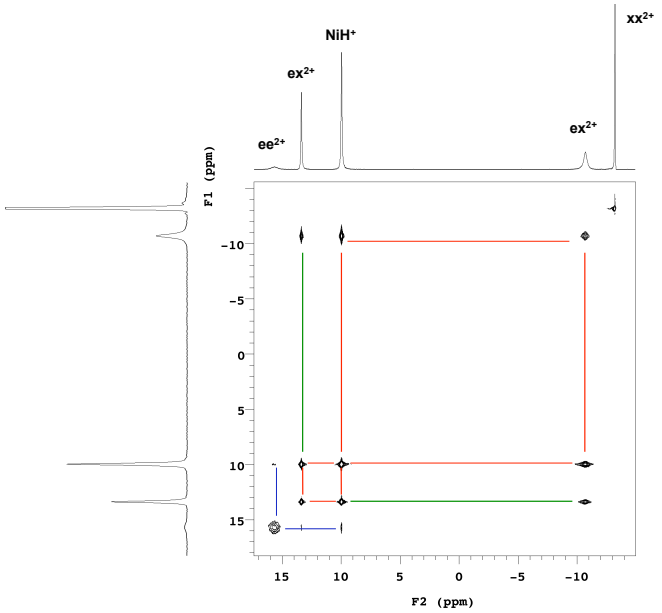

Figure S2: Representative ^{31}P EXSY of 23 mM $[Ni(P^{Cy}_2N^{Bz}_2)_2]^{2+}$ with 10 eq. of aniline and 1 eq. of water, 25 ºC, 100 ms mixing time showing the exchange processes quantified. The exchange between the **ex**$^{2+}$ and **NiH**$^{+}$ species is highlighted in red, the exchange between the **ee**$^{2+}$ isomer and the **NiH**$^{+}$ species is highlighted in blue and the exchange between the inequivalent ^{31}P nuclei of the **ex**$^{2+}$ isomer is highlighted in green.

Cartesian coordinates of the species computationally studied in the paper

The Cartesian coordinates of local minima and transition states are reported below. B stands for aniline, BH^+ stands for anilinium and S stands for the solvent acetonitrile molecule.

ee^{2+}

Ni	0.0653	0.0001	-0.0001
P	0.9344	1.5996	1.2016
P	-1.1042	-0.6060	1.7536
N	1.5087	-0.6450	2.7241
N	-1.0795	1.8189	3.1067
C	1.7286	0.8395	2.7340
H	2.8088	0.9992	2.7158
H	1.3029	1.2386	3.6567
C	0.1189	-1.0464	3.1192
H	-0.1119	-0.5702	4.0748
H	0.1370	-2.1317	3.2470
C	-0.4264	2.5780	2.0512
H	0.0075	3.4711	2.5083
H	-1.1301	2.9148	1.2691
C	-1.9886	0.7910	2.6262
H	-2.7539	1.1953	1.9401
H	-2.5167	0.3801	3.4933
C	2.2038	2.9232	0.7750
H	1.6990	3.5127	-0.0084
C	2.6135	3.8849	1.9016
H	1.7425	4.3837	2.3388
H	3.0947	3.3199	2.7134
C	3.5915	4.9498	1.3909
H	3.0754	5.5885	0.6605
H	3.8826	5.6024	2.2209
C	4.8249	4.3264	0.7435
H	5.4799	5.1076	0.3441
H	5.4090	3.7912	1.5054
C	4.4302	3.3526	-0.3649
H	5.3196	2.8683	-0.7846
H	3.9547	3.9090	-1.1859
C	3.4575	2.2903	0.1539
H	3.9751	1.6822	0.9111
H	3.1825	1.5917	-0.6486
C	-2.3259	-2.0191	1.9086
H	-1.8069	-2.8614	1.4227
C	-3.5921	-1.7152	1.0922
H	-4.1202	-0.8637	1.5445
H	-3.3238	-1.4130	0.0728
C	-4.5329	-2.9226	1.0610
H	-5.4359	-2.6698	0.4941
H	-4.0440	-3.7468	0.5219
C	-4.8978	-3.3810	2.4714
H	-5.5286	-4.2751	2.4272
H	-5.4970	-2.6022	2.9637
C	-3.6475	-3.6598	3.3020
H	-3.1100	-4.5213	2.8811
H	-3.9202	-3.9341	4.3268
C	-2.7079	-2.4484	3.3337
H	-3.2171	-1.6218	3.8477
H	-1.8229	-2.6948	3.9329
C	2.5412	-1.3725	3.5101
H	2.3831	-2.4469	3.4028
H	2.4548	-1.0896	4.5606
C	-1.7595	2.7068	4.0513
H	-2.1692	2.1178	4.8767
H	-2.5837	3.2733	3.5872
P	-1.1047	0.6057	-1.7535
P	0.9344	-1.5995	-1.2015
N	-1.0803	-1.8197	-3.1057
N	1.5078	0.6446	-2.7250
C	-1.9894	-0.7918	-2.6251
H	-2.7543	-1.1960	-1.9385
H	-2.5179	-0.3814	-3.4921
C	-0.4265	-2.5784	-2.0503
H	0.0073	-3.4716	-2.5074
H	-1.1298	-2.9152	-1.2678
C	0.1178	1.0456	-3.1198
H	-0.1133	0.5690	-4.0751
H	0.1356	2.1309	-3.2481
C	1.7279	-0.8398	-2.7345
H	2.8081	-0.9993	-2.7167
H	1.3019	-1.2393	-3.6569
C	-2.3262	2.0190	-1.9089
H	-1.8063	2.8616	-1.4246
C	-2.7095	2.4466	-3.3341
H	-1.8251	2.6916	-3.9346
H	-3.2199	1.6196	-3.8464
C	-3.6484	3.6585	-3.3029
H	-3.1101	4.5203	-2.8836
H	-3.9221	3.9317	-4.3278
C	-4.8981	3.3814	-2.4707
H	-5.5283	4.2758	-2.4270
H	-5.4981	2.6023	-2.9614
C	-4.5319	2.9245	-1.0601
H	-5.4344	2.6729	-0.4920
H	-4.0420	3.7492	-0.5226
C	-3.5916	1.7167	-1.0908
H	-4.1206	0.8647	-1.5413
H	-3.3223	1.4158	-0.0712
C	2.2042	-2.9227	-0.7750
H	1.7000	-3.5118	0.0090
C	3.4582	-2.2893	-0.1550
H	3.9753	-1.6815	-0.9128
H	3.1836	-1.5902	0.6473
C	4.4314	-3.3511	0.3639
H	5.3210	-2.8665	0.7828
H	3.9565	-3.9072	1.1854
C	4.8256	-4.3253	-0.7443
H	5.4810	-5.1063	-0.3449
H	5.4092	-3.7904	-1.5068
C	3.5920	-4.9494	-1.3906
H	3.0764	-5.5878	-0.6596
H	3.8828	-5.6023	-2.2205
C	2.6135	-3.8849	-1.9014
H	3.0941	-3.3202	-2.7137
H	1.7423	-4.3841	-2.3377
C	-1.7606	-2.7080	-4.0497
H	-2.5845	-3.2745	-3.5851
H	-1.0434	-3.4200	-4.4675
C	2.5399	1.3721	-3.5115
H	2.3817	2.4465	-3.4045
H	2.4533	1.0889	-4.5619
H	3.5301	1.1065	-3.1380
H	-2.1707	-2.1193	-4.8751
H	-1.0422	3.4188	4.4690
H	3.5312	-1.1066	3.1364
H	1.5577	-0.8969	1.7038
H	1.5570	0.8969	-1.7048

ee^{2+}:B:S

Ni	-0.7595	-0.2998	0.0776
P	-0.1519	-1.3955	-1.6844

P	-0.4836	1.5248	-1.1147
N	2.0273	0.4866	-2.0612
N	-1.1530	0.3999	-3.5610
C	1.4415	-0.8168	-2.5060
H	2.2204	-1.5632	-2.3276
H	1.2792	-0.7305	-3.5840
C	1.1180	1.6743	-2.0916
H	0.8961	1.8767	-3.1424
H	1.7066	2.4969	-1.6763
C	-1.3209	-0.9654	-3.0910
H	-1.1260	-1.6275	-3.9401
H	-2.3495	-1.1714	-2.7405
C	-1.5978	1.4222	-2.6242
H	-2.6356	1.2569	-2.2900
H	-1.5692	2.3825	-3.1490
C	0.0754	-3.2541	-1.9360
H	-0.9309	-3.6532	-1.7200
C	0.4765	-3.7419	-3.3372
H	-0.2168	-3.3766	-4.1021
H	1.4693	-3.3474	-3.5962
C	0.5266	-5.2730	-3.3968
H	-0.4857	-5.6721	-3.2418
H	0.8328	-5.5890	-4.4000
C	1.4700	-5.8491	-2.3443
H	1.4536	-6.9437	-2.3766
H	2.5018	-5.5466	-2.5728
C	1.0991	-5.3566	-0.9469
H	1.8151	-5.7304	-0.2056
H	0.1158	-5.7659	-0.6709
C	1.0439	-3.8274	-0.8913
H	2.0546	-3.4333	-1.0755
H	0.7757	-3.4819	0.1167
C	-0.5906	3.3196	-0.5660
H	0.3268	3.4245	0.0365
C	-1.7813	3.5717	0.3643
H	-2.7193	3.4544	-0.1980
H	-1.7933	2.8204	1.1623
C	-1.7265	4.9812	0.9607
H	-2.6030	5.1490	1.5973
H	-0.8458	5.0575	1.6149
C	-1.6438	6.0509	-0.1266
H	-1.5498	7.0440	0.3261
H	-2.5811	6.0589	-0.7010
C	-0.4748	5.7881	-1.0738
H	0.4750	5.8962	-0.5310
H	-0.4602	6.5303	-1.8797
C	-0.5499	4.3803	-1.6755
H	-1.4611	4.3113	-2.2854
H	0.2985	4.2237	-2.3532
C	3.2358	0.7759	-2.8909
H	3.6657	1.7234	-2.5633
H	2.9420	0.8398	-3.9402
C	-1.7890	0.5821	-4.8649
H	-1.5783	1.5879	-5.2396
H	-2.8839	0.4492	-4.8287
P	-2.8531	-0.5287	0.7458
P	-0.1472	-0.5965	2.1650
N	-2.5216	0.0730	3.4516
N	-1.6353	-2.8747	1.6074
C	-3.3219	0.4229	2.2896
H	-3.2702	1.4999	2.0533
H	-4.3674	0.1942	2.5253
C	-1.1265	0.4783	3.3580
H	-0.6945	0.3911	4.3583
H	-1.0084	1.5288	3.0388
C	-2.9966	-2.2713	1.4537
H	-3.4989	-2.3087	2.4231
H	-3.5317	-2.9032	0.7409
C	-0.8370	-2.2676	2.7217
H	-0.0209	-2.9595	2.9380
H	-1.4899	-2.1685	3.5908
C	-4.4621	-0.4089	-0.2288
H	-4.2100	-0.8413	-1.2099
C	-5.6761	-1.1695	0.3288
H	-5.4579	-2.2346	0.4685
H	-5.9446	-0.7697	1.3169
C	-6.8829	-1.0351	-0.6083
H	-6.6532	-1.5357	-1.5596
H	-7.7381	-1.5667	-0.1764
C	-7.2392	0.4252	-0.8743
H	-8.0682	0.4874	-1.5872
H	-7.5937	0.8904	0.0562
C	-6.0314	1.2002	-1.3962
H	-6.2817	2.2593	-1.5252
H	-5.7497	0.8203	-2.3889
C	-4.8385	1.0668	-0.4466
H	-5.1057	1.5183	0.5187
H	-3.9821	1.6362	-0.8265
C	1.5519	-0.6910	2.9816
H	1.9631	0.3222	2.8363
C	2.4396	-1.6870	2.2185
H	2.0251	-2.7003	2.3285
H	2.4176	-1.4720	1.1419
C	3.8748	-1.7066	2.7549
H	4.4639	-2.4463	2.2006
H	4.3530	-0.7321	2.5763
C	3.9024	-2.0042	4.2521
H	4.9309	-1.9704	4.6269
H	3.5411	-3.0278	4.4267
C	3.0273	-1.0167	5.0185
H	3.4546	-0.0074	4.9360
H	3.0161	-1.2613	6.0863
C	1.5895	-0.9964	4.4872
H	1.1271	-1.9758	4.6790
H	1.0135	-0.2604	5.0573
C	-3.1375	0.5919	4.6728
H	-3.1825	1.6937	4.6948
H	-2.5704	0.2520	5.5442
C	-1.6912	-4.3567	1.6940
H	-2.2165	-4.7482	0.8210
H	-2.2243	-4.6423	2.6027
H	-0.6754	-4.7541	1.7212
H	-4.1569	0.2050	4.7620
H	-1.3791	-0.1378	-5.5793
H	3.9673	-0.0212	-2.7451
H	2.4177	0.4334	-1.0728
H	-1.1295	-2.5518	0.7371
C	4.9013	2.8759	-0.4537
C	3.8668	2.2801	0.2750
C	5.0791	4.2570	-0.4119
C	4.2377	5.0577	0.3567
C	3.2138	4.4625	1.0916
C	3.0224	3.0837	1.0483
H	5.5845	2.2524	-1.0256
H	5.8932	4.7059	-0.9734
H	2.2265	2.6232	1.6311
H	2.5653	5.0732	1.7135
H	4.3877	6.1315	0.3957
N	3.6416	0.8774	0.1922
H	4.4849	0.3684	-0.0859
H	3.3122	0.5038	1.0754
N	6.0369	-0.6397	-1.0151
C	7.1227	-1.0232	-1.1498
C	8.4871	-1.4981	-1.3097
H	9.1333	-0.6791	-1.6407
H	8.8636	-1.8809	-0.3567
H	8.5249	-2.2999	-2.0520

ee^{2+}:B:S -> eNiH^{2+}:B:S

Ni	0.5426	0.3071	0.0415
P	0.4083	1.2619	-1.8820
P	-0.1702	-1.5340	-0.9983
N	-2.1841	0.0553	-2.3219
N	1.0014	-0.9398	-3.4451
C	-1.1966	1.0536	-2.8392
H	-1.7230	2.0109	-2.8609
H	-0.9660	0.7536	-3.8649
C	-1.6696	-1.3359	-2.1172
H	-1.4405	-1.7358	-3.1080
H	-2.5069	-1.8908	-1.6846
C	1.5220	0.3730	-3.0987
H	1.5850	0.9558	-4.0226
H	2.5360	0.3327	-2.6608
C	1.0575	-1.9150	-2.3662
H	2.0625	-1.9905	-1.9203
H	0.8103	-2.8923	-2.7923
C	0.7335	3.0786	-2.2086

H	1.7491	3.2261	-1.8080
C	0.7304	3.5255	-3.6789
H	1.4534	2.9533	-4.2698
H	-0.2590	3.3421	-4.1229
C	1.0564	5.0183	-3.8029
H	2.0899	5.1883	-3.4700
H	1.0197	5.3099	-4.8581
C	0.1056	5.8780	-2.9749
H	0.3863	6.9336	-3.0504
H	-0.9121	5.7974	-3.3827
C	0.1031	5.4361	-1.5133
H	-0.6167	6.0255	-0.9337
H	1.0929	5.6297	-1.0760
C	-0.2268	3.9466	-1.3797
H	-1.2588	3.7909	-1.7292
H	-0.2099	3.6326	-0.3291
C	-0.6253	-3.2120	-0.2853
H	-1.5411	-2.9803	0.2829
C	0.4201	-3.7188	0.7135
H	1.3584	-3.9365	0.1835
H	0.6432	-2.9369	1.4474
C	-0.0623	-4.9881	1.4218
H	0.7147	-5.3449	2.1073
H	-0.9364	-4.7415	2.0417
C	-0.4386	-6.0818	0.4246
H	-0.8308	-6.9571	0.9531
H	0.4634	-6.4178	-0.1059
C	-1.4609	-5.5749	-0.5897
H	-2.4094	-5.3515	-0.0809
H	-1.6814	-6.3488	-1.3330
C	-0.9643	-4.3122	-1.3030
H	-0.0653	-4.5709	-1.8786
H	-1.7192	-3.9800	-2.0255
C	-3.3532	0.0094	-3.2531
H	-4.1081	-0.6633	-2.8439
H	-3.0171	-0.3451	-4.2290
C	1.6523	-1.4581	-4.6492
H	1.1839	-2.4017	-4.9428
H	2.7314	-1.6355	-4.5085
P	2.5747	-0.1194	0.9509
P	-0.1528	0.8504	2.0954
N	1.8141	-0.3754	3.6263
N	1.9316	2.4947	1.4526
C	2.5945	-1.0241	2.5883
H	2.2834	-2.0694	2.4169
H	3.6362	-1.0544	2.9272
C	0.3783	-0.3916	3.3999
H	-0.1048	-0.1306	4.3450
H	-0.0004	-1.3873	3.1065
C	3.0900	1.5972	1.5143
H	3.5385	1.5826	2.5135
H	3.8303	1.9733	0.8027
C	0.9664	2.2986	2.5427
H	0.3595	3.2034	2.6217
H	1.4708	2.1165	3.4962
C	4.1454	-0.7851	0.1583
H	4.1130	-0.3893	-0.8691
C	5.4668	-0.3287	0.7996
H	5.5340	0.7636	0.8475
H	5.5236	-0.6947	1.8343
C	6.6685	-0.8674	0.0139
H	6.6735	-0.4137	-0.9874
H	7.5941	-0.5464	0.5042
C	6.6305	-2.3879	-0.1152
H	7.4713	-2.7367	-0.7240
H	6.7558	-2.8424	0.8775
C	5.3089	-2.8557	-0.7203
H	5.2673	-3.9502	-0.7524
H	5.2360	-2.5075	-1.7608
C	4.1163	-2.3204	0.0764
H	4.1556	-2.7379	1.0917
H	3.1759	-2.6722	-0.3649
C	-1.8171	1.4581	2.7307
H	-2.4827	0.5824	2.6376
C	-2.3473	2.5772	1.8201
H	-1.6793	3.4473	1.8950
H	-2.3107	2.2666	0.7670
C	-3.7555	3.0240	2.2256
H	-4.0892	3.8371	1.5699
H	-4.4631	2.1925	2.0861
C	-3.7966	3.4646	3.6873
H	-4.8184	3.7364	3.9721
H	-3.1875	4.3712	3.8100
C	-3.2662	2.3648	4.6027
H	-3.9440	1.5001	4.5694
H	-3.2520	2.7061	5.6434
C	-1.8577	1.9144	4.1985
H	-1.1600	2.7517	4.3414
H	-1.5334	1.1158	4.8734
C	2.1506	-0.9216	4.9404
H	1.8915	-1.9891	5.0411
H	1.6220	-0.3623	5.7174
C	2.3191	3.8980	1.2682
H	2.9323	3.9892	0.3677
H	2.8933	4.2748	2.1237
H	1.4234	4.5112	1.1482
H	3.2240	-0.8103	5.1186
H	1.5247	-0.7475	-5.4708
H	-3.7688	1.0142	-3.3491
H	-2.6032	0.3518	-1.3983
H	1.1969	1.7592	0.4223
C	-6.0014	-0.7587	-0.9672
C	-4.8373	-0.8032	-0.1959
C	-6.8046	-1.8912	-1.0811
C	-6.4564	-3.0737	-0.4324
C	-5.3001	-3.1137	0.3429
C	-4.4904	-1.9862	0.4615
H	-6.2940	0.1661	-1.4603
H	-7.7142	-1.8415	-1.6717
H	-3.6049	-2.0144	1.0942
H	-5.0327	-4.0225	0.8739
H	-7.0893	-3.9508	-0.5175
N	-3.9782	0.3370	-0.1195
H	-4.5134	1.1998	-0.1701
H	-3.4747	0.3529	0.7623
N	-5.5983	2.9548	-0.3580
C	-6.2286	3.9264	-0.4119
C	-7.0108	5.1499	-0.4741
H	-7.3809	5.4099	0.5226
H	-6.3909	5.9712	-0.8453
H	-7.8643	5.0206	-1.1451

eNiH^{2+}:B:S

Ni	-0.6045	-0.1442	0.2475
P	-0.0800	-1.2224	-1.7523
P	-0.5526	1.6874	-0.9720
N	2.0060	0.7619	-1.9910
N	-1.1665	0.6926	-3.4735
C	1.4763	-0.5294	-2.5341
H	2.2843	-1.2549	-2.4045
H	1.3143	-0.3764	-3.6045
C	1.0537	1.9110	-1.9208
H	0.8159	2.1918	-2.9494
H	1.6149	2.7187	-1.4432
C	-1.2816	-0.7091	-3.1009
H	-1.0681	-1.3007	-3.9958
H	-2.3007	-0.9825	-2.7723
C	-1.6664	1.6273	-2.4764
H	-2.6966	1.4003	-2.1616
H	-1.6761	2.6246	-2.9287
C	0.1496	-3.0497	-2.1126
H	-0.8538	-3.4609	-1.9203
C	0.5701	-3.4245	-3.5418
H	-0.1294	-3.0277	-4.2859
H	1.5539	-2.9875	-3.7669
C	0.6655	-4.9454	-3.7069
H	-0.3348	-5.3841	-3.5863
H	0.9862	-5.1799	-4.7280
C	1.6197	-5.5618	-2.6878
H	1.6456	-6.6506	-2.8031
H	2.6415	-5.2039	-2.8803
C	1.2092	-5.1901	-1.2653
H	1.9225	-5.5978	-0.5395
H	0.2358	-5.6474	-1.0391
C	1.1004	-3.6735	-1.0822
H	2.1039	-3.2324	-1.1872
H	0.7436	-3.4333	-0.0756
C	-0.6652	3.4137	-0.2579

