

Towards more effective beryllium chelation: An investigation of second-sphere hydrogen bonding

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Supporting Information:

Gibbs free energy ($\Delta G \approx \varepsilon_0 + G_{\text{correction}}$) kJ/mol
xyz cartesian coordinates

HL				C	1.78992	-0.05975	1.28709
$\Delta G =$	-1087.602947			C	0.96116	-0.15389	3.56221
C	-0.67758	2.14381	1.77255	C	-0.36165	-0.11628	3.10568
C	0.46667	1.60046	1.18965	H	1.16036	-0.20489	4.62547
H	-0.58633	2.88808	2.55707	C	-0.55926	-0.05735	1.74607
C	0.29262	0.65084	0.18177	H	-1.19734	-0.13515	3.79114
H	1.45565	1.89843	1.51066	C	-1.94600	-0.02032	1.08831
C	1.46317	-0.04131	-0.52395	H	-2.69303	-0.03705	1.87666
H	1.14444	-0.17333	-1.55970	C	-3.12588	2.19436	0.58407
C	3.00516	1.61321	-1.66121	C	-3.24695	3.33344	-0.21142
C	4.16328	2.38300	-1.67317	H	-3.78222	2.03044	1.42798
H	2.31342	1.64117	-2.49496	C	-1.42491	2.55901	-1.54864
C	4.68428	1.46998	0.47066	C	-2.38729	3.51825	-1.29001
C	5.02676	2.31297	-0.58245	H	-4.00858	4.06969	0.01280
H	4.38945	3.02188	-2.51924	H	-0.72891	2.65328	-2.37140
H	5.33248	1.38517	1.33827	H	-2.45454	4.39051	-1.92511
H	5.94239	2.89039	-0.54692	C	-2.17174	-1.24988	0.20243
C	1.72866	-1.45148	-0.00023	C	-3.30188	-3.26871	-0.40947
C	1.76708	-3.12994	1.72134	C	-1.46121	-2.44901	-1.69312
C	2.50854	-3.55928	-0.50591	C	-2.43956	-3.40605	-1.49289
C	2.29442	-4.02041	0.78980	H	-4.07582	-4.00450	-0.23047
H	1.58179	-3.44284	2.74271	H	-0.76235	-2.50869	-2.51654
H	2.91445	-4.22240	-1.26466	H	-2.51689	-4.24041	-2.17598
H	2.53091	-5.04384	1.05405	C	-2.14755	1.26463	0.27915
C	2.73920	0.79483	-0.55750	C	-3.16644	-2.17923	0.45047
C	1.47927	-1.82878	1.32184	H	-3.82326	-2.05440	1.30066
H	1.06678	-1.11527	2.02342	N	0.48904	-0.03153	0.88300
N	-0.91459	0.25546	-0.23463	N	-1.31313	1.45497	-0.77908
N	3.57122	0.72544	0.49144	N	-1.33612	-1.39208	-0.86196
N	2.23444	-2.30945	-0.90021	C	2.01997	-0.12789	2.67312
C	-1.93321	1.73363	1.34999	H	3.02451	-0.16292	3.06196
H	-2.84017	2.12165	1.78728	C	2.87603	-0.01770	0.28184
C	-3.33425	0.29479	-0.20885	C	4.21584	-0.00656	0.73456
C	-3.33696	-0.40613	-1.43206	C	2.67766	0.01489	-1.13056
C	-4.59659	0.51740	0.48235	C	5.29508	0.02636	-0.12944
C	-4.49046	-0.90253	-2.02244	H	4.42309	-0.01975	1.79436
H	-2.38211	-0.55231	-1.92309	C	3.77646	0.04523	-1.99519
C	-5.76356	-0.02601	-0.16397	C	5.07299	0.05012	-1.50857
C	-5.71767	-0.70506	-1.36543	H	6.30213	0.03437	0.26797
H	-4.44397	-1.42697	-2.97035	H	3.57494	0.06615	-3.05903
H	-6.71153	0.12588	0.34458	H	5.90741	0.07465	-2.19954
H	-6.63663	-1.08525	-1.80402	O	1.45820	0.01836	-1.73643
O	-4.71245	1.13829	1.59961	Al	-0.04325	0.02463	-0.92287
C	-2.03699	0.76985	0.32252				