H	0.2859	3.4764	0.2964
C	-1.7952	3.5774	0.7634
H	-2.7666	3.5142	0.2542
H	-1.7606	2.7601	1.4947
C	-1.6928	4.9339	1.4672
H	-2.5219	5.0455	2.1749
H	-0.7682	4.9599	2.0616
C	-1.6869	6.0872	0.4649
H	-1.5620	7.0414	0.9877
H	-2.6623	6.1356	-0.0395
C	-0.5866	5.9107	-0.5794
H	0.3983	5.9836	-0.0973
H	-0.6314	6.7136	-1.3235
C	-0.6970	4.5546	-1.2854
H	-1.6444	4.5225	-1.8411
H	0.1088	4.4568	-2.0238
C	3.1886	1.1716	-2.8098
H	3.5851	2.1055	-2.4089
H	2.8763	1.3096	-3.8467
C	-1.7909	0.9419	-4.7734
H	-1.6152	1.9792	-5.0728
H	-2.8790	0.7630	-4.7670
P	-2.7630	-0.6749	0.6621
P	-0.2596	-1.0747	2.1902
N	-2.6466	-0.5404	3.4397
N	-1.6586	-3.2172	1.1276
C	-3.3324	0.0237	2.2971
H	-3.2430	1.1245	2.2468
H	-4.3978	-0.2120	2.3968
C	-1.2418	-0.1958	3.5108
H	-0.8703	-0.5186	4.4872
H	-1.0496	0.8902	3.4245
C	-2.9169	-2.5152	0.9446
H	-3.6222	-2.6777	1.7804
H	-3.3816	-2.9245	0.0415
C	-0.9270	-2.8124	2.3156
H	-0.0665	-3.4815	2.4202
H	-1.5287	-2.8871	3.2379
C	-4.2629	-0.2937	-0.4086
H	-3.9331	-0.5002	-1.4378
C	-5.5038	-1.1621	-0.1336
H	-5.2759	-2.2292	-0.2143
H	-5.8577	-0.9908	0.8925
C	-6.6310	-0.8212	-1.1163
H	-6.3155	-1.0999	-2.1319
H	-7.5070	-1.4370	-0.8850
C	-6.9948	0.6606	-1.0837
H	-7.7616	0.8788	-1.8344
H	-7.4355	0.9081	-0.1080
C	-5.7633	1.5330	-1.3145
H	-6.0215	2.5942	-1.2253
H	-5.3931	1.3845	-2.3398
C	-4.6526	1.1905	-0.3184
H	-5.0130	1.4095	0.6953
H	-3.7821	1.8365	-0.4778
C	1.4555	-1.1928	2.9209
H	1.7903	-0.1444	2.9810
C	2.4020	-1.9539	1.9816
H	2.0559	-2.9919	1.8826
H	2.3619	-1.5256	0.9719
C	3.8361	-1.9761	2.5202
H	4.4770	-2.5403	1.8329
H	4.2399	-0.9524	2.5548
C	3.8904	-2.5733	3.9242
H	4.9150	-2.5442	4.3100
H	3.6037	-3.6333	3.8793
C	2.9493	-1.8287	4.8661
H	3.3047	-0.7973	5.0009
H	2.9549	-2.2902	5.8594
C	1.5123	-1.7989	4.3335
H	1.1180	-2.8244	4.3110
H	0.8882	-1.2356	5.0345
C	-3.3422	-0.2213	4.6833
H	-3.3620	0.8607	4.8989
H	-2.8535	-0.7322	5.5176
C	-1.8972	-4.6585	1.1479
H	-2.3897	-4.9625	0.2190
H	-2.5302	-4.9787	1.9932
H	-0.9419	-5.1874	1.2150
H	-4.3734	-0.5814	4.6270
H	-1.3401	0.2917	-5.5284
H	3.9546	0.3974	-2.7388
H	2.4232	0.6377	-1.0123
H	0.7460	0.3101	0.5299
C	4.6994	3.0964	-0.1145
C	3.7455	2.3154	0.5458
C	4.7664	4.4673	0.1254
C	3.8935	5.0730	1.0261
C	2.9508	4.2921	1.6922
C	2.8686	2.9225	1.4506
H	5.4106	2.6229	-0.7870
H	5.5200	5.0607	-0.3837
H	2.1356	2.3161	1.9793
H	2.2823	4.7480	2.4171
H	3.9599	6.1382	1.2214
N	3.6305	0.9249	0.2603
H	4.5018	0.5343	-0.1109
H	3.3679	0.3977	1.0862
N	6.0695	-0.2376	-1.1914
C	7.1711	-0.5297	-1.4058
C	8.5510	-0.8959	-1.6731
H	9.1993	-0.5164	-0.8780
H	8.6498	-1.9842	-1.7202
H	8.8761	-0.4696	-2.6266

NiH^+:BH^+:2S

Ni	-0.5589	-0.1956	0.2115
P	-0.1659	-1.3279	-1.7465
P	-0.6517	1.5794	-1.0941
N	1.8278	0.6791	-2.1896
N	-1.5299	0.4221	-3.4448
C	1.3053	-0.6195	-2.6466
H	2.1182	-1.3440	-2.5350
H	1.0572	-0.5618	-3.7162
C	0.8529	1.7749	-2.1861
H	0.4920	1.9742	-3.2039
H	1.3847	2.6642	-1.8362
C	-1.5192	-0.9578	-2.9822
H	-1.3676	-1.5899	-3.8610
H	-2.4768	-1.2532	-2.5209
C	-1.9299	1.3981	-2.4417
H	-2.8998	1.1561	-1.9835
H	-2.0277	2.3675	-2.9395
C	0.1116	-3.1575	-2.0346
H	-0.8481	-3.6186	-1.7599
C	0.4496	-3.5542	-3.4785
H	-0.3269	-3.2183	-4.1722
H	1.3817	-3.0599	-3.7798
C	0.6327	-5.0677	-3.6099
H	-0.3195	-5.5663	-3.3854
H	0.8857	-5.3184	-4.6461
C	1.7055	-5.5821	-2.6546
H	1.8087	-6.6689	-2.7446
H	2.6749	-5.1462	-2.9313
C	1.3754	-5.1928	-1.2164
H	2.1632	-5.5330	-0.5354
H	0.4504	-5.6999	-0.9103
C	1.1871	-3.6819	-1.0754
H	2.1397	-3.1814	-1.3004
H	0.9302	-3.4259	-0.0428
C	-0.7993	3.3327	-0.4736
H	0.1387	3.4454	0.0921
C	-1.9626	3.5309	0.4998
H	-2.9105	3.3925	-0.0348
H	-1.9313	2.7703	1.2890
C	-1.9323	4.9330	1.1110
H	-2.7868	5.0612	1.7841
H	-1.0274	5.0343	1.7250
C	-1.9331	6.0138	0.0336
H	-1.8662	7.0073	0.4904
H	-2.8856	5.9802	-0.5115
C	-0.7881	5.8060	-0.9544
H	0.1703	5.9434	-0.4367
H	-0.8291	6.5582	-1.7502
C	-0.8301	4.4049	-1.5699
H	-1.7532	4.3022	-2.1540
H	0.0041	4.2790	-2.2670
C	2.9222	1.0484	-3.1030

H	3.3436	2.0109	-2.8045
H	2.5651	1.1272	-4.1381
C	-2.3737	0.5485	-4.6268
H	-2.3134	1.5705	-5.0092
H	-3.4324	0.3190	-4.4188
P	-2.6432	-0.7200	0.8426
P	-0.0375	-0.9183	2.1901
N	-2.3248	-0.3355	3.5886
N	-1.4461	-3.1795	1.4546
C	-3.1052	0.1076	2.4482
H	-3.0369	1.1988	2.2947
H	-4.1544	-0.1352	2.6468
C	-0.9216	0.0326	3.5221
H	-0.4674	-0.2159	4.4849
H	-0.7672	1.1106	3.3439
C	-2.7353	-2.5251	1.3119
H	-3.3593	-2.6147	2.2179
H	-3.2607	-3.0314	0.4979
C	-0.6314	-2.6503	2.5350
H	0.2550	-3.2850	2.6245
H	-1.1570	-2.6524	3.5034
C	-4.2253	-0.4565	-0.1291
H	-3.9595	-0.6932	-1.1676
C	-5.3893	-1.3673	0.2866
H	-5.1089	-2.4206	0.2154
H	-5.6498	-1.1735	1.3352
C	-6.6155	-1.1229	-0.5967
H	-6.3785	-1.4308	-1.6234
H	-7.4388	-1.7607	-0.2574
C	-7.0451	0.3408	-0.5969
H	-7.8811	0.4885	-1.2888
H	-7.4092	0.6104	0.4031
C	-5.8820	1.2540	-0.9690
H	-6.1843	2.3043	-0.9019
H	-5.5918	1.0714	-2.0123
C	-4.6752	1.0089	-0.0646
H	-4.9523	1.2529	0.9681
H	-3.8580	1.6830	-0.3337
C	1.7317	-0.9606	2.7529
H	2.0664	0.0846	2.6847
C	2.5692	-1.8097	1.7889
H	2.2073	-2.8457	1.8138
H	2.4240	-1.4662	0.7582
C	4.0508	-1.7925	2.1681
H	4.6133	-2.4288	1.4771
H	4.4480	-0.7745	2.0503
C	4.2610	-2.2455	3.6096
H	5.3203	-2.1773	3.8791
H	3.9778	-3.3024	3.6997
C	3.4165	-1.4169	4.5728
H	3.7699	-0.3780	4.5618
H	3.5372	-1.7809	5.5983
C	1.9335	-1.4410	4.1950
H	1.5512	-2.4650	4.2921
H	1.3702	-0.8202	4.8969
C	-2.9226	0.1475	4.8267
H	-2.9303	1.2483	4.8929
H	-2.3586	-0.2439	5.6769
C	-1.6338	-4.6138	1.6231
H	-2.2075	-5.0069	0.7801
H	-2.1680	-4.8670	2.5543
H	-0.6578	-5.1055	1.6418
H	-3.9536	-0.2085	4.8949
H	-2.0183	-0.1357	-5.4013
H	3.7042	0.2871	-3.0550
H	2.7393	0.8329	-0.8133
H	0.8196	0.2302	0.2423
C	4.4997	3.2827	-0.3124
C	3.5492	2.4715	0.2983
C	4.5417	4.6378	0.0080
C	3.6413	5.1710	0.9277
C	2.6945	4.3455	1.5316
C	2.6423	2.9891	1.2176
H	5.2037	2.8602	-1.0208
H	5.2851	5.2740	-0.4588
H	1.9107	2.3381	1.6847
H	1.9942	4.7543	2.2513
H	3.6818	6.2252	1.1783
N	3.4910	1.0598	-0.0451
H	4.4108	0.7117	-0.3805
H	3.2510	0.5017	0.7741
N	6.0927	0.0259	-0.8499
C	7.1691	-0.2836	-1.1470
C	8.5145	-0.6711	-1.5186
H	9.2367	-0.0949	-0.9368
H	8.6601	-1.7350	-1.3215
H	8.6728	-0.4791	-2.5817

NiH$^+$

Ni	-0.1944	-0.1568	-0.0399
P	1.1442	-1.0199	-1.6421
P	-0.6538	1.3817	-1.5785
N	2.1287	1.6024	-1.9383
N	-1.3052	-0.9256	-3.0213
C	2.2858	0.2453	-2.4358
H	3.3092	-0.0660	-2.1972
H	2.1913	0.1889	-3.5385
C	0.8632	2.2294	-2.2778
H	0.7390	2.3503	-3.3728
H	0.8765	3.2407	-1.8525
C	0.0311	-1.4835	-3.0884
H	0.5397	-1.2327	-4.0388
H	-0.0687	-2.5749	-3.0581
C	-1.3497	0.5195	-3.1029
H	-2.4024	0.8123	-3.1782
H	-0.8446	0.9101	-4.0062
C	2.2312	-2.5455	-1.5936
H	1.5186	-3.3447	-1.3323
C	2.9082	-2.9203	-2.9203
H	2.1691	-3.0237	-3.7232
H	3.5920	-2.1151	-3.2240
C	3.7069	-4.2208	-2.7846
H	3.0134	-5.0504	-2.5861
H	4.2012	-4.4492	-3.7360
C	4.7316	-4.1349	-1.6555
H	5.2641	-5.0871	-1.5525
H	5.4894	-3.3796	-1.9091
C	4.0636	-3.7567	-0.3348
H	4.8127	-3.6528	0.4589
H	3.3882	-4.5667	-0.0237
C	3.2616	-2.4590	-0.4617
H	3.9568	-1.6289	-0.6578
H	2.7567	-2.2275	0.4841
C	-1.8019	2.8461	-1.3903
H	-1.3104	3.4530	-0.6121
C	-3.1635	2.4032	-0.8419
H	-3.6596	1.7471	-1.5725
H	-3.0213	1.8045	0.0658
C	-4.0686	3.6046	-0.5603
H	-5.0442	3.2570	-0.2008
H	-3.6304	4.2024	0.2520
C	-4.2369	4.4815	-1.8001
H	-4.8526	5.3570	-1.5654
H	-4.7787	3.9174	-2.5729
C	-2.8822	4.9204	-2.3523
H	-2.3870	5.5787	-1.6241
H	-3.0127	5.5107	-3.2667
C	-1.9745	3.7203	-2.6415
H	-2.4222	3.1225	-3.4480
H	-1.0049	4.0724	-3.0127
C	3.2243	2.4339	-2.4205
H	3.1448	3.4372	-1.9896
H	3.2331	2.5346	-3.5214
C	-2.1886	-1.5488	-3.9965
H	-1.8876	-1.3546	-5.0413
H	-3.2082	-1.1758	-3.8588
P	-1.3115	-1.2023	1.4610
P	0.8197	0.7948	1.6702
N	-1.4329	0.8456	3.3660
N	0.5979	-1.3398	3.4992
C	-2.2520	-0.0399	2.5673
H	-2.9573	0.5021	1.9042
H	-2.8591	-0.6345	3.2604
C	-0.4703	1.6882	2.6883
H	0.0409	2.2579	3.4699
H	-0.9386	2.4273	2.0031
C	-0.2036	-2.1587	2.6167
H	-0.8259	-2.7978	3.2511

H 0.3997 -2.8302 1.9691
C 1.5414 -0.4388 2.8713
H 2.3301 -0.9797 2.3111
H 2.0443 0.1187 3.6711
C -2.5946 -2.4620 0.9526
H -2.0136 -3.1777 0.3492
C -3.2715 -3.2324 2.0967
H -2.5337 -3.7226 2.7405
H -3.8336 -2.5342 2.7322
C -4.2374 -4.2897 1.5505
H -3.6638 -5.0501 1.0015
H -4.7197 -4.8081 2.3871
C -5.2839 -3.6759 0.6245
H -5.9343 -4.4575 0.2157
H -5.9314 -3.0015 1.2031
C -4.6193 -2.8922 -0.5047
H -5.3764 -2.4118 -1.1359
H -4.0648 -3.5858 -1.1534
C -3.6547 -1.8331 0.0340
H -4.2277 -1.0838 0.5992
H -3.1680 -1.3090 -0.7964
C 2.2112 2.0475 1.5122
H 1.9540 2.6125 0.6058
C 3.5411 1.3286 1.2301
H 3.8042 0.6865 2.0811
H 3.4286 0.6795 0.3546
C 4.6858 2.3214 1.0164
H 5.6181 1.7716 0.8390
H 4.4919 2.9142 0.1126
C 4.8350 3.2614 2.2092
H 5.6424 3.9808 2.0312
H 5.1221 2.6825 3.0988
C 3.5240 3.9934 2.4782
H 3.2945 4.6492 1.6259
H 3.6160 4.6449 3.3549
C 2.3558 3.0241 2.6888
H 2.5179 2.4646 3.6219
H 1.4386 3.6071 2.8239
C -2.2576 1.6274 4.2690
H -1.6200 2.1916 4.9569
H -2.8858 0.9585 4.8657
C 1.2615 -2.1544 4.5017
H 0.5195 -2.7484 5.0442
H 1.7672 -1.5069 5.2248
H 2.0124 -2.8456 4.0726
H -2.9186 2.3438 3.7438
H -2.1988 -2.6318 -3.8405
H 4.1809 2.0034 -2.1097
H -1.1849 -0.8474 -0.8228

ee^{2+}:H$_2$O:S

Ni -0.2334 0.0675 0.1250
P -0.4570 -1.5440 -1.3172
P -0.1781 1.4287 -1.6995
N 1.8968 -0.4410 -2.4353
N -1.4977 -0.2156 -3.5083
C 0.9676 -1.6086 -2.5266
H 1.5805 -2.4843 -2.3066
H 0.5889 -1.6501 -3.5503
C 1.2935 0.8972 -2.7469
H 1.0240 0.8782 -3.8064
H 2.0983 1.6232 -2.6044
C -1.8323 -1.2576 -2.5506
H -1.9799 -2.1877 -3.1086
H -2.7648 -1.0559 -1.9979
C -1.5289 1.1314 -2.9589
H -2.4951 1.3730 -2.4818
H -1.3946 1.8321 -3.7900
C -0.6523 -3.3203 -0.7896
H -1.6425 -3.3285 -0.3054
C -0.6659 -4.3561 -1.9245
H -1.4360 -4.1279 -2.6701
H 0.3002 -4.3428 -2.4489
C -0.9023 -5.7650 -1.3680
H -1.9116 -5.8157 -0.9362
H -0.8809 -6.4867 -2.1917
C 0.1288 -6.1321 -0.3038
H -0.0877 -7.1254 0.1033
H 1.1241 -6.1955 -0.7662
C 0.1559 -5.0946 0.8162
H 0.9318 -5.3418 1.5498
H -0.8018 -5.1167 1.3563
C 0.3938 -3.6813 0.2766
H 1.3957 -3.6377 -0.1771
H 0.3688 -2.9417 1.0876
C 0.0156 3.2902 -1.7418
H 0.8224 3.4803 -1.0153
C -1.2668 3.9483 -1.2045
H -2.0940 3.7549 -1.9022
H -1.5541 3.5002 -0.2446
C -1.0892 5.4617 -1.0571
H -2.0234 5.9069 -0.6972
H -0.3287 5.6632 -0.2889
C -0.6644 6.1027 -2.3769
H -0.4953 7.1758 -2.2390
H -1.4808 6.0083 -3.1065
C 0.5930 5.4396 -2.9339
H 1.4417 5.6388 -2.2643
H 0.8565 5.8707 -3.9059
C 0.4166 3.9235 -3.0825
H -0.3625 3.7313 -3.8329
H 1.3450 3.4886 -3.4716
C 3.0805 -0.6732 -3.3167
H 3.7779 0.1573 -3.1981
H 2.7475 -0.7358 -4.3540
C -2.3376 -0.3097 -4.7034
H -2.0075 0.4277 -5.4405
H -3.4049 -0.1342 -4.4908
P -2.0587 -0.1393 1.4059
P 0.6036 1.0271 1.8683
N -1.6591 1.9108 3.2102
N -0.1269 -1.3968 3.0015
C -2.6281 1.4226 2.2517
H -2.8791 2.1721 1.4777
H -3.5519 1.1900 2.7925
C -0.4432 2.3894 2.5963
H 0.1645 2.8705 3.3716
H -0.6180 3.1444 1.8048
C -1.5619 -1.1857 2.8764
H -2.0130 -0.7507 3.7858
H -2.0140 -2.1716 2.7232
C 0.6540 -0.2003 3.2681
H 1.6973 -0.5106 3.3881
H 0.3494 0.3181 4.1944
C -3.6869 -0.8691 0.8381
H -3.4019 -1.7313 0.2146
C -4.6116 -1.3846 1.9529
H -4.1029 -2.1182 2.5870
H -4.9057 -0.5519 2.6064
C -5.8733 -2.0201 1.3568
H -5.5890 -2.9202 0.7930
H -6.5261 -2.3575 2.1691
C -6.6189 -1.0560 0.4372
H -7.4841 -1.5546 -0.0122
H -7.0154 -0.2194 1.0292
C -5.6994 -0.5087 -0.6527
H -6.2289 0.2278 -1.2676
H -5.4017 -1.3256 -1.3268
C -4.4474 0.1317 -0.0480
H -4.7535 0.9933 0.5607
H -3.7956 0.5281 -0.8372
C 2.2360 1.9403 1.8359
H 1.9253 2.9628 1.5624
C 3.2206 1.4608 0.7680
H 3.5178 0.4229 0.9653
H 2.7213 1.4558 -0.2103
C 4.4617 2.3571 0.7218
H 5.1674 1.9716 -0.0240
H 4.1680 3.3625 0.3857
C 5.1361 2.4617 2.0892
H 5.9890 3.1467 2.0370
H 5.5409 1.4792 2.3725
C 4.1485 2.9279 3.1568
H 3.8282 3.9572 2.9413
H 4.6289 2.9510 4.1413
C 2.9202 2.0151 3.2123
H 3.2443 1.0092 3.5131
H 2.2262 2.3674 3.9854

C	-2.2428	2.9065	4.1043
H	-2.5677	3.8192	3.5763
H	-1.5103	3.1885	4.8659
C	0.1423	-2.4085	4.0204
H	-0.3764	-3.3365	3.7613
H	-0.1816	-2.1027	5.0298
H	1.2157	-2.6184	4.0544
H	-3.1086	2.4751	4.6145
H	-2.2325	-1.3029	-5.1493
H	3.5600	-1.6015	-3.0088
H	2.2666	-0.4796	-1.4600
H	1.1392	-0.4568	0.2264
O	3.3110	-1.7403	-0.5214
H	4.2794	-1.9171	-0.4616
H	2.9370	-2.0166	0.3208
N	6.0166	-2.3100	-0.3575
C	7.1138	-2.6680	-0.2677
C	8.4898	-3.1177	-0.1555
H	9.1650	-2.2577	-0.1227
H	8.6183	-3.7041	0.7590
H	8.7515	-3.7413	-1.0153

ee^{2+}:H_2O:S --> eNiH^{2+}: H_2O:S

Ni	0.1176	0.0235	-0.0011
P	0.8727	2.0151	0.3738
P	-1.2146	0.3727	1.7706
N	1.0811	1.3597	3.1517
N	-1.4655	3.1063	1.3839
C	1.4205	2.3986	2.1339
H	2.5081	2.5007	2.1498
H	0.9688	3.3347	2.4738
C	-0.3842	1.0963	3.3000
H	-0.8553	2.0434	3.5730
H	-0.4776	0.3795	4.1180
C	-0.5430	3.2371	0.2683
H	-0.1380	4.2532	0.2946
H	-1.0300	3.1002	-0.7144
C	-2.2567	1.8844	1.3808
H	-2.7740	1.7195	0.4227
H	-3.0221	1.9843	2.1565
C	2.2605	2.8395	-0.5756
H	1.9123	2.7991	-1.6198
C	2.5490	4.3076	-0.2237
H	1.6562	4.9293	-0.3498
H	2.8458	4.3879	0.8321
C	3.6774	4.8724	-1.0944
H	3.3416	4.9054	-2.1403
H	3.8754	5.9087	-0.8005
C	4.9473	4.0326	-0.9915
H	5.7227	4.4363	-1.6506
H	5.3466	4.0932	0.0309
C	4.6657	2.5734	-1.3415
H	5.5701	1.9663	-1.2210
H	4.3800	2.5061	-2.4010
C	3.5420	1.9964	-0.4753
H	3.8898	1.9760	0.5686
H	3.3314	0.9546	-0.7467
C	-2.3427	-0.8387	2.6538
H	-1.6121	-1.4600	3.1978
C	-3.0950	-1.7628	1.6920
H	-3.8157	-1.1777	1.1034
H	-2.3906	-2.2106	0.9816
C	-3.8434	-2.8565	2.4601
H	-4.3971	-3.4877	1.7559
H	-3.1113	-3.5093	2.9567
C	-4.7881	-2.2652	3.5046
H	-5.2709	-3.0668	4.0733
H	-5.5937	-1.7148	2.9984
C	-4.0473	-1.3218	4.4497
H	-3.3235	-1.8917	5.0490
H	-4.7448	-0.8614	5.1578
C	-3.3096	-0.2231	3.6759
H	-4.0532	0.3925	3.1516
H	-2.7884	0.4393	4.3788
C	1.6784	1.7093	4.4741
H	1.4975	0.8881	5.1692
H	1.2160	2.6245	4.8481
C	-2.3270	4.2853	1.4910
H	-2.9455	4.2075	2.3894
H	-2.9925	4.4083	0.6208
P	-1.2288	-0.3635	-1.7874
P	1.1424	-1.9373	-0.5150
N	-0.8041	-3.0955	-2.1273
N	1.3583	-0.2580	-2.6734
C	-1.8614	-2.1077	-2.0165
H	-2.5711	-2.3352	-1.2020
H	-2.4316	-2.1231	-2.9520
C	-0.0690	-3.3178	-0.8946
H	0.4988	-4.2447	-1.0110
H	-0.7270	-3.4501	-0.0170
C	-0.0066	-0.2554	-3.2077
H	-0.1598	-1.0593	-3.9358
H	-0.1578	0.7050	-3.7076
C	1.8242	-1.5759	-2.2306
H	2.9142	-1.5412	-2.1623
H	1.5315	-2.3651	-2.9303
C	-2.6978	0.6342	-2.4087
H	-2.4466	1.6746	-2.1493
C	-2.9502	0.5727	-3.9251
H	-2.0616	0.8685	-4.4929
H	-3.1858	-0.4592	-4.2207
C	-4.1180	1.4849	-4.3205
H	-3.8362	2.5298	-4.1281
H	-4.2889	1.4039	-5.3995
C	-5.3918	1.1494	-3.5496
H	-6.1901	1.8504	-3.8154
H	-5.7449	0.1508	-3.8425
C	-5.1451	1.1749	-2.0431
H	-6.0481	0.8735	-1.5006
H	-4.9147	2.2019	-1.7243
C	-3.9851	0.2531	-1.6578
H	-4.2587	-0.7803	-1.9100
H	-3.8293	0.2733	-0.5725
C	2.5849	-2.8769	0.2569
H	2.1585	-3.3236	1.1709
C	3.7098	-1.9120	0.6649
H	4.1528	-1.4725	-0.2405
H	3.3123	-1.0709	1.2464
C	4.8111	-2.6367	1.4445
H	5.6058	-1.9294	1.7078
H	4.4000	-3.0120	2.3949
C	5.3785	-3.8083	0.6459
H	6.1225	-4.3474	1.2415
H	5.9079	-3.4207	-0.2358
C	4.2712	-4.7586	0.1971
H	3.8264	-5.2486	1.0746
H	4.6836	-5.5586	-0.4271
C	3.1701	-4.0269	-0.5796
H	3.5955	-3.6259	-1.5101
H	2.3987	-4.7475	-0.8708
C	-1.3230	-4.3510	-2.6706
H	-2.0672	-4.8287	-2.0116
H	-0.4984	-5.0519	-2.8273
C	2.3091	0.4157	-3.5660
H	1.9639	1.4344	-3.7610
H	2.4076	-0.1104	-4.5239
H	3.2897	0.4610	-3.0875
H	-1.7920	-4.1629	-3.6405
H	-1.7101	5.1837	1.5826
H	2.7526	1.8594	4.3532
H	1.4811	0.4282	2.8874
H	1.0189	0.2757	-1.3291
O	1.3763	-1.2848	2.9200
H	2.1015	-1.9046	3.0645
H	1.1148	-1.3639	1.9799
N	2.8687	-3.1801	4.9511
C	2.9747	-3.8384	5.8975
C	3.1082	-4.6650	7.0837
H	3.6219	-5.5974	6.8320
H	3.6874	-4.1372	7.8467
H	2.1209	-4.9035	7.4893

eNiH^{2+}:H_2O:S

Ni	-0.2340	0.0675	0.1254
P	-0.4534	-1.5473	-1.3138
P	-0.1742	1.4244	-1.7021
N	1.9029	-0.4464	-2.4288

N	-1.4888	-0.2242	-3.5105
C	0.9742	-1.6143	-2.5196
H	1.5867	-2.4894	-2.2962
H	0.5978	-1.6580	-3.5441
C	1.3002	0.8912	-2.7445
H	1.0335	0.8701	-3.8047
H	2.1045	1.6175	-2.6014
C	-1.8256	-1.2642	-2.5513
H	-1.9716	-2.1955	-3.1076
H	-2.7596	-1.0615	-2.0014
C	-1.5216	1.1240	-2.9643
H	-2.4891	1.3666	-2.4903
H	-1.3852	1.8229	-3.7966
C	-0.6493	-3.3225	-0.7828
H	-1.6404	-3.3299	-0.3004
C	-0.6606	-4.3608	-1.9155
H	-1.4294	-4.1343	-2.6629
H	0.3064	-4.3484	-2.4382
C	-0.8977	-5.7685	-1.3563
H	-1.9077	-5.8185	-0.9262
H	-0.8746	-6.4920	-2.1784
C	0.1316	-6.1330	-0.2895
H	-0.0853	-7.1255	0.1193
H	1.1278	-6.1971	-0.7500
C	0.1565	-5.0931	0.8284
H	0.9312	-5.3385	1.5639
H	-0.8022	-5.1142	1.3668
C	0.3950	-3.6809	0.2861
H	1.3978	-3.6379	-0.1659
H	0.3684	-2.9395	1.0953
C	0.0189	3.2859	-1.7475
H	0.8243	3.4776	-1.0199
C	-1.2647	3.9444	-1.2135
H	-2.0906	3.7495	-1.9124
H	-1.5537	3.4976	-0.2534
C	-1.0879	5.4581	-1.0682
H	-2.0229	5.9035	-0.7106
H	-0.3288	5.6610	-0.2990
C	-0.6611	6.0971	-2.3883
H	-0.4926	7.1704	-2.2518
H	-1.4763	6.0012	-3.1192
C	0.5975	5.4335	-2.9421
H	1.4450	5.6340	-2.2715
H	0.8624	5.8630	-3.9144
C	0.4219	3.9170	-3.0885
H	-0.3558	3.7232	-3.8399
H	1.3512	3.4817	-3.4753
C	3.0886	-0.6803	-3.3071
H	3.7856	0.1506	-3.1888
H	2.7578	-0.7451	-4.3451
C	-2.3256	-0.3212	-4.7075
H	-1.9938	0.4146	-5.4455
H	-3.3935	-0.1454	-4.4982
P	-2.0629	-0.1368	1.4017
P	0.5979	1.0315	1.8687
N	-1.6687	1.9178	3.2023
N	-0.1351	-1.3900	3.0057
C	-2.6349	1.4270	2.2422
H	-2.8837	2.1745	1.4656
H	-3.5602	1.1957	2.7809
C	-0.4513	2.3952	2.5906
H	0.1541	2.8782	3.3665
H	-0.6240	3.1484	1.7970
C	-1.5698	-1.1796	2.8762
H	-2.0235	-0.7423	3.7833
H	-2.0213	-2.1659	2.7242
C	0.6447	-0.1926	3.2716
H	1.6878	-0.5023	3.3953
H	0.3375	0.3279	4.1958
C	-3.6893	-0.8682	0.8314
H	-3.4025	-1.7306	0.2088
C	-4.6157	-1.3838	1.9448
H	-4.1074	-2.1166	2.5803
H	-4.9116	-0.5510	2.5973
C	-5.8757	-2.0209	1.3468
H	-5.5895	-2.9210	0.7840
H	-6.5296	-2.3584	2.1581
C	-6.6204	-1.0580	0.4252
H	-7.4843	-1.5577	-0.0255
H	-7.0188	-0.2214	1.0160
C	-5.6993	-0.5104	-0.6633
H	-6.2284	0.2252	-1.2795
H	-5.3997	-1.3274	-1.3364
C	-4.4492	0.1315	-0.0566
H	-4.7573	0.9930	0.5512
H	-3.7963	0.5282	-0.8447
C	2.2301	1.9451	1.8389
H	1.9200	2.9668	1.5623
C	3.2178	1.4637	0.7750
H	3.5148	0.4264	0.9754
H	2.7213	1.4563	-0.2046
C	4.4588	2.3603	0.7304
H	5.1667	1.9735	-0.0125
H	4.1657	3.3648	0.3913
C	5.1293	2.4682	2.0993
H	5.9821	3.1534	2.0480
H	5.5335	1.4866	2.3858
C	4.1385	2.9363	3.1629
H	3.8186	3.9648	2.9443
H	4.6161	2.9618	4.1486
C	2.9104	2.0231	3.2169
H	3.2339	1.0181	3.5207
H	2.2141	2.3767	3.9871
C	-2.2553	2.9155	4.0922
H	-2.5788	3.8269	3.5610
H	-1.5250	3.1997	4.8551
C	0.1316	-2.3992	4.0277
H	-0.3861	-3.3279	3.7693
H	-0.1951	-2.0911	5.0355
H	1.2050	-2.6087	4.0651
H	-3.1224	2.4853	4.6010
H	-2.2192	-1.3153	-5.1510
H	3.5675	-1.6078	-2.9963
H	2.2706	-0.4829	-1.4526
H	1.1384	-0.4564	0.2317
O	3.3172	-1.7391	-0.5103
H	4.2859	-1.9141	-0.4530
H	2.9460	-2.0145	0.3331
N	6.0247	-2.3048	-0.3554
C	7.1216	-2.6640	-0.2667
C	8.4973	-3.1149	-0.1561
H	9.1733	-2.2553	-0.1241
H	8.6264	-3.7016	0.7582
H	8.7576	-3.7388	-1.0165

eNiH^{2+}:H$_2$O:B:2S

Ni	1.3147	-0.0398	-0.3194
P	0.8401	-0.8034	1.8320
P	1.1906	1.9502	0.5902
N	-1.3192	1.0989	1.7766
N	1.8659	1.4034	3.2058
C	-0.7301	-0.0532	2.5239
H	-1.5080	-0.8213	2.5363
H	-0.5593	0.2867	3.5490
C	-0.4222	2.2586	1.5014
H	-0.1977	2.7296	2.4611
H	-1.0229	2.9403	0.8939
C	2.0418	-0.0333	3.0531
H	1.8745	-0.4861	4.0346
H	3.0662	-0.3073	2.7427
C	2.3126	2.1937	2.0686
H	3.3529	1.9740	1.7817
H	2.2696	3.2494	2.3575
C	0.6874	-2.5580	2.4775
H	1.6985	-2.9656	2.3230
C	0.3114	-2.7171	3.9583
H	1.0170	-2.1919	4.6118
H	-0.6784	-2.2745	4.1407
C	0.2640	-4.1956	4.3594
H	1.2736	-4.6227	4.2812
H	-0.0270	-4.2769	5.4126
C	-0.6945	-4.9867	3.4735
H	-0.6870	-6.0446	3.7572
H	-1.7214	-4.6281	3.6347
C	-0.3260	-4.8311	2.0003
H	-1.0425	-5.3656	1.3654
H	0.6555	-5.2930	1.8232
C	-0.2663	-3.3595	1.5811

H	-1.2796	-2.9334	1.6403
H	0.0619	-3.2690	0.5408
C	1.2295	3.5275	-0.4165
H	0.2825	3.4461	-0.9758
C	2.3592	3.5540	-1.4511
H	3.3283	3.6196	-0.9377
H	2.3608	2.6193	-2.0252
C	2.2094	4.7591	-2.3841
H	3.0382	4.7753	-3.1008
H	1.2881	4.6442	-2.9731
C	2.1548	6.0701	-1.6014
H	1.9986	6.9120	-2.2842
H	3.1239	6.2427	-1.1123
C	1.0535	6.0398	-0.5434
H	0.0713	5.9939	-1.0347
H	1.0638	6.9619	0.0481
C	1.2050	4.8335	0.3905
H	2.1465	4.9362	0.9473
H	0.3957	4.8353	1.1315
C	-2.5150	1.5951	2.5255
H	-3.0065	2.3640	1.9306
H	-2.1917	2.0030	3.4854
C	2.4866	1.8805	4.4415
H	2.2647	2.9429	4.5778
H	3.5820	1.7519	4.4483
P	3.4785	-0.5763	-0.6813
P	0.9654	-1.2768	-2.0757
N	3.3216	-0.8958	-3.4404
N	2.4409	-3.1889	-0.7154
C	4.0052	-0.1334	-2.4173
H	3.8801	0.9579	-2.5440
H	5.0761	-0.3502	-2.4980
C	1.9063	-0.6057	-3.5397
H	1.5292	-1.0951	-4.4423
H	1.6836	0.4742	-3.6307
C	3.6812	-2.4339	-0.6786
H	4.3725	-2.7065	-1.4973
H	4.1777	-2.6851	0.2647
C	1.6647	-2.9992	-1.9284
H	0.8133	-3.6872	-1.8886
H	2.2374	-3.2212	-2.8459
C	4.9817	0.0059	0.2881
H	4.6748	-0.0566	1.3427
C	6.2481	-0.8526	0.1201
H	6.0584	-1.9027	0.3622
H	6.5808	-0.8245	-0.9268
C	7.3769	-0.3326	1.0187
H	7.0861	-0.4659	2.0705
H	8.2708	-0.9470	0.8650
C	7.6878	1.1387	0.7583
H	8.4584	1.4916	1.4519
H	8.1039	1.2514	-0.2526
C	6.4302	1.9957	0.8820
H	6.6499	3.0395	0.6306
H	6.0816	1.9899	1.9254
C	5.3163	1.4723	-0.0282
H	5.6511	1.5506	-1.0711
H	4.4256	2.1051	0.0538
C	-0.7533	-1.5262	-2.7550
H	-1.0676	-0.5073	-3.0368
C	-1.7139	-2.0498	-1.6786
H	-1.3912	-3.0520	-1.3630
H	-1.6763	-1.4101	-0.7900
C	-3.1468	-2.1343	-2.2084
H	-3.8110	-2.5215	-1.4286
H	-3.5107	-1.1224	-2.4396
C	-3.2321	-2.9960	-3.4650
H	-4.2572	-2.9985	-3.8510
H	-2.9898	-4.0376	-3.2099
C	-2.2649	-2.4988	-4.5355
H	-2.5796	-1.5040	-4.8817
H	-2.2889	-3.1545	-5.4128
C	-0.8281	-2.4141	-4.0085
H	-0.4782	-3.4264	-3.7630
H	-0.1780	-2.0406	-4.8063
C	3.9894	-0.7632	-4.7317
H	3.9726	0.2697	-5.1200
H	3.5050	-1.4162	-5.4631
C	2.7219	-4.6078	-0.5134
H	3.2438	-4.7475	0.4383
H	3.3452	-5.0421	-1.3141
H	1.7816	-5.1654	-0.4705
H	5.0320	-1.0799	-4.6375
H	2.0713	1.3370	5.2948
H	-3.2132	0.7702	2.6798
H	-1.7251	0.8032	0.8315
H	-0.0362	0.3460	-0.6806
O	-2.6813	0.9730	-0.4348
H	-2.3806	0.7303	-1.3148
H	-3.7057	0.8727	-0.4257
N	-5.3208	0.7732	-0.2964
C	-5.6131	0.7667	1.0911
H	-5.7120	1.5975	-0.7608
H	-5.6696	-0.0738	-0.7538
C	-5.5407	-0.4287	1.8165
C	-5.8952	1.9595	1.7655
C	-5.7453	-0.4249	3.1948
H	-5.3515	-1.3604	1.2893
C	-6.0910	1.9546	3.1447
H	-5.9779	2.8837	1.1996
C	-6.0121	0.7663	3.8692
H	-5.7096	-1.3624	3.7430
H	-6.3241	2.8858	3.6537
H	-6.1803	0.7648	4.9418
N	-6.4305	3.3835	-1.5199
C	-6.9985	4.3247	-1.8884
C	-7.7117	5.5049	-2.3498
H	-7.1804	5.9632	-3.1887
H	-8.7192	5.2314	-2.6776
H	-7.7922	6.2368	-1.5404
N	-6.5932	-1.8536	-1.3425
C	-7.3774	-2.6858	-1.5389
C	-8.3655	-3.7256	-1.7801
H	-7.9920	-4.4491	-2.5136
H	-8.5841	-4.2494	-0.8483
H	-9.2913	-3.2846	-2.1632