HL Be (II)

$\Delta G = -1102.257071$

C	-1.69975	-0.00109	-1.30112
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HL Al (III)

$\Delta G = -1329.760349$

C	-0.89206	-0.00257	-3.58252	C	0.53834	-0.00010	-3.18065
C	0.43005	-0.00194	-3.12342	H	-0.98497	-0.00017	-4.70336
H	-1.09274	-0.00338	-4.64725	C	0.73975	-0.00006	-1.82285
C	0.62366	-0.00100	-1.75672	H	1.37678	-0.00012	-3.86280
H	1.26869	-0.00222	-3.80640	C	2.08153	-0.00002	-1.09883
C	1.99153	-0.00026	-1.07470	H	2.90932	-0.00003	-1.80068
H	2.77794	-0.00046	-1.82496	C	3.04125	2.24303	-0.20611
C	3.10217	2.20432	-0.35380	C	2.89695	3.28404	0.71363
C	3.11957	3.29075	0.51921	H	3.85907	2.22354	-0.91322
H	3.83759	2.10713	-1.14159	C	0.92592	2.23485	1.57809
C	1.20026	2.38197	1.61939	C	1.83328	3.28006	1.61233
C	2.15651	3.38320	1.52026	H	3.61514	4.09429	0.72502
H	3.87858	4.05670	0.41620	H	0.07363	2.16182	2.23906
H	0.42446	2.40007	2.37462	H	1.70163	4.07475	2.33321
H	2.14152	4.21353	2.21344	C	2.10934	-1.22543	-0.19326
C	2.11754	-1.24016	-0.19212	C	2.89702	-3.28396	0.71382
C	3.12121	-3.28905	0.52260	C	0.92596	-2.23476	1.57822
C	1.20141	-2.38010	1.62183	C	1.83334	-3.27995	1.61252
C	2.15816	-3.38097	1.52372	H	3.61522	-4.09419	0.72526
H	3.88058	-4.05473	0.42038	H	0.07367	-2.16171	2.23918
H	0.42560	-2.39783	2.37704	H	1.70171	-4.07460	2.33344
H	2.14355	-4.21061	2.21772	C	2.10931	1.22545	-0.19333
C	2.11690	1.24064	-0.19343	C	3.04129	-2.24300	-0.20597
C	3.10330	-2.20351	-0.35149	H	3.85912	-2.22352	-0.91309
H	3.83868	-2.10675	-1.13938	N	-0.31011	-0.00003	-0.96014
N	-0.41013	-0.00065	-0.89389	N	1.07901	1.23945	0.68681
N	1.18766	1.33610	0.77961	N	1.07904	-1.23941	0.68688
N	1.18832	-1.33508	0.78099	C	-1.84500	-0.00011	-2.74803
C	-1.94814	-0.00216	-2.68794	H	-2.85781	-0.00013	-3.12008
H	-2.95877	-0.00271	-3.06636	C	-2.63759	-0.00002	-0.32970
C	-2.75235	-0.00042	-0.26994	C	-4.01030	-0.00002	-0.64743
C	-4.11138	-0.00028	-0.65212	C	-2.27566	0.00001	1.03348
C	-2.44617	0.00014	1.12863	C	-4.97511	0.00001	0.34537
C	-5.14151	0.00026	0.27184	H	-4.32620	-0.00003	-1.68188
H	-4.37111	-0.00052	-1.70248	C	-3.24423	0.00004	2.03371
C	-3.51303	0.00060	2.05181	C	-4.58911	0.00004	1.68991
C	-4.83302	0.00065	1.63834	H	-6.02403	0.00001	0.07770
H	-6.17160	0.00037	-0.06282	H	-2.92373	0.00006	3.06793
H	-3.25796	0.00095	3.10537	H	-5.33964	0.00006	2.47131
H	-5.62743	0.00104	2.37670	O	-0.97005	0.00002	1.43826
O	-1.21199	0.00021	1.62137	B	0.09591	0.00001	0.54027
Be	0.04205	0.00021	0.74551				

HL Ca (II)