NiH^+: H_2O:BH^+:3S

Ni	1.3223	-0.0342	-0.2521
P	1.2775	-0.8741	1.9237
P	0.8544	1.8760	0.7423
N	-1.2356	0.4641	2.0983
N	2.0056	1.4979	3.2221
C	-0.3450	-0.4935	2.7722
H	-0.8964	-1.4374	2.8433
H	-0.1308	-0.1557	3.7987
C	-0.6525	1.7883	1.8607
H	-0.3846	2.2740	2.8109
H	-1.4331	2.3893	1.3804
C	2.4331	0.1244	3.0157
H	2.4710	-0.3506	4.0004
H	3.4508	0.0536	2.5869
C	2.1036	2.3536	2.0524
H	3.1136	2.3563	1.6115
H	1.8847	3.3780	2.3720
C	1.6182	-2.6155	2.5352
H	2.6812	-2.7659	2.2891
C	1.4224	-2.8602	4.0393
H	2.0303	-2.1758	4.6414
H	0.3740	-2.6719	4.3107
C	1.7728	-4.3038	4.4161
H	2.8452	-4.4718	4.2431
H	1.6045	-4.4512	5.4889
C	0.9624	-5.3086	3.6019
H	1.2526	-6.3321	3.8637
H	-0.1026	-5.2111	3.8575
C	1.1500	-5.0702	2.1058
H	0.5323	-5.7657	1.5250
H	2.1951	-5.2792	1.8363
C	0.8131	-3.6295	1.7124
H	-0.2633	-3.4606	1.8686
H	1.0165	-3.4650	0.6497
C	0.4379	3.4423	-0.1985
H	-0.5232	3.1638	-0.6632
C	1.4141	3.7452	-1.3387
H	2.3921	4.0206	-0.9208
H	1.5675	2.8452	-1.9470
C	0.9032	4.9012	-2.2029

H	1.6267	5.1183	-2.9970
H	-0.0265	4.5919	-2.7027
C	0.6395	6.1517	-1.3653
H	0.2292	6.9499	-1.9935
H	1.5919	6.5290	-0.9671
C	-0.3078	5.8530	-0.2047
H	-1.3013	5.5940	-0.5986
H	-0.4419	6.7438	0.4193
C	0.2079	4.6956	0.6578
H	1.1566	5.0001	1.1205
H	-0.4942	4.4984	1.4771
C	-2.4340	0.6280	2.9330
H	-3.1411	1.3027	2.4409
H	-2.1929	1.0410	3.9249
C	2.6930	2.0972	4.3618
H	2.2851	3.0939	4.5552
H	3.7818	2.1934	4.2063
P	3.4763	-0.0725	-0.9036
P	1.0286	-1.3191	-1.9777
N	3.0339	-0.4246	-3.6310
N	3.0609	-2.8551	-0.8906
C	3.6603	0.4720	-2.6814
H	3.2823	1.5082	-2.7627
H	4.7324	0.4983	-2.9071
C	1.5883	-0.4675	-3.5407
H	1.2204	-1.0390	-4.3981
H	1.1172	0.5331	-3.5804
C	4.0910	-1.8363	-0.9830
H	4.7185	-1.9430	-1.8873
H	4.7449	-1.9688	-0.1146
C	2.1066	-2.8420	-1.9846
H	1.4439	-3.7044	-1.8550
H	2.5848	-2.9280	-2.9762
C	4.9303	0.8283	-0.1199
H	4.7790	0.7063	0.9632
C	6.3222	0.2701	-0.4644
H	6.4005	-0.7948	-0.2253
H	6.5048	0.3657	-1.5439
C	7.4145	1.0303	0.2978
H	7.2951	0.8417	1.3743
H	8.3948	0.6275	0.0199
C	7.3596	2.5328	0.0353
H	8.1159	3.0501	0.6355
H	7.6092	2.7295	-1.0168
C	5.9706	3.0913	0.3348
H	5.9223	4.1570	0.0829
H	5.7664	3.0133	1.4129
C	4.8929	2.3306	-0.4412
H	5.0674	2.4758	-1.5158
H	3.9030	2.7504	-0.2330
C	-0.6693	-1.9607	-2.4104
H	-1.2583	-1.0465	-2.5904
C	-1.2950	-2.7034	-1.2219
H	-0.6947	-3.5967	-0.9995
H	-1.2703	-2.0714	-0.3284
C	-2.7308	-3.1340	-1.5247
H	-3.1338	-3.6881	-0.6691
H	-3.3538	-2.2352	-1.6305
C	-2.8103	-3.9781	-2.7943
H	-3.8523	-4.2317	-3.0203
H	-2.2885	-4.9317	-2.6315
C	-2.1754	-3.2517	-3.9772
H	-2.7668	-2.3567	-4.2196
H	-2.1891	-3.8846	-4.8715
C	-0.7333	-2.8292	-3.6766
H	-0.1201	-3.7302	-3.5377
H	-0.3267	-2.3026	-4.5466
C	3.4771	-0.1422	-4.9917
H	3.1761	0.8604	-5.3428
H	3.0604	-0.8877	-5.6752
C	3.6773	-4.1724	-0.7712
H	4.3380	-4.1913	0.1010
H	4.2711	-4.4534	-1.6586
H	2.9005	-4.9289	-0.6247
H	4.5675	-0.2120	-5.0428
H	2.5269	1.4860	5.2536
H	-2.9168	-0.3442	3.0700
H	-2.1095	0.1506	0.6301
H	-0.1172	-0.0198	-0.3630
O	-2.7528	0.1875	-0.1409
H	-2.2178	0.4321	-0.9027
H	-4.3897	0.4989	-0.0823
N	-5.4374	0.6327	-0.0146
C	-6.1263	-0.6523	0.1054
H	-5.6359	1.2375	0.8058
H	-5.7678	1.1397	-0.8636
C	-6.3159	-1.4226	-1.0365
C	-6.5688	-1.0780	1.3516
C	-6.9626	-2.6503	-0.9215
H	-5.9777	-1.0631	-2.0040
C	-7.2133	-2.3090	1.4542
H	-6.4233	-0.4541	2.2287
C	-7.4094	-3.0948	0.3213
H	-7.1242	-3.2562	-1.8075
H	-7.5683	-2.6489	2.4220
H	-7.9171	-4.0504	0.4052
N	-6.0868	2.3439	2.2626
C	-6.5887	3.0461	3.0238
C	-7.2271	3.9288	3.9833
H	-6.5735	4.0836	4.8465
H	-7.4381	4.8968	3.5197
H	-8.1681	3.4888	4.3265
N	-6.5081	1.9479	-2.3428
C	-7.1411	2.4655	-3.1501
C	-7.9429	3.1136	-4.1720
H	-8.0155	2.4715	-5.0546
H	-8.9503	3.3047	-3.7908
H	-7.4871	4.0647	-4.4616

ex^{2+}

Ni	-0.0250	-0.0198	-0.0701
P	-0.6994	1.5225	-1.4620
P	1.2260	-0.8389	-1.6647
N	-1.3168	-0.8147	-2.8058
N	1.4474	1.4418	-3.2327
C	-1.4762	0.6710	-2.9532
H	-2.5501	0.8712	-2.9754
H	-1.0195	0.9705	-3.8984
C	0.0747	-1.3005	-3.0898
H	0.3902	-0.8826	-4.0480
H	0.0130	-2.3893	-3.1648
C	0.7513	2.3404	-2.3253
H	0.3822	3.1843	-2.9152
H	1.4147	2.7530	-1.5427
C	2.2594	0.4334	-2.5701
H	2.9719	0.8747	-1.8498
H	2.8490	-0.0750	-3.3397
C	-1.8636	2.9685	-1.1964
H	-1.2815	3.6358	-0.5392
C	-2.2665	3.7642	-2.4474
H	-1.3889	4.1215	-2.9970
H	-2.8259	3.1130	-3.1350
C	-3.1517	4.9596	-2.0778
H	-2.5660	5.6674	-1.4748
H	-3.4407	5.4938	-2.9895
C	-4.3890	4.5234	-1.2974
H	-4.9822	5.3973	-1.0083
H	-5.0330	3.9117	-1.9454
C	-4.0023	3.7163	-0.0598
H	-4.8982	3.3631	0.4638
H	-3.4627	4.3656	0.6445
C	-3.1116	2.5243	-0.4212
H	-3.6928	1.8194	-1.0365
H	-2.8138	1.9751	0.4807
C	2.3386	-2.3483	-1.6427
H	1.6770	-3.1368	-1.2464
C	3.4832	-2.1536	-0.6374
H	4.1451	-1.3493	-0.9897
H	3.0814	-1.8249	0.3302
C	4.3015	-3.4370	-0.4706
H	5.1286	-3.2607	0.2266
H	3.6665	-4.2123	-0.0172
C	4.8328	-3.9398	-1.8118
H	5.3699	-4.8842	-1.6748
H	5.5646	-3.2207	-2.2057
C	3.7023	-4.1175	-2.8229
H	3.0327	-4.9232	-2.4901
H	4.1025	-4.4274	-3.7944

C	2.8938	-2.8261	-2.9926
H	3.5524	-2.0563	-3.4168
H	2.0906	-2.9894	-3.7219
C	-2.3412	-1.5695	-3.5746
H	-2.2310	-2.6357	-3.3695
H	-2.1984	-1.3830	-4.6405
C	2.2464	2.1915	-4.2030
H	3.0587	2.7697	-3.7319
H	1.6030	2.8846	-4.7522
P	0.8745	0.8027	1.7102
P	-1.2097	-1.2876	1.1913
N	0.6208	-1.4666	3.3680
N	-1.2617	0.3342	3.4980
C	1.6390	-0.5076	2.8321
H	2.3951	-1.0742	2.2813
H	2.1151	-0.0501	3.7055
C	-0.0919	-2.2990	2.3427
H	-0.6744	-3.0271	2.9125
H	0.6540	-2.8360	1.7482
C	-0.4280	1.4137	2.9281
H	0.0580	1.9073	3.7747
H	-1.0479	2.1656	2.4147
C	-2.1440	-0.3466	2.5306
H	-2.8120	0.3734	2.0344
H	-2.7710	-1.0384	3.1043
C	2.1974	2.1341	1.7929
H	1.8372	2.8770	1.0642
C	2.4244	2.8534	3.1291
H	1.5023	3.3265	3.4847
H	2.7341	2.1314	3.8993
C	3.5074	3.9318	2.9929
H	3.1370	4.7233	2.3265
H	3.6733	4.4017	3.9684
C	4.8138	3.3708	2.4377
H	5.5451	4.1760	2.3111
H	5.2491	2.6671	3.1614
C	4.5820	2.6523	1.1106
H	5.5153	2.2105	0.7435
H	4.2566	3.3771	0.3508
C	3.5195	1.5607	1.2547
H	3.8978	0.7986	1.9518
H	3.3510	1.0550	0.2958
C	-2.4987	-2.5764	0.7036
H	-2.0112	-3.1158	-0.1250
C	-3.7243	-1.8416	0.1315
H	-4.2211	-1.2839	0.9377
H	-3.4140	-1.0884	-0.6078
C	-4.7343	-2.8179	-0.4757
H	-5.5992	-2.2642	-0.8587
H	-4.2784	-3.3297	-1.3363
C	-5.1762	-3.8558	0.5535
H	-5.8658	-4.5733	0.0969
H	-5.7355	-3.3549	1.3560
C	-3.9738	-4.5856	1.1452
H	-3.4879	-5.1850	0.3624
H	-4.2952	-5.2912	1.9189
C	-2.9425	-3.6174	1.7403
H	-3.3847	-3.1158	2.6131
H	-2.0898	-4.2027	2.1028
C	1.2044	-2.3210	4.4337
H	0.4179	-2.9354	4.8755
H	1.6443	-1.6850	5.2040
C	-2.0531	0.8498	4.6252
H	-1.3865	1.2835	5.3750
H	-2.6102	0.0308	5.0877
H	-2.7658	1.6207	4.2991
H	1.9763	-2.9646	4.0042
H	2.6904	1.4999	-4.9247
H	-3.3351	-1.2364	-3.2716
H	-0.1661	-0.8044	3.7509
H	-1.4215	-0.9678	-1.7675

ex^{2+}:B:2S

Ni	-1.4740	-0.0074	-0.0088
P	-3.3022	-0.6795	0.9594
P	-2.6990	1.1229	-1.4087
N	-3.6493	-1.4803	-1.6615
N	-5.0258	1.3301	0.0948
C	-4.3383	-1.5860	-0.3321
H	-4.3880	-2.6497	-0.0877
H	-5.3446	-1.1755	-0.4350
C	-3.7914	-0.1335	-2.3070
H	-4.8500	0.1346	-2.3040
H	-3.4417	-0.2453	-3.3369
C	-4.4854	0.7347	1.3089
H	-5.3302	0.3545	1.8908
H	-3.9545	1.4675	1.9430
C	-4.0781	2.1420	-0.6539
H	-3.6255	2.9386	-0.0367
H	-4.6333	2.6343	-1.4592
C	-3.5303	-1.7731	2.4658
H	-3.1778	-1.1330	3.2914
C	-4.9629	-2.2231	2.7886
H	-5.6393	-1.3673	2.8904
H	-5.3527	-2.8368	1.9630
C	-5.0026	-3.0542	4.0761
H	-4.7149	-2.4164	4.9237
H	-6.0309	-3.3803	4.2680
C	-4.0643	-4.2560	4.0003
H	-4.0801	-4.8089	4.9457
H	-4.4233	-4.9513	3.2278
C	-2.6392	-3.8202	3.6665
H	-1.9842	-4.6932	3.5635
H	-2.2366	-3.2226	4.4969
C	-2.5928	-2.9856	2.3843
H	-2.8915	-3.6215	1.5357
H	-1.5694	-2.6516	2.1754
C	-2.1558	2.1825	-2.8584
H	-1.4623	1.5185	-3.4015
C	-1.3460	3.3863	-2.3543
H	-2.0050	4.0541	-1.7809
H	-0.5670	3.0477	-1.6585
C	-0.7308	4.1692	-3.5172
H	-0.1870	5.0400	-3.1327
H	0.0090	3.5345	-4.0278
C	-1.7957	4.6078	-4.5213
H	-1.3281	5.1210	-5.3685
H	-2.4634	5.3391	-4.0447
C	-2.6175	3.4179	-5.0128
H	-1.9749	2.7413	-5.5940
H	-3.4092	3.7541	-5.6913
C	-3.2383	2.6449	-3.8436
H	-3.9509	3.3042	-3.3302
H	-3.8169	1.7961	-4.2292
C	-4.0247	-2.5844	-2.5806
H	-3.4346	-2.5067	-3.4954
H	-5.0869	-2.5071	-2.8200
C	-6.2396	2.0930	0.3823
H	-6.0549	2.9600	1.0390
H	-6.9760	1.4451	0.8665
P	-0.0625	0.9394	1.3325
P	0.1790	-1.1853	-0.7217
N	2.1684	0.9606	-0.5503
N	1.7890	-1.1233	1.5630
C	1.3873	1.7477	0.4633
H	0.9780	2.6233	-0.0493
H	2.1390	2.0967	1.1777
C	1.4961	-0.0488	-1.4375
H	2.3278	-0.6231	-1.8539
H	1.0106	0.4994	-2.2513
C	0.8517	-0.3300	2.3505
H	1.4347	0.1764	3.1258
H	0.0953	-0.9541	2.8629
C	1.1687	-2.0393	0.6130
H	0.4912	-2.7563	1.1131
H	1.9727	-2.6202	0.1464
C	-0.4447	2.2646	2.6100
H	-1.1292	1.7303	3.2902
C	0.7177	2.8163	3.4480
H	1.2953	2.0135	3.9197
H	1.4114	3.3702	2.7997
C	0.1990	3.7711	4.5294
H	-0.4282	3.2085	5.2352
H	1.0436	4.1619	5.1081
C	-0.6104	4.9164	3.9251
H	-1.0086	5.5589	4.7179
H	0.0524	5.5480	3.3163
C	-1.7469	4.3888	3.0516

H	-2.2813	5.2191	2.5755
H	-2.4796	3.8659	3.6832
C	-1.2323	3.4224	1.9816
H	-0.5813	3.9732	1.2859
H	-2.0627	3.0268	1.3866
C	0.1461	-2.5206	-2.0608
H	-0.5222	-2.0963	-2.8288
C	-0.5338	-3.7750	-1.4841
H	0.1078	-4.2059	-0.7036
H	-1.4769	-3.5102	-0.9832
C	-0.7663	-4.8395	-2.5582
H	-1.2390	-5.7212	-2.1098
H	-1.4667	-4.4546	-3.3146
C	0.5462	-5.2223	-3.2382
H	0.3646	-5.9574	-4.0295
H	1.2039	-5.7096	-2.5049
C	1.2414	-3.9904	-3.8103
H	0.6323	-3.5755	-4.6262
H	2.2050	-4.2635	-4.2543
C	1.4629	-2.9022	-2.7522
H	2.1892	-3.2601	-2.0096
H	1.9178	-2.0340	-3.2409
C	2.9033	1.9270	-1.4215
H	3.5452	1.3661	-2.1027
H	3.5229	2.5705	-0.7936
C	2.6630	-1.8751	2.4607
H	3.2086	-1.1891	3.1132
H	3.4025	-2.4337	1.8816
H	2.1016	-2.5895	3.0885
H	2.1781	2.5190	-1.9841
H	-6.6742	2.4575	-0.5531
H	-3.8245	-3.5405	-2.0943
H	2.9545	0.4473	-0.0318
H	-2.6228	-1.5148	-1.4005
N	4.7101	0.0908	0.2415
C	5.2422	-0.5998	-0.8801
H	5.1382	1.0124	0.3444
H	4.8857	-0.4291	1.1042
C	5.1026	-1.9892	-0.9798
C	5.8642	0.0955	-1.9239
C	5.5721	-2.6642	-2.1031
H	4.6543	-2.5413	-0.1574
C	6.3220	-0.5865	-3.0492
H	6.0170	1.1688	-1.8359
C	6.1757	-1.9678	-3.1486
H	5.4762	-3.7453	-2.1550
H	6.8121	-0.0328	-3.8449
H	6.5442	-2.4975	-4.0212
N	6.0041	-1.3946	2.6094
C	6.8998	-1.8523	3.1854
C	8.0238	-2.4255	3.9063
H	7.7414	-3.3877	4.3429
H	8.8660	-2.5812	3.2261
H	8.3388	-1.7535	4.7097
N	5.6161	3.1143	0.4312
C	6.4168	3.9326	0.6156
C	7.4203	4.9571	0.8482
H	7.2076	5.8390	0.2372
H	7.4228	5.2495	1.9022
H	8.4117	4.5772	0.5850

ex^{2+}:B:2S --> ex'^{2+}:B:2S

Ni	-0.8052	0.1217	0.1293
P	-2.3316	1.4771	-0.6320
P	-2.3365	-0.8201	1.3688
N	-2.5465	1.8595	2.1014
N	-4.5688	-0.0922	-0.1243
C	-3.1151	2.3924	0.8184
H	-2.8505	3.4515	0.7745
H	-4.2002	2.2780	0.8553
C	-3.0806	0.5111	2.4828
H	-4.1706	0.5526	2.4323
H	-2.7646	0.3341	3.5143
C	-3.8535	0.5510	-1.2162
H	-4.5414	1.2581	-1.6893
H	-3.5328	-0.1660	-1.9945
C	-3.8988	-1.2591	0.4286
H	-3.6387	-1.9996	-0.3488
H	-4.5978	-1.7439	1.1174
C	-2.1663	2.8506	-1.8951
H	-1.9599	2.3068	-2.8316
C	-3.4002	3.7373	-2.1177
H	-4.2761	3.1412	-2.3969
H	-3.6571	4.2570	-1.1829
C	-3.1370	4.7869	-3.2035
H	-2.9889	4.2783	-4.1665
H	-4.0236	5.4198	-3.3203
C	-1.9104	5.6361	-2.8808
H	-1.7219	6.3514	-3.6884
H	-2.1052	6.2318	-1.9774
C	-0.6808	4.7593	-2.6539
H	0.1842	5.3737	-2.3780
H	-0.4189	4.2533	-3.5947
C	-0.9325	3.7053	-1.5723
H	-1.0852	4.2184	-0.6096
H	-0.0577	3.0560	-1.4449
C	-2.1903	-2.2161	2.6168
H	-1.3830	-1.8650	3.2812
C	-1.7023	-3.5026	1.9359
H	-2.4734	-3.8628	1.2396
H	-0.8108	-3.2900	1.3314
C	-1.4045	-4.5983	2.9634
H	-1.0900	-5.5136	2.4487
H	-0.5583	-4.2822	3.5910
C	-2.6153	-4.8767	3.8523
H	-2.3626	-5.6252	4.6107
H	-3.4210	-5.3106	3.2437
C	-3.1172	-3.5977	4.5187
H	-2.3582	-3.2253	5.2214
H	-4.0158	-3.8017	5.1110
C	-3.4241	-2.5106	3.4825
H	-4.2488	-2.8602	2.8471
H	-3.7815	-1.6074	3.9926
C	-2.6582	2.8380	3.2150
H	-2.1481	2.4413	4.0945
H	-3.7132	3.0012	3.4421
C	-5.9376	-0.4240	-0.5205
H	-5.9787	-1.1673	-1.3343
H	-6.4537	0.4808	-0.8538
P	0.1435	-1.0318	-1.4262
P	1.1785	0.6020	0.8123
N	2.4593	-1.8853	0.0458
N	2.0428	1.0732	-1.8835
C	1.3105	-2.3603	-0.7849
H	0.7293	-3.0544	-0.1714
H	1.7533	-2.9234	-1.6133
C	2.1133	-0.9967	1.2012
H	3.0655	-0.7813	1.6923
H	1.4934	-1.5840	1.8861
C	1.3297	-0.0334	-2.4745
H	2.0096	-0.7328	-2.9960
H	0.6735	0.3703	-3.2629
C	2.3231	1.3195	-0.4896
H	2.2527	2.4016	-0.3156
H	3.3544	1.0426	-0.2028
C	-0.7165	-2.0405	-2.7628
H	-1.4980	-1.3437	-3.1060
C	0.1051	-2.4639	-3.9897
H	0.5811	-1.6012	-4.4676
H	0.9117	-3.1471	-3.6844
C	-0.7837	-3.1760	-5.0176
H	-1.5146	-2.4566	-5.4129
H	-0.1713	-3.4932	-5.8689
C	-1.5196	-4.3690	-4.4131
H	-2.1818	-4.8211	-5.1589
H	-0.7925	-5.1445	-4.1331
C	-2.3169	-3.9564	-3.1774
H	-2.7947	-4.8298	-2.7193
H	-3.1264	-3.2734	-3.4722
C	-1.4202	-3.2611	-2.1502
H	-0.6661	-3.9834	-1.8046
H	-1.9995	-2.9653	-1.2673
C	1.7643	1.5982	2.3111
H	1.3589	1.0273	3.1634
C	1.0963	2.9808	2.3164
H	1.4794	3.5753	1.4744
H	0.0159	2.8860	2.1459
C	1.3675	3.7340	3.6215