$\Delta G = -1765.133379$

HL B(III)				C	-1.85751	-0.20375	1.23694
$\Delta G = -1112.127021$				C	-0.95836	-0.51822	3.45991
C	-1.60695	-0.00005	-1.36588	C	0.31193	-0.29057	2.94263
C	-0.78660	-0.00013	-3.63892				

H	-1.09482	-0.72798	4.51449	C	0.53052	-0.35108	-1.71759
C	0.44590	-0.05987	1.57499	H	1.17832	-0.52362	-3.75544
H	1.18425	-0.30091	3.58319	C	1.93319	-0.17050	-1.14126
C	1.86409	0.17022	1.03736	H	2.64210	-0.25523	-1.96204
H	2.48803	0.27415	1.92309	C	2.99588	2.14654	-1.02866
C	3.54890	-1.69820	0.79082	C	3.09245	3.39569	-0.42132
C	4.04272	-2.81127	0.11885	H	3.61159	1.89329	-1.88226
H	4.03225	-1.33813	1.69021	C	1.39524	2.70969	1.11674
C	2.27509	-2.54120	-1.46003	C	2.27881	3.68409	0.67027
C	3.39240	-3.24584	-1.03204	H	3.79263	4.13177	-0.79750
H	4.91905	-3.32958	0.48959	H	0.73599	2.88606	1.95792
H	1.74087	-2.84829	-2.35284	H	2.32253	4.64274	1.17035
H	3.73694	-4.10776	-1.58850	C	2.25675	-1.24260	-0.11811
C	2.03734	1.47738	0.26849	C	3.54714	-3.07304	0.73647
C	3.01540	3.66998	0.10002	C	1.67036	-2.18963	1.92523
C	1.57183	2.78474	-1.57986	C	2.71042	-3.10341	1.84939
C	2.36299	3.82891	-1.11866	H	4.36776	-3.77420	0.64617
H	3.64323	4.45757	0.49959	H	0.98833	-2.17038	2.76719
H	1.04405	2.86821	-2.52399	H	2.85462	-3.82021	2.64671
H	2.46059	4.73587	-1.70112	C	2.08983	1.21998	-0.52139
C	2.41827	-1.04482	0.29557	C	3.31866	-2.12980	-0.26087
C	2.85064	2.48026	0.80117	H	3.95174	-2.07862	-1.13711
H	3.34737	2.32761	1.75099	N	-0.50188	-0.31968	-0.84830
N	-0.60596	-0.03229	0.73539	N	1.30730	1.50384	0.53580
N	1.79399	-1.46387	-0.81662	N	1.45126	-1.28041	0.95824
N	1.40871	1.63349	-0.90769	C	-2.03084	-0.48534	-2.66261
C	-2.04483	-0.47623	2.60442	H	-3.04687	-0.48331	-3.02915
H	-3.04097	-0.66702	2.97870	C	-2.89180	-0.21349	-0.31889
C	-3.05622	-0.08370	0.37104	C	-4.16954	-0.71114	-0.64836
C	-4.20062	0.53616	0.90959	C	-2.73237	0.49018	0.91552
C	-3.11636	-0.62109	-0.95664	C	-5.27437	-0.50614	0.16126
C	-5.39456	0.63473	0.20779	H	-4.29211	-1.28775	-1.55717
H	-4.14031	0.97242	1.90085	C	-3.88025	0.71529	1.71004
C	-4.36125	-0.53358	-1.63775	C	-5.12350	0.23075	1.34338
C	-5.46873	0.08017	-1.07644	H	-6.23845	-0.91313	-0.11812
H	-6.24885	1.13546	0.64772	H	-3.74831	1.27278	2.63037
H	-4.41153	-0.96130	-2.63377	H	-5.97924	0.41207	1.98490
H	-6.39492	0.13593	-1.63997	O	-1.57430	0.96570	1.34927
O	-2.08865	-1.18489	-1.53628	Co	-0.03295	-0.00889	1.02632
Ca	-0.14038	-0.16569	-1.77373				

HL Co (III)

$\Delta G = -2469.956572$

HL Co (II)

$\Delta G = -2470.174092$

C	-1.78640	-0.35727	-1.28319	C	-1.72793	1.08831	-0.82966
C	-0.97690	-0.57497	-3.55388	C	-0.88611	2.39378	-2.70139
C	0.33273	-0.49533	-3.08127	C	0.38038	1.84640	-2.50280
H	-1.16940	-0.67508	-4.61529	H	-1.06273	3.09250	-3.50919
				C	0.57061	1.00065	-1.43055
				H	1.20662	2.07394	-3.16207

C	1.92603	0.35482	-1.18966	H	4.69418	0.02933	0.09928
H	2.57232	0.58896	-2.03076	C	3.79686	2.20578	1.08652
C	3.75515	1.54959	0.16434	C	3.23426	3.34023	1.63424
C	4.19928	1.98249	1.41187	H	4.87140	2.09125	1.03038
H	4.33554	1.72230	-0.73210	C	1.08069	2.39557	1.19199
C	2.21422	1.07173	2.39198	C	1.84149	3.43435	1.70379
C	3.42043	1.74057	2.54008	H	3.86228	4.13981	2.00673
H	5.14433	2.50375	1.50012	H	-0.00089	2.45119	1.20217
H	1.56691	0.85989	3.23393	H	1.34865	4.29819	2.12867
H	3.73335	2.06344	3.52365	C	3.06812	-1.28138	-0.23717
C	1.76694	-1.15100	-1.08014	C	3.48714	-3.59136	-0.85238
C	2.19804	-3.42381	-1.69392	C	1.26950	-2.74766	-0.52179
C	0.72010	-2.88052	0.10874	C	2.10845	-3.81179	-0.82426
C	1.34420	-3.83812	-0.67607	H	4.17213	-4.39493	-1.09278
H	2.69333	-4.15252	-2.32324	H	0.19481	-2.87509	-0.48741
H	0.04105	-3.14285	0.90882	H	1.68367	-4.78450	-1.03269
H	1.15172	-4.88532	-0.48690	C	2.97761	1.15437	0.60500
C	2.54054	0.88502	0.08982	C	3.96468	-2.32931	-0.55807
C	2.41208	-2.06334	-1.90198	H	5.02714	-2.12356	-0.55659
H	3.06886	-1.70995	-2.68561	N	-1.27423	0.88659	-0.76802
N	-0.44136	0.69412	-0.57303	N	1.61360	1.28645	0.64497
N	1.79709	0.65768	1.18230	N	1.71679	-1.51019	-0.24474
N	0.94458	-1.57183	-0.10331	C	-3.17155	1.51586	-1.90907
C	-1.92393	2.00227	-1.88546	H	-4.24262	1.54566	-2.05938
H	-2.91202	2.38850	-2.07437	C	-3.22438	-0.03671	0.18166
C	-2.88272	0.53372	-0.10902	C	-4.59535	0.04373	0.48240
C	-4.20112	0.82188	-0.52409	C	-2.41422	-1.03222	0.82981
C	-2.73574	-0.37483	0.97338	C	-5.19007	-0.81077	1.39616
C	-5.30274	0.25343	0.09122	H	-5.19392	0.80374	-0.00750
H	-4.38163	1.48880	-1.35384	C	-3.05260	-1.89365	1.74763
C	-3.85908	-0.96545	1.58104	C	-4.40536	-1.78442	2.02846
C	-5.13204	-0.64792	1.15005	H	-6.24636	-0.72394	1.61964
H	-6.29647	0.50246	-0.25909	H	-2.44537	-2.64939	2.23244
H	-3.68900	-1.65348	2.39945	H	-4.85664	-2.46132	2.74578
H	-5.99331	-1.09791	1.62921	O	-1.11200	-1.22913	0.60446
O	-1.55020	-0.65543	1.48876	Cr	0.24485	-0.03063	-0.11461
Co	0.08670	-0.25692	0.96679				

HL Cr(III)

$\Delta G = -2131.748214$

HL Cr(II)