H	0.8942	4.7223	3.5854
H	0.9024	3.1897	4.4565
C	2.8662	3.8721	3.8809
H	3.0396	4.3585	4.8466
H	3.3069	4.5289	3.1180
C	3.5583	2.5123	3.8405
H	3.2118	1.8960	4.6822
H	4.6401	2.6302	3.9674
C	3.2764	1.7736	2.5264
H	3.6993	2.3563	1.6971
H	3.8067	0.8146	2.5365
C	3.2296	-3.0635	0.5461
H	4.1409	-2.7125	1.0325
H	3.4932	-3.6992	-0.3010
C	2.3661	2.1248	-2.8303
H	2.9268	1.7335	-3.6907
H	2.9941	2.8817	-2.3537
H	1.4666	2.6245	-3.2236
H	2.6135	-3.6255	1.2509
H	-6.4817	-0.8253	0.3393
H	-2.1960	3.7796	2.9145
H	3.1608	-1.3935	-0.6156
H	-1.5399	1.6641	1.8598
N	4.4339	-0.9255	-1.6645
C	5.6971	-0.8140	-0.9934
H	4.5103	-1.5482	-2.4651
H	4.0977	-0.0255	-2.0082
C	6.1370	0.4155	-0.5028
C	6.4694	-1.9592	-0.7876
C	7.3378	0.4940	0.1998
H	5.5609	1.3176	-0.6960
C	7.6716	-1.8709	-0.0916
H	6.1437	-2.9164	-1.1898
C	8.1075	-0.6465	0.4109
H	7.6798	1.4571	0.5662
H	8.2733	-2.7635	0.0502
H	9.0475	-0.5803	0.9487
N	4.7222	-2.4077	-4.0942
C	5.0655	-2.9466	-5.0599
C	5.4953	-3.6214	-6.2714
H	5.8428	-2.8867	-7.0039
H	6.3142	-4.3109	-6.0475
H	4.6643	-4.1860	-6.7030

ex$^{i\,2+}$:B:2S

Ni	-1.3952	0.0226	0.1001
P	-3.0473	0.9584	-0.9679
P	-2.8253	-1.3180	1.0431
N	-3.8264	1.1999	1.6725
N	-4.8706	-1.1379	-0.8386
C	-4.2843	1.6061	0.3014
H	-4.2927	2.6985	0.2844
H	-5.2941	1.2195	0.1512
C	-4.0679	-0.2469	1.9828
H	-5.1069	-0.4777	1.7386
H	-3.9047	-0.3648	3.0573
C	-4.1551	-0.3074	-1.7966
H	-4.9033	0.2130	-2.4019
H	-3.5281	-0.9003	-2.4878
C	-4.0402	-2.1115	-0.1462
H	-3.4722	-2.7502	-0.8460
H	-4.7084	-2.7676	0.4209
C	-3.0179	2.3617	-2.2078
H	-2.5004	1.9177	-3.0738
C	-4.3774	2.8962	-2.6805
H	-4.9964	2.0995	-3.1081
H	-4.9347	3.3028	-1.8234
C	-4.2011	4.0088	-3.7200
H	-3.7433	3.5846	-4.6247
H	-5.1847	4.3883	-4.0186
C	-3.3263	5.1420	-3.1899
H	-3.1864	5.9051	-3.9633
H	-3.8395	5.6380	-2.3533
C	-1.9750	4.6136	-2.7137
H	-1.3720	5.4271	-2.2929
H	-1.4142	4.2222	-3.5748
C	-2.1336	3.4990	-1.6762
H	-2.5938	3.9258	-0.7703
H	-1.1578	3.0913	-1.3868
C	-2.5597	-2.6737	2.3166
H	-1.9824	-2.1592	3.1032
C	-1.6683	-3.7816	1.7378
H	-2.2043	-4.2949	0.9265
H	-0.7707	-3.3399	1.2862
C	-1.2829	-4.8051	2.8090
H	-0.6746	-5.5999	2.3617
H	-0.6538	-4.3139	3.5663
C	-2.5173	-5.3971	3.4873
H	-2.2174	-6.0871	4.2833
H	-3.0823	-5.9923	2.7563
C	-3.4181	-4.2998	4.0500
H	-2.8972	-3.7779	4.8654
H	-4.3234	-4.7349	4.4876
C	-3.8080	-3.2856	2.9688
H	-4.4095	-3.8020	2.2087
H	-4.4516	-2.5122	3.4062
C	-4.3560	2.0943	2.7331
H	-3.9149	1.8153	3.6917
H	-5.4413	1.9887	2.7818
C	-6.0127	-1.7966	-1.4710
H	-5.7137	-2.5055	-2.2617
H	-6.6720	-1.0448	-1.9144
P	0.1409	-0.7675	-1.2102
P	0.2124	1.0098	1.1549
N	2.1572	-1.1330	0.8504
N	0.9989	1.8887	-1.3678
C	1.4303	-1.7764	-0.2908
H	0.9093	-2.6498	0.1116
H	2.2177	-2.1260	-0.9659
C	1.3707	-0.3181	1.8304
H	2.1240	0.1048	2.5006
H	0.7482	-1.0114	2.4043
C	1.2018	0.5838	-1.9649
H	2.2660	0.2748	-1.9752
H	0.8895	0.6543	-3.0135
C	1.3702	1.9774	0.0302
H	1.2715	3.0273	0.3260
H	2.4267	1.7059	0.2164
C	-0.0811	-1.9071	-2.6889
H	-0.8303	-1.3587	-3.2836
C	1.1443	-2.1476	-3.5838
H	1.5942	-1.2026	-3.9070
H	1.9201	-2.6892	-3.0248
C	0.7581	-2.9762	-4.8150
H	0.0638	-2.3931	-5.4365
H	1.6481	-3.1553	-5.4287
C	0.1037	-4.2997	-4.4248
H	-0.2034	-4.8490	-5.3213
H	0.8407	-4.9322	-3.9096
C	-1.0957	-4.0740	-3.5060
H	-1.5204	-5.0330	-3.1876
H	-1.8874	-3.5480	-4.0587
C	-0.7069	-3.2467	-2.2782
H	0.0167	-3.8232	-1.6833
H	-1.5783	-3.0761	-1.6354
C	0.1849	2.1320	2.6757
H	-0.2966	1.5125	3.4507
C	-0.7280	3.3368	2.4030
H	-0.2828	3.9617	1.6155
H	-1.6941	3.0036	2.0016
C	-0.9316	4.1915	3.6561
H	-1.5718	5.0499	3.4207
H	-1.4614	3.6004	4.4177
C	0.4045	4.6644	4.2245
H	0.2448	5.2307	5.1483
H	0.8762	5.3559	3.5123
C	1.3379	3.4843	4.4805
H	0.9240	2.8568	5.2826
H	2.3127	3.8381	4.8350
C	1.5324	2.6276	3.2234
H	2.0408	3.2293	2.4574
H	2.2045	1.7963	3.4637
C	2.8915	-2.1947	1.6049
H	3.5461	-1.7169	2.3369
H	3.4943	-2.7702	0.9007
C	1.6618	2.9239	-2.1525
H	2.7608	2.8280	-2.1542
H	1.4037	3.9086	-1.7495

H	1.3060	2.8799	-3.1867
H	2.1669	-2.8431	2.1022
H	-6.5849	-2.3448	-0.7169
H	-4.0969	3.1273	2.4957
H	2.9663	-0.5306	0.4482
H	-2.7724	1.2574	1.6007
N	4.5597	-0.0213	0.0478
C	5.1684	-1.0020	-0.7913
H	4.6461	0.9102	-0.3702
H	5.0037	0.0041	0.9681
C	5.8601	-2.0847	-0.2390
C	5.0323	-0.9129	-2.1804
C	6.3932	-3.0705	-1.0666
H	6.0036	-2.1381	0.8377
C	5.5725	-1.9005	-3.0001
H	4.5320	-0.0518	-2.6163
C	6.2481	-2.9876	-2.4492
H	6.9375	-3.9004	-0.6255
H	5.4735	-1.8122	-4.0782
H	6.6711	-3.7532	-3.0916
N	5.4089	-0.2250	3.0769
C	6.2113	-0.1625	3.9123
C	7.2168	-0.0824	4.9576
H	7.6861	-1.0595	5.1039
H	7.9889	0.6412	4.6802
H	6.7584	0.2339	5.8990
N	5.3102	2.6153	-1.2888
C	6.0944	3.3344	-1.7490
C	7.0780	4.2350	-2.3254
H	7.3565	5.0038	-1.5990
H	7.9747	3.6774	-2.6107
H	6.6683	4.7220	-3.2149

e^{r+}:BH^{+}:2S

Ni	-1.1685	0.0488	0.1102
P	-2.9493	0.1688	-1.1350
P	-2.3993	-0.7679	1.7075
N	-3.6775	1.6270	1.0950
N	-4.5089	-1.7329	0.1651
C	-4.2217	1.2475	-0.2517
H	-4.3657	2.1784	-0.8053
H	-5.1795	0.7454	-0.1029
C	-3.7293	0.5172	2.1016
H	-4.7408	0.1057	2.1021
H	-3.5141	0.9713	3.0725
C	-3.9182	-1.4375	-1.1325
H	-4.7357	-1.3649	-1.8561
H	-3.2401	-2.2378	-1.4817
C	-3.5531	-2.1500	1.1797
H	-2.9397	-3.0067	0.8480
H	-4.1250	-2.4814	2.0528
C	-3.1275	0.7541	-2.9059
H	-2.5991	-0.0262	-3.4780
C	-4.5544	0.8727	-3.4601
H	-5.0997	-0.0737	-3.3725
H	-5.1181	1.6162	-2.8772
C	-4.5402	1.3131	-4.9281
H	-4.0730	0.5244	-5.5346
H	-5.5697	1.4136	-5.2895
C	-3.7754	2.6209	-5.1164
H	-3.7483	2.8941	-6.1769
H	-4.3083	3.4323	-4.5999
C	-2.3576	2.5116	-4.5593
H	-1.8330	3.4698	-4.6570
H	-1.7895	1.7819	-5.1545
C	-2.3548	2.0674	-3.0943
H	-2.8251	2.8568	-2.4860
H	-1.3301	1.9402	-2.7255
C	-1.9297	-1.2872	3.4507
H	-1.3506	-0.4230	3.8167
C	-0.9819	-2.4947	3.4027
H	-1.5246	-3.3679	3.0127
H	-0.1605	-2.2997	2.7020
C	-0.4334	-2.8287	4.7922
H	0.2151	-3.7106	4.7326
H	0.1968	-1.9967	5.1396
C	-1.5602	-3.0626	5.7965
H	-1.1470	-3.2498	6.7936
H	-2.1149	-3.9687	5.5148
C	-2.5195	-1.8749	5.8368
H	-1.9960	-0.9928	6.2325
H	-3.3505	-2.0767	6.5217
C	-3.0710	-1.5505	4.4436
H	-3.6737	-2.4023	4.1007
H	-3.7507	-0.6922	4.5111
C	-4.2811	2.8797	1.6155
H	-3.7787	3.1627	2.5422
H	-5.3427	2.7130	1.8075
C	-5.5827	-2.7168	0.0377
H	-5.2241	-3.6980	-0.3175
H	-6.3362	-2.3507	-0.6656
P	0.4231	-1.1531	-0.7462
P	0.3579	1.5481	0.4338
N	2.5525	-0.2602	0.9607
N	0.9889	1.1424	-2.2662
C	1.8401	-1.4470	0.4442
H	1.4091	-2.0126	1.2844
H	2.5977	-2.0864	-0.0236
C	1.7003	0.8059	1.5279
H	2.3855	1.5887	1.8690
H	1.1706	0.4247	2.4155
C	1.3061	-0.2662	-2.1462
H	2.3986	-0.4560	-2.0813
H	0.9702	-0.7502	-3.0705
C	1.3223	1.9670	-1.1260
H	1.0506	2.9966	-1.3839
H	2.4117	1.9904	-0.9092
C	0.2715	-2.8775	-1.4788
H	-0.5489	-2.7508	-2.2042
C	1.4865	-3.4339	-2.2362
H	1.8273	-2.7390	-3.0120
H	2.3283	-3.5712	-1.5429
C	1.1536	-4.7871	-2.8763
H	0.3828	-4.6397	-3.6459
H	2.0381	-5.1756	-3.3940
C	0.6551	-5.7947	-1.8424
H	0.3804	-6.7351	-2.3323
H	1.4705	-6.0338	-1.1448
C	-0.5319	-5.2394	-1.0577
H	-0.8423	-5.9478	-0.2809
H	-1.3917	-5.1166	-1.7320
C	-0.1955	-3.8883	-0.4224
H	0.6022	-4.0363	0.3200
H	-1.0604	-3.4920	0.1219
C	0.2605	3.2644	1.2220
H	-0.0826	3.0563	2.2492
C	-0.8207	4.1037	0.5267
H	-0.5135	4.3122	-0.5085
H	-1.7548	3.5332	0.4461
C	-1.0628	5.4319	1.2479
H	-1.8256	6.0119	0.7151
H	-1.4617	5.2317	2.2532
C	0.2284	6.2383	1.3694
H	0.0491	7.1593	1.9343
H	0.5582	6.5466	0.3672
C	1.3278	5.4140	2.0341
H	1.0528	5.2099	3.0787
H	2.2647	5.9820	2.0652
C	1.5579	4.0832	1.3080
H	1.9267	4.2927	0.2938
H	2.3514	3.5303	1.8235
C	3.4621	-0.7156	2.0299
H	4.0833	0.1192	2.3716
H	4.1104	-1.5093	1.6472
C	1.5410	1.6942	-3.4905
H	2.6503	1.6964	-3.5052
H	1.2032	2.7268	-3.6217
H	1.1969	1.1120	-4.3505
H	2.9040	-1.1085	2.8914
H	-6.0675	-2.8596	1.0079
H	-4.1614	3.6723	0.8751
H	-2.6402	1.7358	0.9124
N	4.7422	0.6453	-0.3798
H	4.6422	1.6836	-0.4761
H	4.9124	0.2728	-1.3147
C	5.8597	0.3170	0.5068
C	6.0940	1.1198	1.6186
H	5.4792	1.9951	1.8067

C	7.1477	0.7988	2.4711
H	7.3438	1.4230	3.3371
C	7.9537	-0.3068	2.2080
H	8.7774	-0.5478	2.8721
C	7.7120	-1.0938	1.0846
H	8.3481	-1.9458	0.8670
C	6.6604	-0.7842	0.2249
H	6.4813	-1.3888	-0.6607
H	3.7693	0.2340	-0.0350
N	4.5663	3.4776	-0.6107
C	4.7453	4.6136	-0.7474
C	4.9712	6.0366	-0.9192
H	4.3412	6.6033	-0.2274
H	6.0203	6.2739	-0.7195
H	4.7301	6.3330	-1.9442
N	5.1590	0.1604	-3.1521
C	5.5300	0.3434	-4.2338
C	5.9954	0.5742	-5.5886
H	5.3277	0.0849	-6.3038
H	6.0144	1.6478	-5.7980
H	7.0050	0.1717	-5.7115

ex^{2+}:H_2O:S

Ni	0.5952	0.0837	-0.0743
P	2.1925	1.4037	0.6021
P	2.0524	-0.9278	-1.3457
N	2.2447	1.7338	-2.1437
N	4.3800	-0.2049	-0.0128
C	2.9050	2.2780	-0.9099
H	2.6650	3.3432	-0.8696
H	3.9831	2.1387	-1.0108
C	2.7331	0.3712	-2.5384
H	3.8244	0.3976	-2.5671
H	2.3422	0.1816	-3.5417
C	3.7265	0.4502	1.1109
H	4.4474	1.1478	1.5475
H	3.4336	-0.2573	1.9073
C	3.6769	-1.3713	-0.5252
H	3.4783	-2.1238	0.2581
H	4.3260	-1.8447	-1.2693
C	2.1532	2.7902	1.8638
H	2.0273	2.2506	2.8171
C	3.4106	3.6656	1.9751
H	4.3057	3.0616	2.1598
H	3.5776	4.1954	1.0257
C	3.2611	4.7025	3.0942
H	3.1980	4.1815	4.0598
H	4.1613	5.3255	3.1360
C	2.0191	5.5683	2.8982
H	1.9118	6.2706	3.7316
H	2.1384	6.1784	1.9914
C	0.7639	4.7079	2.7683
H	-0.1135	5.3360	2.5746
H	0.5763	4.1912	3.7205
C	0.9098	3.6657	1.6564
H	0.9871	4.1862	0.6886
H	0.0155	3.0334	1.5970
C	1.7892	-2.3593	-2.5297
H	0.9177	-2.0338	-3.1224
C	1.3773	-3.6180	-1.7517
H	2.2183	-3.9521	-1.1274
H	0.5555	-3.3803	-1.0634
C	0.9764	-4.7520	-2.6989
H	0.7188	-5.6462	-2.1196
H	0.0693	-4.4590	-3.2488
C	2.0895	-5.0667	-3.6971
H	1.7618	-5.8434	-4.3962
H	2.9539	-5.4787	-3.1578
C	2.5187	-3.8155	-4.4603
H	1.6910	-3.4690	-5.0956
H	3.3518	-4.0451	-5.1335
C	2.9284	-2.6885	-3.5054
H	3.8157	-3.0121	-2.9450
H	3.2269	-1.8063	-4.0854
C	2.2937	2.6934	-3.2768
H	1.7284	2.2865	-4.1170
H	3.3334	2.8461	-3.5720
C	5.7659	-0.5425	0.3114
H	5.8468	-1.2809	1.1266
H	6.3048	0.3612	0.6101
P	-0.4503	-0.9397	1.5196
P	-1.3495	0.5964	-0.8257
N	-2.6019	-1.9667	-0.1576
N	-2.7413	0.7771	1.6865
C	-1.6041	-2.2881	0.9133
H	-0.9468	-3.0808	0.5417
H	-2.2052	-2.6967	1.7311
C	-2.2832	-0.9889	-1.2420
H	-3.2508	-0.7694	-1.7012
H	-1.6592	-1.4943	-1.9873
C	-1.5964	0.2341	2.4277
H	-2.0116	-0.2623	3.3105
H	-0.9360	1.0425	2.7880
C	-2.4576	1.4587	0.4180
H	-1.9525	2.4219	0.6021
H	-3.4268	1.6870	-0.0413
C	0.3178	-1.8365	2.9848
H	0.8125	-1.0100	3.5223
C	-0.6197	-2.5502	3.9701
H	-1.4150	-1.8885	4.3310
H	-1.1119	-3.3943	3.4675
C	0.1704	-3.0957	5.1657
H	0.6007	-2.2547	5.7275
H	-0.5138	-3.6091	5.8502
C	1.2851	-4.0383	4.7173
H	1.8637	-4.3789	5.5825
H	0.8413	-4.9374	4.2667
C	2.2034	-3.3639	3.7003
H	2.9600	-4.0701	3.3394
H	2.7485	-2.5429	4.1882
C	1.4143	-2.8020	2.5147
H	0.9561	-3.6362	1.9623
H	2.0833	-2.2912	1.8139
C	-1.7751	1.6059	-2.3711
H	-1.1066	1.1737	-3.1346
C	-1.3527	3.0690	-2.1512
H	-2.0100	3.5264	-1.3992
H	-0.3374	3.1227	-1.7318
C	-1.4562	3.8864	-3.4407
H	-1.1574	4.9232	-3.2476
H	-0.7537	3.4872	-4.1876
C	-2.8742	3.8352	-4.0053
H	-2.9273	4.3860	-4.9503
H	-3.5580	4.3422	-3.3104
C	-3.3289	2.3930	-4.2090
H	-2.7208	1.9256	-4.9965
H	-4.3656	2.3640	-4.5622
C	-3.2067	1.5592	-2.9265
H	-3.9122	1.9463	-2.1780
H	-3.5143	0.5326	-3.1533
C	-3.0877	-3.2361	-0.7647
H	-3.9128	-3.0141	-1.4444
H	-3.4463	-3.8909	0.0318
C	-3.4769	1.7025	2.5616
H	-3.7808	1.1826	3.4746
H	-4.3771	2.0559	2.0499
H	-2.8666	2.5759	2.8400
H	-2.2752	-3.7210	-1.3116
H	6.2603	-0.9528	-0.5740
H	1.8558	3.6426	-2.9640
H	-3.4932	-1.5998	0.3939
H	1.2532	1.5522	-1.8253
O	-4.5077	-1.2339	1.3284
H	-4.0262	-0.3958	1.5616
H	-5.4330	-1.0267	1.0617
N	-7.1271	-0.6786	0.6158
C	-8.2821	-0.6232	0.5607
C	-9.7308	-0.5548	0.4926
H	-10.1706	-1.1978	1.2605
H	-10.0669	0.4729	0.6573
H	-10.0777	-0.8887	-0.4894

ex^{2+}: H_2O:S --> ex'^{2+}: H_2O:S

Ni	0.0083	-0.0377	-0.1809
P	-0.6377	1.5145	-1.5666
P	1.4726	-0.6797	-1.6687
N	-0.9144	-0.7753	-3.1024