$\Delta G = -2131.841939$

C	-2.61311	0.82762	-0.82218	C	-1.81195	0.75885	-1.05313
C	-2.31369	2.10345	-2.84701	C	-0.95621	1.81468	-3.06277
C	-0.91571	1.96995	-2.78055	C	0.32234	1.36893	-2.73834
H	-2.75251	2.61992	-3.69416	H	-1.12510	2.39131	-3.96360
C	-0.41397	1.28592	-1.67224	C	0.50294	0.68999	-1.54882
H	-0.28191	2.34259	-3.57438	H	1.16783	1.56186	-3.38431
C	3.61325	-0.02101	0.12526	C	1.90623	0.23119	-1.16067
				H	2.55049	0.40794	-2.01776

C	3.55931	1.85265	-0.07299
C	3.96072	2.56049	1.05714
H	4.10872	1.92405	-1.00231
C	2.10919	1.62498	2.24349
C	3.22620	2.44469	2.23376
H	4.83745	3.19496	1.01804
H	1.50242	1.50399	3.13271
H	3.50576	2.97803	3.13214
C	1.95580	-1.25276	-0.83443
C	2.74131	-3.48956	-1.17763
C	1.21237	-2.95745	0.58057
C	1.97130	-3.90072	-0.09342
H	3.34283	-4.20365	-1.72625
H	0.59042	-3.22189	1.42691
H	1.95157	-4.93279	0.22894
C	2.43239	1.04626	0.00853
C	2.73397	-2.14902	-1.55421
H	3.32263	-1.80049	-2.39235
N	-0.53002	0.42784	-0.70335
N	1.72632	0.94041	1.14772
N	1.21184	-1.66190	0.21086
C	-2.01042	1.50501	-2.22856
H	-3.00049	1.84988	-2.48050
C	-2.97805	0.32935	-0.25623
C	-4.26776	0.35723	-0.82931
C	-2.87665	-0.15538	1.07012
C	-5.39317	-0.03659	-0.12424
H	-4.39666	0.66319	-1.85757
C	-4.01866	-0.54207	1.78572
C	-5.26993	-0.48012	1.19616
H	-6.36288	-0.00813	-0.60530
H	-3.88736	-0.89594	2.80066
H	-6.14603	-0.78795	1.75461
O	-1.69538	-0.26814	1.68852
Cr	0.01820	-0.25615	1.13320

HL Cu(II)

$\Delta G = -2727.87861$

C	-1.81960	0.07834	-1.34054
C	-0.98099	0.42758	-3.58194
C	0.32469	0.30534	-3.10593
H	-1.16015	0.62046	-4.63288
C	0.50641	0.07836	-1.75037
H	1.17664	0.40446	-3.76523
C	1.90869	0.01993	-1.14005
H	2.61604	0.05808	-1.96560
C	3.14016	2.18570	-0.60788

C	3.34807	3.28071	0.22667
H	3.71118	2.06514	-1.51966
C	1.65228	2.41874	1.67343
C	2.59212	3.40187	1.38876
H	4.09021	4.02732	-0.02929
H	1.03784	2.46963	2.56445
H	2.72303	4.23733	2.06401
C	2.16540	-1.27415	-0.38266
C	3.38196	-3.30982	-0.01373
C	1.57374	-2.65193	1.40281
C	2.56780	-3.56518	1.08626
H	4.16653	-4.00340	-0.29060
H	0.91136	-2.80578	2.24553
H	2.69278	-4.45379	1.69041
C	2.17997	1.24168	-0.25182
C	3.17907	-2.15119	-0.75681
H	3.79751	-1.92521	-1.61553
N	-0.54226	-0.05300	-0.91757
N	1.45377	1.36301	0.87198
N	1.38150	-1.53352	0.68138
C	-2.04805	0.33247	-2.70559
H	-3.05515	0.47764	-3.06764
C	-2.92869	-0.02084	-0.37046
C	-4.21386	-0.36814	-0.83765
C	-2.77173	0.26485	1.02194
C	-5.32170	-0.40606	-0.00792
H	-4.33964	-0.63480	-1.87961
C	-3.92003	0.24701	1.84456
C	-5.16843	-0.07964	1.34459
H	-6.28937	-0.68867	-0.40374
H	-3.78520	0.48851	2.89249
H	-6.02443	-0.09399	2.01051
O	-1.61710	0.57897	1.60233
Cu	-0.05059	-0.20841	1.02135