N	1.6781	1.6990	-3.0932
C	-1.1897	0.6992	-3.1743
H	-2.2704	0.8094	-3.2910
H	-0.6762	1.0970	-4.0519
C	0.5368	-1.1276	-3.2462
H	0.9221	-0.6158	-4.1304
H	0.5790	-2.2096	-3.3965
C	0.8073	2.4975	-2.2441
H	0.4216	3.3229	-2.8501
H	1.3431	2.9440	-1.3859
C	2.4898	0.7276	-2.3760
H	3.0642	1.1881	-1.5527
H	3.2134	0.3147	-3.0861
C	-1.9497	2.8299	-1.3328
H	-1.4935	3.5031	-0.5881
C	-2.3188	3.6650	-2.5677
H	-1.4364	4.1441	-3.0063
H	-2.7421	3.0113	-3.3443
C	-3.3558	4.7378	-2.2162
H	-2.9053	5.4590	-1.5200
H	-3.6182	5.3002	-3.1189
C	-4.6035	4.1270	-1.5833
H	-5.3118	4.9151	-1.3062
H	-5.1161	3.4946	-2.3222
C	-4.2435	3.2867	-0.3599
H	-5.1403	2.8152	0.0591
H	-3.8396	3.9440	0.4240
C	-3.2039	2.2142	-0.6968
H	-3.6530	1.4950	-1.4000
H	-2.9216	1.6450	0.1976
C	2.6942	-2.1037	-1.6102
H	2.0514	-2.9675	-1.3704
C	3.6769	-1.9215	-0.4448
H	4.3129	-1.0453	-0.6367
H	3.1233	-1.7080	0.4794
C	4.5653	-3.1558	-0.2671
H	5.2780	-2.9856	0.5483
H	3.9397	-4.0094	0.0331
C	5.3058	-3.5028	-1.5576
H	5.8935	-4.4168	-1.4212
H	6.0234	-2.7038	-1.7908
C	4.3351	-3.6681	-2.7247
H	3.6927	-4.5428	-2.5495
H	4.8824	-3.8653	-3.6529
C	3.4578	-2.4238	-2.9034
H	4.1051	-1.5781	-3.1714
H	2.7727	-2.5752	-3.7468
C	-1.7703	-1.5512	-4.0386
H	-1.6011	-2.6177	-3.8805
H	-1.5099	-1.2841	-5.0643
C	2.5180	2.5546	-3.9321
H	3.2187	3.1725	-3.3460
H	1.8862	3.2203	-4.5269
P	0.6902	0.7637	1.7015
P	-1.2066	-1.3915	0.9653
N	0.5483	-1.6580	3.2489
N	-2.0048	0.7757	2.6581
C	1.4361	-0.5100	2.8719
H	2.3213	-0.9366	2.3928
H	1.7378	-0.0464	3.8160
C	-0.0752	-2.3995	2.1046
H	-0.6164	-3.2334	2.5585
H	0.7421	-2.8021	1.4995
C	-0.7043	1.4033	2.7720
H	-0.3501	1.4600	3.8164
H	-0.8141	2.4483	2.4428
C	-2.3086	-0.5791	2.2556
H	-3.2936	-0.5639	1.7718
H	-2.4125	-1.2797	3.1053
C	1.9562	2.1336	1.9490
H	1.6234	2.8846	1.2145
C	2.0187	2.8165	3.3237
H	1.0377	3.1990	3.6241
H	2.3273	2.0917	4.0913
C	3.0231	3.9760	3.3056
H	2.6513	4.7577	2.6283
H	3.0716	4.4281	4.3023
C	4.4102	3.5276	2.8527
H	5.0875	4.3867	2.8045
H	4.8343	2.8396	3.5979
C	4.3475	2.8263	1.4973
H	5.3388	2.4597	1.2078
H	4.0397	3.5451	0.7244
C	3.3553	1.6612	1.5251
H	3.7226	0.9119	2.2415
H	3.3107	1.1669	0.5471
C	-2.3504	-2.8087	0.4486
H	-1.6675	-3.5079	-0.0628
C	-3.3706	-2.3130	-0.5865
H	-4.0618	-1.6032	-0.1091
H	-2.8662	-1.7489	-1.3819
C	-4.1770	-3.4701	-1.1831
H	-4.9085	-3.0806	-1.9008
H	-3.5002	-4.1292	-1.7463
C	-4.8794	-4.2782	-0.0943
H	-5.4008	-5.1340	-0.5358
H	-5.6503	-3.6553	0.3803
C	-3.8869	-4.7517	0.9643
H	-3.1894	-5.4755	0.5198
H	-4.4097	-5.2784	1.7701
C	-3.0904	-3.5810	1.5529
H	-3.7867	-2.9065	2.0692
H	-2.4038	-3.9676	2.3156
C	1.3028	-2.6065	4.1241
H	2.1200	-3.0492	3.5520
H	0.6246	-3.3882	4.4702
C	-3.1154	1.6336	3.0374
H	-3.0360	2.6124	2.5456
H	-3.1760	1.8220	4.1219
H	-4.0614	1.1792	2.7315
H	1.6987	-2.0572	4.9797
H	3.0992	1.9359	-4.6218
H	-2.8182	-1.3122	-3.8506
H	-1.1266	-1.0146	-2.0993
H	-0.2049	-1.2766	3.8749
O	-1.1072	-0.5328	5.0987
H	-1.7287	0.0438	4.6243
H	-1.5549	-0.8624	5.8857
N	-2.3396	-1.4234	7.3779
C	-2.7511	-1.8205	8.3845
C	-3.2660	-2.3191	9.6471
H	-2.5005	-2.9156	10.1520
H	-3.5473	-1.4839	10.2948
H	-4.1455	-2.9458	9.4739

ex'$^{2+}$: H_2O:2S

Ni	0.6387	0.0252	0.1156
P	2.5271	-0.6463	-0.7420
P	1.7652	1.4462	1.3159
N	2.9827	-0.9711	1.9894
N	4.0847	1.6024	-0.2280
C	3.6252	-1.2625	0.6643
H	3.7275	-2.3485	0.5978
H	4.6115	-0.7934	0.6609
C	3.0113	0.4830	2.3579
H	4.0323	0.8440	2.2167
H	2.7334	0.5450	3.4130
C	3.6609	0.7327	-1.3157
H	4.5587	0.2767	-1.7508
H	3.1530	1.2899	-2.1223
C	3.0187	2.4294	0.3179
H	2.4759	2.9855	-0.4672
H	3.4785	3.1689	0.9847
C	2.9008	-1.9629	-2.0139
H	3.9891	-2.1349	-1.9840
C	2.1753	-3.2731	-1.6871
H	2.4456	-3.6357	-0.6855
H	1.0957	-3.0669	-1.6715
C	2.4906	-4.3538	-2.7255
H	3.5585	-4.6077	-2.6730
H	1.9428	-5.2717	-2.4821
C	2.1492	-3.8863	-4.1393
H	2.4298	-4.6529	-4.8696
H	1.0607	-3.7562	-4.2253
C	2.8420	-2.5656	-4.4676
H	2.5457	-2.2128	-5.4620
H	3.9290	-2.7225	-4.5060
C	2.5278	-1.4880	-3.4258

H	1.4526	-1.2588	-3.4453
H	3.0582	-0.5630	-3.6818
C	1.2753	2.7315	2.5911
H	2.2021	3.0479	3.0962
C	0.3190	2.1501	3.6379
H	-0.5803	1.7840	3.1191
H	0.7598	1.2775	4.1386
C	-0.0822	3.1976	4.6796
H	-0.7840	2.7572	5.3973
H	0.8058	3.4919	5.2555
C	-0.6914	4.4332	4.0199
H	-0.9288	5.1887	4.7764
H	-1.6460	4.1593	3.5451
C	0.2480	5.0157	2.9664
H	1.1522	5.4009	3.4573
H	-0.2188	5.8708	2.4646
C	0.6519	3.9670	1.9264
H	-0.2377	3.6565	1.3570
H	1.3443	4.4129	1.2028
C	3.5247	-1.8307	3.0740
H	2.9674	-1.6440	3.9935
H	4.5785	-1.5899	3.2252
C	5.2205	2.4271	-0.6399
H	4.9695	3.1215	-1.4594
H	6.0391	1.7832	-0.9741
P	-0.8560	0.8057	-1.2433
P	-0.8842	-1.3278	0.8119
N	-3.1488	0.4465	0.4764
N	-1.3261	-1.8744	-1.9078
C	-2.3565	1.4537	-0.2985
H	-2.0125	2.2069	0.4156
H	-3.0705	1.9224	-0.9847
C	-2.3891	-0.3846	1.4640
H	-3.1241	-1.0802	1.8836
H	-2.0540	0.2905	2.2559
C	-1.6989	-0.5218	-2.2743
H	-2.7966	-0.3596	-2.2840
H	-1.3616	-0.3577	-3.3033
C	-1.7221	-2.2875	-0.5766
H	-1.4047	-3.3284	-0.4526
H	-2.8213	-2.2857	-0.4261
C	-0.7997	2.1797	-2.5231
H	-1.7717	2.1556	-3.0429
C	-0.6212	3.5665	-1.8904
H	-1.4299	3.7875	-1.1827
H	0.3138	3.5755	-1.3116
C	-0.5723	4.6653	-2.9568
H	-1.5489	4.7229	-3.4575
H	-0.4136	5.6363	-2.4742
C	0.5145	4.3973	-3.9950
H	0.4956	5.1706	-4.7703
H	1.5018	4.4620	-3.5149
C	0.3459	3.0148	-4.6208
H	1.1586	2.8098	-5.3268
H	-0.5859	2.9861	-5.2027
C	0.3079	1.9196	-3.5519
H	1.2727	1.8894	-3.0265
H	0.1842	0.9393	-4.0285
C	-0.9240	-2.6766	2.1282
H	-1.9171	-3.1491	2.0592
C	-0.7534	-2.1156	3.5463
H	0.2053	-1.5746	3.6044
H	-1.5317	-1.3789	3.7785
C	-0.7796	-3.2264	4.6008
H	-0.6220	-2.7939	5.5954
H	-1.7804	-3.6794	4.6159
C	0.2589	-4.3077	4.3133
H	0.1812	-5.1134	5.0508
H	1.2683	-3.8838	4.4264
C	0.0981	-4.8643	2.9006
H	-0.8592	-5.3976	2.8246
H	0.8792	-5.6020	2.6841
C	0.1346	-3.7509	1.8505
H	1.1305	-3.2799	1.8563
H	0.0136	-4.1791	0.8486
C	-4.2782	1.1334	1.1733
H	-4.8964	0.3818	1.6665
H	-4.8768	1.6658	0.4327
C	-1.7822	-2.8285	-2.9068
H	-2.8850	-2.8891	-2.9827
H	-1.4077	-3.8276	-2.6643
H	-1.3932	-2.5490	-3.8904
H	-3.8762	1.8336	1.9077
H	5.5774	3.0137	0.2115
H	3.4236	-2.8787	2.7875
H	-3.6510	-0.1941	-0.2001
H	1.9636	-1.1649	1.8188
O	-4.8946	-0.9570	-0.9624
H	-5.8559	-0.7418	-0.8665
H	-4.8281	-1.5948	-1.6792
N	-7.5591	-0.3956	-0.7377
C	-8.7130	-0.3136	-0.7769
C	-10.1599	-0.2111	-0.8265
H	-10.4546	0.6376	-1.4504
H	-10.5840	-1.1262	-1.2499
H	-10.5611	-0.0683	0.1810
N	-5.4533	-2.7072	-2.9086
C	-5.9401	-3.2559	-3.8042
C	-6.5500	-3.9450	-4.9272
H	-6.0542	-4.9068	-5.0879
H	-7.6107	-4.1232	-4.7283
H	-6.4556	-3.3423	-5.8350

[eNiH^{2+}: H$_2$O:B:2S]$_x$

Ni	1.7525	0.0396	-0.0369
P	3.5424	1.0500	0.6858
P	3.0132	-1.1587	-1.3425
N	3.6906	1.4482	-2.0447
N	5.4160	-0.9023	0.0419
C	4.4201	1.8324	-0.7899
H	4.3666	2.9211	-0.7169
H	5.4591	1.5122	-0.8886
C	3.9409	0.0350	-2.4780
H	5.0202	-0.1310	-2.4880
H	3.5433	-0.0522	-3.4926
C	4.8832	-0.1650	1.1788
H	5.7141	0.3831	1.6330
H	4.4636	-0.8297	1.9563
C	4.5137	-1.9065	-0.5004
H	4.1610	-2.6128	0.2723
H	5.0759	-2.4883	-1.2379
C	3.7033	2.3993	1.9741
H	3.4269	1.8850	2.9091
C	5.0958	3.0190	2.1581
H	5.8469	2.2568	2.3939
H	5.4155	3.4973	1.2204
C	5.0863	4.0772	3.2671
H	4.8751	3.5875	4.2282
H	6.0844	4.5202	3.3572
C	4.0404	5.1581	3.0059
H	4.0290	5.8803	3.8295
H	4.3159	5.7213	2.1024
C	2.6546	4.5449	2.8175
H	1.9188	5.3242	2.5857
H	2.3317	4.0810	3.7608
C	2.6475	3.4836	1.7141
H	2.8611	3.9762	0.7515
H	1.6603	3.0140	1.6281
C	2.5532	-2.4810	-2.5965
H	1.7755	-1.9850	-3.2012
C	1.8994	-3.6801	-1.8946
H	2.6423	-4.1775	-1.2545
H	1.0985	-3.3328	-1.2292
C	1.3541	-4.6910	-2.9073
H	0.9240	-5.5499	-2.3790
H	0.5336	-4.2257	-3.4735
C	2.4390	-5.1519	-3.8790
H	2.0147	-5.8337	-4.6238
H	3.1988	-5.7253	-3.3296
C	3.1040	-3.9626	-4.5686
H	2.3728	-3.4548	-5.2136
H	3.9132	-4.3033	-5.2239
C	3.6581	-2.9625	-3.5477
H	4.4532	-3.4573	-2.9741
H	4.1274	-2.1226	-4.0748
C	3.9148	2.4175	-3.1473
H	3.2867	2.1461	-3.9976
H	4.9657	2.3890	-3.4409

C	6.7105	-1.4990	0.3680
H	7.1311	-1.9740	-0.5232
H	6.6429	-2.2582	1.1656
P	0.6028	-0.8970	1.5401
P	-0.1094	0.9332	-0.6773
N	-1.8091	-1.3065	-0.0014
N	-0.3975	1.6824	1.9955
C	-0.7977	-1.9637	0.8823
H	-0.3413	-2.7751	0.3083
H	-1.3769	-2.4036	1.7000
C	-1.3022	-0.4597	-1.1259
H	-2.2042	-0.0816	-1.6142
H	-0.7806	-1.1210	-1.8246
C	-0.3548	0.3499	2.5660
H	-1.3600	-0.0499	2.8090
H	0.1837	0.4233	3.5182
C	-1.0591	1.7855	0.7067
H	-1.0820	2.8484	0.4429
H	-2.1130	1.4498	0.7345
C	1.2186	-2.0512	2.8895
H	2.0388	-1.4617	3.3318
C	0.2370	-2.4094	4.0156
H	-0.2013	-1.5123	4.4665
H	-0.5970	-3.0005	3.6110
C	0.9381	-3.2350	5.1009
H	1.7075	-2.6145	5.5819
H	0.2172	-3.4969	5.8834
C	1.5834	-4.4938	4.5255
H	2.1166	-5.0389	5.3119
H	0.7983	-5.1693	4.1568
C	2.5347	-4.1541	3.3795
H	2.9449	-5.0696	2.9378
H	3.3897	-3.5834	3.7695
C	1.8324	-3.3279	2.2990
H	1.0391	-3.9419	1.8476
H	2.5305	-3.0736	1.4930
C	-0.4804	2.0936	-2.1212
H	-0.1285	1.5334	-3.0036
C	0.3805	3.3592	-1.9934
H	0.0653	3.9273	-1.1065
H	1.4304	3.0935	-1.8127
C	0.2561	4.2587	-3.2254
H	0.8685	5.1584	-3.0923
H	0.6552	3.7304	-4.1039
C	-1.1998	4.6395	-3.4850
H	-1.2780	5.2403	-4.3974
H	-1.5601	5.2729	-2.6622
C	-2.0788	3.3964	-3.5915
H	-1.7973	2.8247	-4.4874
H	-3.1289	3.6810	-3.7227
C	-1.9445	2.4943	-2.3585
H	-2.3247	3.0326	-1.4792
H	-2.5879	1.6175	-2.4905
C	-2.7222	-2.3540	-0.5527
H	-2.1427	-3.0433	-1.1704
H	-3.5015	-1.8753	-1.1477
C	-0.9640	2.6263	2.9475
H	-0.3957	2.5939	3.8820
H	-2.0248	2.4215	3.1860
H	-0.8982	3.6420	2.5455
H	-3.1809	-2.8856	0.2820
H	7.4040	-0.7185	0.6937
H	3.6557	3.4202	-2.8037
H	2.6783	1.4298	-1.7389
H	-2.4616	-0.7272	0.6243
O	-3.6869	-0.2730	1.5000
H	-3.6472	0.2624	2.2976
H	-4.6429	-0.1815	1.1226
N	-6.0837	-0.0695	0.4302
C	-5.9387	-0.6353	-0.8584
H	-6.7740	-0.5726	0.9956
H	-6.3363	0.9222	0.3855
C	-5.3828	0.1220	-1.8979
C	-6.2695	-1.9751	-1.0905
C	-5.1639	-0.4569	-3.1466
H	-5.1602	1.1729	-1.7287
C	-6.0427	-2.5455	-2.3407
H	-6.7199	-2.5581	-0.2916
C	-5.4837	-1.7950	-3.3742
H	-4.7603	0.1493	-3.9535
H	-6.3191	-3.5823	-2.5107
H	-5.3232	-2.2401	-4.3512
N	-8.1614	-1.6361	2.0463
C	-9.0891	-2.1041	2.5588
C	-10.2527	-2.6898	3.2023
H	-11.0719	-2.7842	2.4838
H	-10.0090	-3.6823	3.5917
H	-10.5822	-2.0571	4.0314
N	-6.9265	2.8626	0.1875
C	-7.6784	3.7393	0.0940
C	-8.6223	4.8380	-0.0224
H	-8.0998	5.7586	-0.2976
H	-9.3678	4.6126	-0.7903
H	-9.1352	4.9957	0.9307

[NiH$^+$: H_2O:BH^+:2S]$_x$

Ni	-1.9435	0.0243	0.0829
P	-3.6644	0.7608	-1.0156
P	-3.2476	-1.3874	1.0927
N	-4.4372	1.0705	1.6132
N	-5.3223	-1.4615	-0.7670
C	-4.9457	1.3673	0.2328
H	-5.0474	2.4528	0.1622
H	-5.9194	0.8879	0.1158
C	-4.5588	-0.3712	2.0038
H	-5.5811	-0.6959	1.7986
H	-4.3647	-0.4164	3.0786
C	-4.6732	-0.6294	-1.7710
H	-5.4598	-0.2027	-2.4009
H	-4.0015	-1.2092	-2.4307
C	-4.4178	-2.3314	-0.0297
H	-3.8149	-2.9694	-0.7003
H	-5.0327	-2.9985	0.5838
C	-3.7601	2.0937	-2.3289
H	-3.2376	1.6347	-3.1843
C	-5.1603	2.5178	-2.7933
H	-5.7405	1.6613	-3.1550
H	-5.7194	2.9414	-1.9458
C	-5.0774	3.5751	-3.8999
H	-4.6149	3.1263	-4.7904
H	-6.0888	3.8774	-4.1941
C	-4.2614	4.7882	-3.4594
H	-4.1856	5.5112	-4.2792
H	-4.7854	5.3010	-2.6398
C	-2.8701	4.3709	-2.9875
H	-2.3097	5.2432	-2.6298
H	-2.3051	3.9645	-3.8390
C	-2.9368	3.3111	-1.8849
H	-3.4034	3.7595	-0.9927
H	-1.9315	2.9826	-1.5945
C	-2.8614	-2.6652	2.4156
H	-2.2597	-2.0927	3.1410
C	-1.9630	-3.7689	1.8381
H	-2.5265	-4.3409	1.0867
H	-1.1088	-3.3221	1.3148
C	-1.4803	-4.7242	2.9323
H	-0.8671	-5.5170	2.4880
H	-0.8286	-4.1743	3.6271
C	-2.6512	-5.3266	3.7069
H	-2.2823	-5.9664	4.5161
H	-3.2333	-5.9758	3.0376
C	-3.5608	-4.2359	4.2684
H	-3.0151	-3.6571	5.0273
H	-4.4236	-4.6807	4.7770
C	-4.0471	-3.2884	3.1661
H	-4.6716	-3.8599	2.4662
H	-4.6935	-2.5193	3.6067
C	-5.0136	1.9764	2.6370
H	-4.5296	1.7875	3.5969
H	-6.0856	1.7880	2.7209
C	-6.4088	-2.2389	-1.3590
H	-6.9359	-2.7906	-0.5749
H	-6.0557	-2.9630	-2.1133
P	-0.3306	-0.7026	-1.1818
P	-0.4030	1.1413	1.1208
N	1.7325	-0.7251	0.7717
N	0.3540	2.0111	-1.4303
C	1.0230	-1.5565	-0.2105

H	0.5540	-2.4216	0.2867
H	1.7817	-1.9461	-0.8991
C	0.8775	-0.0733	1.7752
H	1.5548	0.4386	2.4653
H	0.3191	-0.8269	2.3566
C	0.6387	0.6950	-1.9749
H	1.7202	0.4523	-1.9617
H	0.3366	0.7139	-3.0285
C	0.6537	2.1930	-0.0229
H	0.4230	3.2364	0.2193
H	1.7256	2.0493	0.2175
C	-0.4940	-1.8808	-2.6354
H	-1.2737	-1.3962	-3.2458
C	0.7421	-2.0807	-3.5247
H	1.1390	-1.1225	-3.8788
H	1.5429	-2.5604	-2.9442
C	0.4081	-2.9710	-4.7275
H	-0.3212	-2.4522	-5.3657
H	1.3063	-3.1163	-5.3388
C	-0.1648	-4.3181	-4.2918
H	-0.4379	-4.9155	-5.1687
H	0.6094	-4.8864	-3.7565
C	-1.3748	-4.1340	-3.3777
H	-1.7401	-5.1058	-3.0261
H	-2.1972	-3.6780	-3.9472
C	-1.0381	-3.2417	-2.1811
H	-0.2833	-3.7479	-1.5618
H	-1.9198	-3.1003	-1.5456
C	-0.5345	2.2987	2.6098
H	-0.9726	1.6590	3.3940
C	-1.5303	3.4295	2.3149
H	-1.1234	4.0785	1.5261
H	-2.4636	3.0223	1.9052
C	-1.8107	4.2802	3.5558
H	-2.5124	5.0853	3.3065
H	-2.3002	3.6588	4.3204
C	-0.5193	4.8598	4.1293
H	-0.7288	5.4225	5.0456
H	-0.0965	5.5776	3.4121
C	0.5002	3.7576	4.4045
H	0.1292	3.1093	5.2111
H	1.4420	4.1892	4.7624
C	0.7667	2.9031	3.1596
H	1.2332	3.5321	2.3882
H	1.4957	2.1258	3.4133
C	2.7073	-1.5728	1.4732
H	2.2162	-2.3731	2.0486
H	3.2992	-0.9610	2.1606
C	0.9873	3.0423	-2.2324
H	0.6753	2.9460	-3.2770
H	2.0955	2.9986	-2.2070
H	0.6836	4.0317	-1.8759
H	3.3832	-2.0329	0.7458
H	-7.1254	-1.5654	-1.8381
H	-4.8446	3.0122	2.3383
H	-3.3870	1.1989	1.5122
H	2.9902	0.2239	0.0016
O	3.8289	0.6055	-0.3963
H	3.5688	1.3915	-0.8867
H	5.4979	0.3800	-0.0693
N	6.5329	0.2273	0.0070
C	6.9598	-0.9141	-0.8036
H	7.0172	1.0966	-0.3147
H	6.7857	0.0844	1.0070
C	8.2268	-1.4486	-0.5985
C	6.1034	-1.4174	-1.7752
C	8.6423	-2.5166	-1.3887
H	8.8786	-1.0391	0.1677
C	6.5326	-2.4854	-2.5603
H	5.1188	-0.9784	-1.9070
C	7.7982	-3.0342	-2.3694
H	9.6288	-2.9434	-1.2378
H	5.8752	-2.8871	-3.3253
H	8.1283	-3.8652	-2.9847
N	7.9712	2.5175	-0.9295
C	8.6753	3.3409	-1.3366
C	9.5594	4.3727	-1.8480
H	9.3550	5.3242	-1.3487
H	10.6018	4.0943	-1.6676
H	9.4077	4.4961	-2.9243
N	7.4103	-0.2175	2.7271
C	7.9158	-0.4133	3.7502
C	8.5483	-0.6613	5.0338
H	7.9795	-0.1770	5.8327
H	8.5901	-1.7367	5.2293
H	9.5665	-0.2616	5.0330

eNiH^{2+}: H$_2$O:B:2 H$_2$O

Ni	0.9703	-0.1084	-0.3218
P	0.0815	-0.2322	1.8326
P	0.9625	2.0566	0.0303
N	-1.7873	1.7643	0.9342
N	1.1525	2.1628	2.7817
C	-1.4623	0.8083	2.0366
H	-2.3292	0.1459	2.1091
H	-1.3935	1.3961	2.9558
C	-0.7207	2.7251	0.5259
H	-0.5868	3.4266	1.3525
H	-1.1355	3.2575	-0.3342
C	1.1671	0.7280	3.0268
H	0.7887	0.5690	4.0408
H	2.1842	0.2983	2.9929
C	1.8648	2.5822	1.5838
H	2.8985	2.2044	1.5510
H	1.9171	3.6761	1.5920
C	-0.3919	-1.7434	2.8363
H	0.5679	-2.2691	2.9571
C	-0.9941	-1.4878	4.2261
H	-0.3239	-0.8858	4.8498
H	-1.9304	-0.9199	4.1276
C	-1.2978	-2.8060	4.9467
H	-0.3545	-3.3333	5.1461
H	-1.7456	-2.5910	5.9233
C	-2.2162	-3.7001	4.1181
H	-2.3928	-4.6477	4.6381
H	-3.1978	-3.2162	4.0106
C	-1.6211	-3.9577	2.7361
H	-2.3034	-4.5650	2.1298
H	-0.6955	-4.5402	2.8452
C	-1.3041	-2.6525	2.0008
H	-2.2489	-2.1316	1.7814
H	-0.8193	-2.8601	1.0415
C	1.3580	3.3131	-1.3002
H	0.5196	3.1548	-1.9992
C	2.6462	2.9931	-2.0659
H	3.5116	3.1252	-1.4021
H	2.6410	1.9436	-2.3848
C	2.8022	3.9215	-3.2739
H	3.7392	3.6936	-3.7944
H	1.9906	3.7206	-3.9878
C	2.7657	5.3914	-2.8591
H	2.8294	6.0354	-3.7425
H	3.6486	5.6184	-2.2450
C	1.5016	5.7124	-2.0643
H	0.6211	5.6083	-2.7140
H	1.5162	6.7534	-1.7234
C	1.3470	4.7828	-0.8551
H	2.1835	4.9618	-0.1656
H	0.4278	5.0344	-0.3112
C	-3.0007	2.5479	1.3239
H	-3.3187	3.1432	0.4683
H	-2.7518	3.1937	2.1683
C	1.6315	2.9000	3.9512
H	1.5257	3.9747	3.7769
H	2.6882	2.6898	4.1869
P	3.0841	-0.8901	-0.1268
P	0.7667	-1.7273	-1.7640
N	3.3463	-1.9059	-2.7020
N	1.7427	-3.3264	0.2786
C	3.9442	-0.9629	-1.7819
H	3.9858	0.0636	-2.1908
H	4.9760	-1.2824	-1.5977
C	2.0164	-1.5328	-3.1357
H	1.7336	-2.2013	-3.9535
H	1.9527	-0.4965	-3.5180
C	3.0463	-2.6919	0.3671
H	3.8219	-3.2245	-0.2135

H	3.3459	-2.7265	1.4198
C	1.2082	-3.4005	-1.0701
H	0.2812	-3.9824	-1.0273
H	1.8910	-3.9021	-1.7780
C	4.4692	-0.1927	0.9396
H	3.9866	0.0634	1.8944
C	5.6198	-1.1681	1.2464
H	5.2544	-2.0919	1.7052
H	6.1227	-1.4560	0.3128
C	6.6424	-0.5191	2.1874
H	6.1655	-0.3357	3.1609
H	7.4595	-1.2251	2.3718
C	7.1853	0.7939	1.6301
H	7.8688	1.2569	2.3498
H	7.7763	0.5911	0.7261
C	6.0502	1.7542	1.2829
H	6.4460	2.6672	0.8239
H	5.5341	2.0633	2.2040
C	5.0455	1.0970	0.3335
H	5.5589	0.8575	-0.6070
H	4.2470	1.8008	0.0735
C	-0.8250	-2.0158	-2.6933
H	-0.9538	-1.0880	-3.2753
C	-2.0209	-2.1603	-1.7424
H	-1.8905	-3.0635	-1.1298
H	-2.0625	-1.3126	-1.0491
C	-3.3354	-2.2765	-2.5188
H	-4.1730	-2.3884	-1.8216
H	-3.5137	-1.3395	-3.0696
C	-3.2992	-3.4361	-3.5113
H	-4.2291	-3.4739	-4.0898
H	-3.2379	-4.3844	-2.9590
C	-2.1023	-3.3161	-4.4496
H	-2.2238	-2.4305	-5.0895
H	-2.0505	-4.1796	-5.1216
C	-0.7849	-3.1986	-3.6761
H	-0.6135	-4.1315	-3.1214
H	0.0384	-3.1017	-4.3910
C	4.2282	-2.1692	-3.8353
H	4.4080	-1.2750	-4.4564
H	3.7905	-2.9476	-4.4667
C	1.8032	-4.6605	0.8704
H	2.1393	-4.5871	1.9093
H	2.4892	-5.3390	0.3346
H	0.8053	-5.1088	0.8666
H	5.1918	-2.5357	-3.4701
H	1.0261	2.6384	4.8236
H	-3.7995	1.8576	1.5986
H	-2.0984	1.2524	0.0518
H	-0.2620	0.2645	-0.9923
O	-2.9328	1.1093	-1.3297
H	-2.5581	0.6285	-2.0731
H	-3.9461	0.9792	-1.3705
N	-5.5941	0.8375	-1.3104
C	-5.9504	1.1275	0.0305
H	-6.0223	1.5037	-1.9612
H	-5.8827	-0.1155	-1.5561
C	-5.7998	0.1465	1.0200
C	-6.3836	2.4069	0.3966
C	-6.0843	0.4446	2.3518
H	-5.4767	-0.8522	0.7347
C	-6.6569	2.6969	1.7312
H	-6.5199	3.1604	-0.3750
C	-6.5069	1.7222	2.7171
H	-5.9868	-0.3313	3.1065
H	-7.0054	3.6903	1.9996
H	-6.7365	1.9495	3.7534
O	-6.9850	2.8949	-2.9095
O	-6.6746	-1.9042	-1.4665
H	-7.0221	-2.3604	-2.2457
H	-7.4019	-1.9143	-0.8277
H	-6.7307	3.4439	-3.6637
H	-7.9520	2.9098	-2.9026

e^+: H_2O:BH+:2S

Ni	-0.8455	0.1390	-0.0935
P	-1.5503	1.2900	-1.8239
P	-2.8404	-0.7953	0.0112
N	-3.3929	1.9302	0.1315
N	-3.6518	-0.3561	-2.6209
C	-3.0971	2.2437	-1.3057
H	-2.9289	3.3197	-1.3699
H	-3.9664	1.9576	-1.9005
C	-4.0658	0.6067	0.3237
H	-4.9470	0.5731	-0.3209
H	-4.3787	0.5737	1.3703
C	-2.3809	0.1757	-3.0929
H	-2.5913	0.7572	-3.9939
H	-1.6616	-0.6150	-3.3700
C	-3.5372	-1.4019	-1.6180
H	-2.9152	-2.2465	-1.9625
H	-4.5428	-1.7983	-1.4367
C	-0.6597	2.5850	-2.8676
H	0.2850	2.0824	-3.1294
C	-1.3281	3.0402	-4.1725
H	-1.5406	2.1900	-4.8288
H	-2.2935	3.5170	-3.9460
C	-0.4352	4.0287	-4.9335
H	0.4670	3.4997	-5.2722
H	-0.9542	4.3636	-5.8384
C	-0.0290	5.2247	-4.0768
H	0.6552	5.8733	-4.6344
H	-0.9163	5.8324	-3.8496
C	0.6168	4.7702	-2.7695
H	0.8549	5.6341	-2.1380
H	1.5692	4.2643	-2.9859
C	-0.3048	3.8121	-2.0109
H	-1.2235	4.3617	-1.7595
H	0.1432	3.5075	-1.0578
C	-3.5248	-2.0977	1.1890
H	-3.0827	-1.8277	2.1617
C	-2.9987	-3.4903	0.8051
H	-3.4365	-3.7898	-0.1574
H	-1.9126	-3.4682	0.6559
C	-3.3731	-4.5336	1.8605
H	-2.9947	-5.5169	1.5590
H	-2.8774	-4.2824	2.8099
C	-4.8847	-4.5851	2.0727
H	-5.1333	-5.2974	2.8667
H	-5.3653	-4.9596	1.1580
C	-5.4429	-3.2048	2.4099
H	-5.0653	-2.8852	3.3918
H	-6.5345	-3.2435	2.4958
C	-5.0514	-2.1573	1.3605
H	-5.5211	-2.4198	0.4025
H	-5.4647	-1.1864	1.6575
C	-4.1192	3.0302	0.8156
H	-4.2349	2.7817	1.8720
H	-5.1015	3.1521	0.3556
C	-4.4759	-0.8110	-3.7404
H	-4.0268	-1.6587	-4.2847
H	-4.6263	0.0114	-4.4456
P	0.8424	-1.2449	-0.2891
P	0.0825	0.7486	1.7742
N	1.1425	-1.8042	2.4811
N	2.6626	0.8832	0.4443
C	0.8925	-2.4219	1.1693
H	-0.0665	-2.9618	1.1812
H	1.6860	-3.1603	1.0112
C	0.1630	-0.7790	2.8708
H	0.4103	-0.4867	3.8962
H	-0.8560	-1.2009	2.8814
C	2.5615	-0.4936	-0.0690
H	3.1432	-1.1530	0.5847
H	3.0566	-0.5005	-1.0452
C	1.9277	1.1636	1.6905
H	2.0308	2.2370	1.8784
H	2.4341	0.6429	2.5109
C	1.2131	-2.4070	-1.7200
H	1.3517	-1.7018	-2.5565
C	2.4779	-3.2725	-1.6172
H	3.3640	-2.6674	-1.3926
H	2.3685	-3.9930	-0.7945
C	2.7068	-4.0554	-2.9156
H	2.9071	-3.3480	-3.7328
H	3.6039	-4.6768	-2.8149
C	1.4975	-4.9173	-3.2706
H	1.6663	-5.4337	-4.2217

H	1.3733	-5.7008	-2.5094
C	0.2242	-4.0771	-3.3440
H	-0.6447	-4.7150	-3.5427
H	0.2979	-3.3757	-4.1876
C	0.0003	-3.2837	-2.0540
H	-0.1832	-3.9870	-1.2280
H	-0.8945	-2.6572	-2.1401
C	-0.4628	2.0372	3.0454
H	-1.4626	1.6843	3.3503
C	-0.6317	3.4075	2.3737
H	0.3508	3.7738	2.0400
H	-1.2379	3.3184	1.4622
C	-1.2435	4.4379	3.3266
H	-1.3271	5.4075	2.8218
H	-2.2666	4.1277	3.5861
C	-0.4201	4.5716	4.6059
H	-0.9024	5.2725	5.2956
H	0.5616	5.0016	4.3614
C	-0.2280	3.2142	5.2765
H	-1.1987	2.8378	5.6290
H	0.4071	3.3114	6.1640
C	0.3880	2.1901	4.3161
H	1.3992	2.5253	4.0454
H	0.5042	1.2348	4.8395
C	1.1276	-2.8700	3.4974
H	0.1466	-3.3651	3.5600
H	1.3629	-2.4489	4.4798
C	2.4160	1.8748	-0.6054
H	3.1282	1.7147	-1.4206
H	2.5734	2.8791	-0.2012
H	1.3953	1.7991	-0.9952
H	1.8785	-3.6260	3.2482
H	-5.4572	-1.1221	-3.3704
H	-3.5480	3.9545	0.7157
H	2.8652	-1.4390	2.7522
H	-2.4347	1.7720	0.5533
O	3.8426	-1.3077	2.9211
H	4.8246	-0.1358	2.1448
H	4.0713	-1.7816	3.7270
H	6.6309	2.0991	-0.1767
H	8.3370	1.2646	-1.7665
C	6.8300	1.0331	-0.2553
C	7.7890	0.5612	-1.1478
H	4.1660	0.8672	0.9569
N	5.1259	0.6056	1.4679
C	6.1463	0.1209	0.5410
H	8.8021	-1.1668	-1.9331
C	8.0495	-0.8048	-1.2400
H	5.4604	1.4133	1.9939
C	7.3533	-1.7042	-0.4361
C	6.3939	-1.2449	0.4639
H	5.8537	-1.9350	1.1062
H	7.5637	-2.7672	-0.4982
N	6.2825	2.6375	2.9811
C	6.8028	3.4152	3.6627
C	7.4562	4.3898	4.5179
H	8.3718	3.9628	4.9373
H	7.7145	5.2828	3.9415
H	6.7917	4.6765	5.3379
N	4.5545	-2.6709	5.1597
C	4.9000	-3.2573	6.0961
C	5.3343	-3.9932	7.2699
H	6.2665	-4.5232	7.0535
H	5.5040	-3.3057	8.1035
H	4.5724	-4.7221	7.5605