HL Fe(II)

$\Delta G = -2351.116474$

C	-1.81913	-0.40315	-1.24833
C	-1.00886	-0.66204	-3.51500
C	0.30060	-0.56484	-3.04308
H	-1.20032	-0.78125	-4.57465
C	0.49936	-0.39354	-1.68369
H	1.14550	-0.59749	-3.71798
C	1.90998	-0.18984	-1.13229
H	2.59874	-0.29128	-1.96830
C	2.99899	2.11255	-1.11497
C	3.14188	3.37411	-0.54387

H	3.57951	1.82640	-1.98280	C	-1.85189	1.82958	-2.10847
C	1.48964	2.75967	1.06973	C	-2.92516	2.70608	-2.11199
C	2.37473	3.70565	0.56914	H	-4.58076	3.45358	-0.95604
H	3.84186	4.08638	-0.96383	H	-1.18685	1.72687	-2.95778
H	0.86620	2.97128	1.93022	H	-3.11587	3.31396	-2.98582
H	2.45550	4.67499	1.04337	C	-2.02374	-1.25016	0.72451
C	2.27124	-1.23956	-0.09996	C	-2.89238	-3.47996	0.78637
C	3.61623	-3.04167	0.73578	C	-1.21861	-2.83408	-0.79436
C	1.77060	-2.16026	1.97396	C	-2.05050	-3.81122	-0.27115
C	2.81777	-3.06275	1.87705	H	-3.55519	-4.22224	1.21335
H	4.44221	-3.73397	0.62814	H	-0.54331	-3.03860	-1.61514
H	1.12232	-2.14089	2.84220	H	-2.03179	-4.80735	-0.69164
H	2.99731	-3.76397	2.68118	C	-2.35881	1.12163	0.05848
C	2.09424	1.21605	-0.55211	C	-2.88035	-2.18233	1.29183
C	3.33994	-2.11650	-0.26529	H	-3.52546	-1.89400	2.11092
H	3.94206	-2.06926	-1.16344	N	0.48960	0.34295	0.76743
N	-0.53279	-0.35765	-0.80959	N	-1.58197	1.06233	-1.03537
N	1.35590	1.54087	0.52449	N	-1.21276	-1.58304	-0.29586
N	1.50066	-1.26694	1.00225	C	1.99554	1.12508	2.44456
C	-2.06202	-0.55889	-2.62636	H	2.99674	1.37803	2.75264
H	-3.07716	-0.56348	-2.99480	C	2.93949	0.25584	0.31568
C	-2.93136	-0.23282	-0.29783	C	4.25075	0.29327	0.83243
C	-4.21079	-0.72415	-0.63660	C	2.80394	-0.13614	-1.03820
C	-2.78811	0.50006	0.92280	C	5.35533	-0.00791	0.05120
C	-5.32760	-0.48408	0.14490	H	4.42456	0.53985	1.86910
H	-4.32446	-1.32460	-1.53079	C	3.92485	-0.43345	-1.83210
C	-3.95016	0.76390	1.68555	C	5.19511	-0.36590	-1.29249
C	-5.19166	0.28534	1.30867	H	6.34375	0.02897	0.49176
H	-6.29082	-0.88769	-0.14235	H	3.75625	-0.71973	-2.86253
H	-3.82842	1.34613	2.59184	H	6.05805	-0.59954	-1.90421
H	-6.05798	0.49637	1.92643	O	1.61208	-0.24585	-1.61458
O	-1.63445	0.96853	1.37208	Fe	-0.04052	-0.18230	-1.04051
Fe	-0.05445	0.01118	1.08576				

HL K(I)

$\Delta G = -1687.507056$

HL Fe (III)