eNiH^{2+}:Et$_3$N

Ni	0.7317	0.0360	0.2111
P	-0.4265	1.5531	-0.8099
P	-0.1331	-1.3375	-1.2356
N	-2.7836	-0.0938	-1.5601
N	-0.1221	0.5065	-3.4117
C	-2.2757	1.2486	-1.1040
H	-2.7450	1.4386	-0.1336
H	-2.6728	1.9783	-1.8136
C	-2.0222	-1.2814	-1.0613
H	-2.4927	-2.1531	-1.5222
H	-2.1951	-1.3345	0.0183
C	0.2517	1.6223	-2.5572
H	-0.1034	2.5275	-3.0608
H	1.3461	1.7230	-2.4393
C	0.2230	-0.8500	-3.0047
H	1.3040	-1.0539	-3.1147
H	-0.2928	-1.5276	-3.6953
C	-0.5626	3.3913	-0.3836
H	0.4994	3.6910	-0.3609
C	-1.2863	4.3287	-1.3622
H	-0.9009	4.2242	-2.3821
H	-2.3553	4.0761	-1.3980
C	-1.1494	5.7898	-0.9171
H	-0.0912	6.0829	-0.9662
H	-1.6825	6.4379	-1.6212
C	-1.6745	5.9983	0.5013
H	-1.5207	7.0363	0.8148
H	-2.7602	5.8271	0.5174
C	-1.0012	5.0443	1.4864
H	-1.4317	5.1614	2.4878
H	0.0649	5.3039	1.5684
C	-1.1323	3.5888	1.0295
H	-2.1978	3.3163	1.0351
H	-0.6481	2.9079	1.7433
C	0.0731	-3.2052	-1.3269
H	-0.3755	-3.5447	-0.3781
C	1.5613	-3.5827	-1.2906
H	2.0457	-3.2457	-2.2187
H	2.0592	-3.0577	-0.4680
C	1.7445	-5.0962	-1.1491
H	2.8129	-5.3407	-1.1546
H	1.3555	-5.4140	-0.1708
C	1.0181	-5.8574	-2.2561
H	1.1137	-6.9371	-2.0991
H	1.4963	-5.6402	-3.2216
C	-0.4557	-5.4629	-2.3236
H	-0.9687	-5.7915	-1.4086
H	-0.9504	-5.9717	-3.1584
C	-0.6211	-3.9465	-2.4787
H	-0.1717	-3.6442	-3.4341
H	-1.6887	-3.7008	-2.5416
C	-3.0215	-0.1408	-3.0324
H	-3.3824	-1.1369	-3.2940
H	-2.0880	0.1048	-3.5449
C	0.3176	0.7384	-4.7845
H	-0.0762	-0.0479	-5.4364
H	1.4168	0.7455	-4.8809
P	2.9050	0.3686	0.2324
P	0.8947	-0.6801	2.2716
N	3.5958	-1.3708	2.2867
N	2.0046	1.8477	2.4134
C	3.9213	-1.0521	0.9058
H	3.7923	-1.9161	0.2304
H	4.9790	-0.7707	0.8715
C	2.2707	-1.9420	2.4718
H	2.2295	-2.3475	3.4864
H	2.0646	-2.7772	1.7790
C	3.2489	1.6145	1.6105
H	4.0402	1.2966	2.2929
H	3.5125	2.5771	1.1649
C	1.6489	0.7015	3.3125
H	0.9090	1.0766	4.0234
H	2.5522	0.3882	3.8393
C	4.0371	1.0407	-1.1085
H	3.4870	1.9130	-1.4981
C	5.4316	1.5181	-0.6745
H	5.3709	2.2682	0.1234
H	6.0059	0.6738	-0.2696
C	6.2001	2.1067	-1.8635
H	5.6855	3.0135	-2.2122
H	7.1959	2.4222	-1.5330
C	6.3097	1.1072	-3.0126
H	6.8235	1.5652	-3.8644
H	6.9291	0.2559	-2.6971
C	4.9328	0.6000	-3.4363
H	5.0288	-0.1592	-4.2209
H	4.3549	1.4293	-3.8699
C	4.1615	0.0185	-2.2488
H	4.6899	-0.8728	-1.8817
H	3.1667	-0.3159	-2.5670
C	-0.4037	-1.3452	3.4554

H	-0.6879	-2.3081	2.9999
C	-1.6396	-0.4376	3.4400
H	-1.3736	0.5498	3.8490
H	-1.9572	-0.2629	2.4041
C	-2.7806	-1.0231	4.2753
H	-3.6347	-0.3359	4.2705
H	-3.1242	-1.9578	3.8085
C	-2.3367	-1.3082	5.7086
H	-3.1532	-1.7710	6.2732
H	-2.1082	-0.3592	6.2143
C	-1.1025	-2.2054	5.7316
H	-1.3604	-3.1967	5.3332
H	-0.7618	-2.3639	6.7606
C	0.0418	-1.6139	4.9010
H	0.3662	-0.6731	5.3697
H	0.8989	-2.2945	4.9379
C	4.6232	-2.2318	2.8723
H	4.6886	-3.2162	2.3791
H	4.4093	-2.3912	3.9330
C	2.0429	3.1433	3.1391
H	2.2217	3.9495	2.4257
H	2.8480	3.1179	3.8757
H	1.0876	3.3022	3.6419
H	5.5989	-1.7434	2.7946
H	-0.0663	1.6991	-5.1403
H	-3.7912	0.5937	-3.2727
H	-3.8069	-0.1754	-1.1487
H	-0.4273	0.7336	0.9301
N	-5.4476	-0.2666	-0.7121
C	-5.7344	-1.6675	-0.3137
C	-6.3150	0.1044	-1.8605
C	-5.7404	0.6368	0.4255
H	-5.0339	-1.9298	0.4844
H	-6.7460	-1.7163	0.1222
C	-5.6240	-2.6974	-1.4277
H	-5.7068	-3.6983	-0.9939
H	-6.4168	-2.6052	-2.1738
H	-4.6598	-2.6452	-1.9467
H	-7.3569	-0.1670	-1.6237
C	-6.2673	1.5709	-2.2656
H	-6.0156	-0.5149	-2.7100
H	-6.7695	1.6893	-3.2302
H	-6.7805	2.2236	-1.5553
H	-5.2410	1.9403	-2.3808
C	-4.9899	0.3178	1.7066
H	-5.4875	1.6522	0.1089
H	-6.8247	0.6272	0.6254
H	-5.1480	1.1290	2.4238
H	-5.3313	-0.6044	2.1829
H	-3.9100	0.2335	1.5350

eNiH^{2+}: H$_2$O:Et$_3$N

Ni	-0.8302	-0.1860	0.0580
P	-0.7002	-1.2714	-1.8060
P	-0.3846	1.6235	-1.0946
N	1.7363	0.1839	-2.3578
N	-1.5756	0.7974	-3.4560
C	0.8676	-0.9518	-2.7993
H	1.4981	-1.8435	-2.7527
H	0.6113	-0.7555	-3.8442
C	1.0672	1.5202	-2.2883
H	0.7461	1.7710	-3.3020
H	1.8453	2.2113	-1.9585
C	-1.9330	-0.5435	-3.0221
H	-1.9750	-1.1725	-3.9162
H	-2.9290	-0.5844	-2.5426
C	-1.6935	1.8215	-2.4274
H	-2.6874	1.8214	-1.9497
H	-1.5610	2.7925	-2.9149
C	-0.8655	-3.1211	-2.1567
H	-1.8876	-3.3463	-1.8055
C	-0.7662	-3.5818	-3.6199
H	-1.4833	-3.0526	-4.2560
H	0.2347	-3.3526	-4.0129
C	-1.0086	-5.0906	-3.7433
H	-2.0452	-5.3124	-3.4525
H	-0.9116	-5.3899	-4.7925
C	-0.0493	-5.8925	-2.8681
H	-0.2736	-6.9620	-2.9388
H	0.9779	-5.7654	-3.2379
C	-0.1217	-5.4332	-1.4134
H	0.6099	-5.9753	-0.8028
H	-1.1151	-5.6773	-1.0084
C	0.1179	-3.9256	-1.2936
H	1.1478	-3.7098	-1.6147
H	0.0688	-3.6031	-0.2444
C	-0.0668	3.3677	-0.4701
H	0.9118	3.2547	0.0264
C	-1.0763	3.7869	0.6035
H	-2.0740	3.8818	0.1510
H	-1.1480	3.0057	1.3693
C	-0.6847	5.1238	1.2392
H	-1.4370	5.4155	1.9810
H	0.2608	4.9960	1.7863
C	-0.5184	6.2200	0.1885
H	-0.1869	7.1507	0.6614
H	-1.4934	6.4352	-0.2709
C	0.4685	5.7986	-0.8981
H	1.4740	5.7002	-0.4646
H	0.5373	6.5693	-1.6737
C	0.0608	4.4658	-1.5359
H	-0.9065	4.6038	-2.0378
H	0.7836	4.1922	-2.3148
C	2.9222	0.2706	-3.2580
H	3.5896	1.0435	-2.8774

H	2.5900	0.5195	-4.2675
C	-2.3298	1.1740	-4.6510
H	-1.9848	2.1471	-5.0119
H	-3.4159	1.2380	-4.4687
P	-2.7932	-0.0883	1.0626
P	0.0373	-0.7470	1.9937
N	-1.9362	0.2242	3.6981
N	-1.9234	-2.6788	1.5921
C	-2.8176	0.8148	2.7041
H	-2.5836	1.8767	2.5144
H	-3.8388	0.7752	3.0993
C	-0.5202	0.3726	3.3963
H	0.0363	0.1157	4.3019
H	-0.2496	1.4094	3.1270
C	-3.1452	-1.8222	1.7160
H	-3.4650	-1.8341	2.7604
H	-3.9105	-2.2913	1.0934
C	-0.8382	-2.3229	2.5629
H	-0.1339	-3.1575	2.5626
H	-1.2900	-2.2115	3.5504
C	-4.4843	0.3814	0.3783
H	-4.4830	-0.0404	-0.6392
C	-5.7154	-0.1645	1.1195
H	-5.6884	-1.2574	1.2000
H	-5.7364	0.2272	2.1461
C	-7.0095	0.2440	0.4047
H	-7.0403	-0.2394	-0.5821
H	-7.8695	-0.1393	0.9650
C	-7.1131	1.7573	0.2341
H	-8.0198	2.0131	-0.3243
H	-7.2119	2.2305	1.2212
C	-5.8802	2.3169	-0.4718
H	-5.9367	3.4095	-0.5346
H	-5.8459	1.9438	-1.5056
C	-4.5957	1.9105	0.2546
H	-4.6040	2.3552	1.2594
H	-3.7199	2.3243	-0.2588
C	1.7987	-1.1835	2.4989
H	2.3329	-0.2209	2.4262
C	2.4140	-2.1433	1.4708
H	1.8674	-3.0986	1.4938
H	2.2951	-1.7349	0.4612
C	3.8906	-2.4167	1.7630
H	4.2837	-3.1338	1.0328
H	4.4528	-1.4835	1.6170
C	4.1011	-2.9300	3.1853
H	5.1690	-3.0681	3.3867
H	3.6373	-3.9215	3.2872
C	3.4888	-1.9774	4.2086
H	4.0294	-1.0204	4.1905
H	3.6008	-2.3771	5.2224
C	2.0052	-1.7184	3.9241
H	1.4547	-2.6619	4.0503

H	1.6125	-1.0240	4.6745
C	-2.2449	0.7428	5.0307
H	-2.0665	1.8276	5.1194
H	-1.6309	0.2299	5.7765
C	-2.2579	-4.1264	1.6285
H	-2.9910	-4.3454	0.8502
H	-2.6758	-4.3716	2.6067
H	-1.3524	-4.7101	1.4567
H	-3.2950	0.5471	5.2660
H	-2.1569	0.4393	-5.4427
H	3.4379	-0.6911	-3.2615
H	2.1485	0.0400	-1.4023
H	0.6565	-0.0356	0.2346
O	3.3257	0.6188	-0.2569
H	2.9667	0.7435	0.6269
H	4.3213	0.8728	-0.2086
N	5.9257	1.2988	-0.1625
C	6.6214	0.5146	-1.2068
C	6.5014	0.9901	1.1649
C	6.0721	2.7437	-0.4465
H	6.3262	0.9286	-2.1755
H	7.7093	0.6696	-1.1220
C	6.2998	-0.9729	-1.1910
H	6.7402	-1.4499	-2.0721
H	6.7065	-1.4869	-0.3156
H	5.2178	-1.1414	-1.2079
H	7.5214	1.4030	1.2276
C	5.6686	1.4798	2.3400
H	6.5996	-0.0961	1.2377
H	6.1479	1.1761	3.2756
H	5.5656	2.5682	2.3724
H	4.6641	1.0409	2.3251
C	5.1914	3.2474	-1.5795
H	5.8084	3.2897	0.4626
H	7.1299	2.9722	-0.6538
H	5.3154	4.3290	-1.6882
H	5.4449	2.8003	-2.5463
H	4.1367	3.0464	-1.3624

B:2S

N	0.0046	-0.3126	-0.7748
H	-0.8461	-0.8415	-0.6323
H	0.8578	-0.8336	-0.6187
C	-0.0047	1.0014	-0.3703
C	-1.2152	1.6972	-0.1896
H	-2.1528	1.1671	-0.3392
C	-1.2169	3.0383	0.1722
H	-2.1685	3.5486	0.3046
C	-0.0232	3.7320	0.3681
H	-0.0303	4.7806	0.6506
C	1.1798	3.0488	0.1933
H	2.1243	3.5675	0.3425
C	1.1962	1.7078	-0.1683
H	2.1409	1.1860	-0.3011
N	-2.7814	-1.8322	-0.2194
C	-3.8660	-2.1209	0.0673
C	-5.2272	-2.4839	0.4273
H	-5.9149	-2.2175	-0.3804
H	-5.2963	-3.5606	0.6071
H	-5.5303	-1.9555	1.3357
N	2.7986	-1.8089	-0.1956
C	3.8894	-2.0930	0.0718
C	5.2582	-2.4504	0.4075
H	5.5578	-1.9611	1.3388
H	5.3457	-3.5331	0.5352
H	5.9370	-2.1343	-0.3897

B:3H_2O:4S

N	-0.1061	0.0134	-0.2727
H	0.3261	0.5801	-1.0186
H	0.4609	-0.0753	0.5760
C	-1.4363	0.3046	-0.0244
C	-2.2527	0.8585	-1.0294
H	-1.8110	1.0860	-1.9957
C	-3.5949	1.1261	-0.7828
H	-4.2012	1.5636	-1.5727
C	-4.1666	0.8486	0.4626
H	-5.2138	1.0663	0.6526
C	-3.3610	0.2915	1.4604
H	-3.7833	0.0703	2.4380
C	-2.0173	0.0207	1.2273
H	-1.3909	-0.4022	2.0090
O	0.6115	-2.7261	-0.1112
H	0.2853	-1.8516	-0.4390
H	-0.1809	-3.2972	-0.1182
O	1.1723	-1.1351	2.0747
H	0.9806	-1.8938	1.4767
H	2.1417	-1.1035	2.0966
O	0.9759	1.7479	-2.2877
H	1.9404	1.7120	-2.1447
H	0.7112	2.5975	-1.8891
N	-2.0473	-3.8329	-0.3163
C	-3.0762	-3.3238	-0.4753
C	-4.3610	-2.6785	-0.6756
H	-4.2956	-1.6267	-0.3745
H	-4.6465	-2.7306	-1.7302
H	-5.1290	-3.1753	-0.0756
N	4.1653	-1.5702	1.1791
C	3.9320	-2.2736	0.2854
C	3.5894	-3.1466	-0.8219
H	3.9655	-2.7292	-1.7604
H	4.0247	-4.1386	-0.6707
H	2.4917	-3.2206	-0.8592
N	3.7212	1.6709	-1.2627
C	4.4391	1.6108	-0.3555
C	5.3290	1.5198	0.7889
H	5.1757	0.5533	1.2813
H	6.3707	1.6011	0.4654
H	5.1143	2.3264	1.4959
N	-0.0691	3.9245	-0.6071
C	-0.8824	3.8817	0.2178
C	-1.9026	3.8196	1.2497
H	-1.4452	3.5880	2.2156
H	-2.4239	4.7785	1.3234
H	-2.6237	3.0320	1.0057

BH^+:3S

N	-0.0763	-0.0017	-0.1806
H	-1.0587	-0.3435	-0.2159
H	-0.0708	0.9841	-0.5224
C	0.4702	-0.0859	1.1742
C	-0.1856	-0.8491	2.1311
H	-1.1079	-1.3663	1.8838
C	0.3584	-0.9353	3.4109
H	-0.1454	-1.5280	4.1678
C	1.5395	-0.2650	3.7175
H	1.9591	-0.3348	4.7162
C	2.1830	0.4971	2.7442
H	3.1031	1.0214	2.9819
C	1.6501	0.5905	1.4619
H	2.1432	1.1846	0.6978
H	0.4908	-0.5805	-0.8405
N	-2.8255	-0.9206	-0.2996
C	-3.9302	-1.2563	-0.3828
C	-5.3150	-1.6773	-0.4881
H	-5.9433	-1.0678	0.1678
H	-5.6635	-1.5640	-1.5186
H	-5.4099	-2.7271	-0.1954
N	1.5633	-1.6207	-1.8840
C	2.2444	-2.2967	-2.5307
C	3.1008	-3.1450	-3.3419
H	2.9826	-4.1907	-3.0435
H	2.8346	-3.0442	-4.3982
H	4.1470	-2.8545	-3.2094
N	-0.0736	2.7408	-1.0508
C	-0.0680	3.8587	-1.3560
C	-0.0727	5.2596	-1.7452
H	0.5871	5.8333	-1.0881
H	0.2750	5.3602	-2.7772
H	-1.0873	5.6613	-1.6714

BH^+:3 H_2O:5S

N	-0.2020	-0.8101	-0.1347
H	-1.1163	-0.3593	-0.4421
H	0.0048	-0.6492	0.8866

C	-0.1819	-2.2306	-0.4554
C	-0.9268	-2.6948	-1.5343
H	-1.5386	-2.0019	-2.1048
C	-0.8877	-4.0519	-1.8451
H	-1.4689	-4.4259	-2.6827
C	-0.1130	-4.9256	-1.0850
H	-0.0883	-5.9831	-1.3304
C	0.6238	-4.4432	-0.0052
H	1.2217	-5.1231	0.5944
C	0.5937	-3.0890	0.3179
H	1.1531	-2.6933	1.1614
H	0.6091	-0.3118	-0.5667
O	2.1953	0.5031	-0.3129
H	2.9789	-0.0119	-0.6002
H	2.3457	1.4168	-0.6323
O	1.1633	-0.3589	2.1007
H	1.7592	0.1222	1.4888
H	1.0791	0.1800	2.9111
O	-2.5086	0.1208	-1.0953
H	-2.6840	1.0651	-1.2830
H	-3.3182	-0.2225	-0.6645
N	4.4951	-1.0205	-1.0717
C	5.4156	-1.6910	-1.2768
C	6.5722	-2.5314	-1.5346
H	6.6251	-2.7805	-2.5984
H	7.4882	-2.0074	-1.2475
H	6.4994	-3.4573	-0.9573
N	2.7479	3.1410	-1.3164
C	3.1036	4.1542	-1.7495
C	3.5507	5.4265	-2.2921
H	4.3885	5.2688	-2.9780
H	2.7348	5.9113	-2.8365
H	3.8770	6.0858	-1.4828
N	1.0319	1.2120	4.5346
C	1.0486	1.6557	5.6041
C	1.0691	2.2123	6.9469
H	1.8948	2.9227	7.0477
H	0.1285	2.7317	7.1536
H	1.2002	1.4133	7.6822
N	-4.8992	-0.9316	0.1265
C	-5.8802	-1.4291	0.4862
C	-7.1124	-2.0530	0.9364
H	-7.3207	-1.7715	1.9723
H	-7.9475	-1.7305	0.3080
H	-7.0255	-3.1417	0.8764
N	-3.2111	2.8684	-1.6559
C	-3.6913	3.8710	-1.9793
C	-4.2947	5.1290	-2.3864
H	-4.5340	5.7342	-1.5076
H	-3.6040	5.6886	-3.0242
H	-5.2156	4.9395	-2.9460

H_2O:2S

O	-0.0002	1.9915	0.0002
H	-0.7598	1.3952	0.0060
H	0.7598	1.3957	-0.0060
N	2.4392	0.0833	-0.0102
C	3.5222	-0.3271	-0.0035
C	4.8821	-0.8421	0.0050
H	5.3194	-0.7697	-0.9949
H	5.4988	-0.2655	0.7004
H	4.8880	-1.8906	0.3164
N	-2.4386	0.0817	0.0096
C	-3.5221	-0.3277	0.0033
C	-4.8824	-0.8413	-0.0047
H	-4.9356	-1.7627	-0.5917
H	-5.2116	-1.0551	1.0162
H	-5.5603	-0.1046	-0.4451

S

N	-0.0004	-0.0186	-1.4376
C	0.0003	-0.0029	-0.2780
C	0.0001	0.0148	1.1769
H	0.7797	-0.6474	1.5646
H	0.1879	1.0281	1.5439
H	-0.9673	-0.3221	1.5606

H_2O

O	0.0000	0.1183	0.0000
H	0.7586	-0.4731	0.0000
H	-0.7586	-0.4731	0.0000