$\Delta G = -2350.913228$

C	1.77896	0.57874	1.16603	C	-2.02651	-0.83465	-0.38030
C	0.95255	1.34881	3.31741	C	-1.20473	-2.98018	-1.11781
C	-0.33828	1.01937	2.92006	C	0.08032	-2.45583	-1.09647
H	1.14010	1.76660	4.29837	H	-1.37564	-4.00841	-1.41708
C	-0.53336	0.53146	1.64125	C	0.25404	-1.12721	-0.69224
H	-1.18393	1.15051	3.58101	H	0.93386	-3.05565	-1.38996
C	-1.94245	0.19373	1.18256	C	1.67608	-0.54991	-0.72342
H	-2.61576	0.33368	2.02368	H	2.11943	-0.92851	-1.64796
C	-3.45079	1.97448	0.12054	C	1.85196	1.55839	-2.10125
C	-3.73419	2.77872	-0.98125	C	1.90352	2.94420	-2.20625
H	-4.06378	2.00656	1.01132	H	1.91072	0.93566	-2.98602
				C	1.71056	3.04053	0.17014

C	1.83360	3.70787	-1.04432	H	3.45051	4.42285	-0.85791
H	2.00240	3.41770	-3.17629	H	0.74204	3.05468	2.18244
H	1.65291	3.60027	1.09931	H	2.12643	4.88941	1.22555
H	1.87522	4.78958	-1.07299	C	2.34919	-1.06092	0.01221
C	2.55697	-1.08570	0.40423	C	3.91764	-2.75919	0.66913
C	4.68244	-1.92345	1.16303	C	1.99962	-2.21004	1.98158
C	2.79947	-1.69263	2.61142	C	3.14579	-2.97840	1.80673
C	4.12865	-2.06217	2.43311	H	4.81862	-3.33497	0.49206
H	5.71338	-2.19992	0.97426	H	1.36842	-2.34791	2.85353
H	2.33114	-1.78489	3.58711	H	3.41995	-3.72420	2.54205
H	4.70580	-2.44733	3.26444	C	1.96445	1.41300	-0.36789
C	1.72501	0.97129	-0.83788	C	3.51456	-1.78757	-0.24188
C	3.88583	-1.43073	0.13507	H	4.09252	-1.59425	-1.13719
H	4.28332	-1.31783	-0.86664	N	-0.55590	-0.15534	-0.68947
N	-0.76559	-0.34365	-0.32843	N	1.25888	1.66882	0.74475
N	1.65518	1.70641	0.28031	N	1.60596	-1.27296	1.10876
N	2.02538	-1.21402	1.62761	C	-2.01396	-0.97938	-2.38868
C	-2.27085	-2.16133	-0.76154	H	-3.00238	-1.27890	-2.70787
H	-3.28599	-2.53767	-0.77547	C	-2.95119	-0.18907	-0.18853
C	-3.16916	0.07478	-0.09623	C	-4.21798	0.05207	-0.76117
C	-4.15841	0.21419	-1.07913	C	-2.82430	-0.17868	1.25457
C	-3.29177	0.77147	1.16184	C	-5.36114	0.27350	-0.00749
C	-5.26475	1.04696	-0.91405	H	-4.30266	0.09496	-1.84130
H	-4.04265	-0.33186	-2.01156	C	-4.03291	0.02658	1.99427
C	-4.43853	1.61970	1.29042	C	-5.25640	0.24795	1.39162
C	-5.38900	1.75336	0.28910	H	-6.30968	0.47116	-0.49287
H	-6.00294	1.14753	-1.70134	H	-3.94704	0.01439	3.07648
H	-4.55089	2.15977	2.22647	H	-6.13700	0.41152	2.00596
H	-6.23966	2.41148	0.44460	O	-1.71344	-0.35735	1.89154
O	-2.45013	0.62783	2.12853	Li	-0.02423	0.05332	1.26671
K	0.05629	0.70749	2.46027				

HL Mg (II)

$\Delta G = -1287.592403$

HL Li (I)

$\Delta G = -1095.118333$

C	-1.81177	-0.44621	-1.09669	C	-1.82719	0.34534	-1.16132
C	-0.93878	-1.13848	-3.24663	C	-0.96648	0.86788	-3.36624
C	0.34204	-0.78946	-2.81847	C	0.32238	0.58327	-2.91708
H	-1.09150	-1.54170	-4.24153	H	-1.13162	1.18016	-4.39078
C	0.48338	-0.31690	-1.51711	C	0.48276	0.23664	-1.58405
H	1.20197	-0.89971	-3.46710	H	1.17681	0.64977	-3.57750
C	1.87630	0.01144	-0.96930	C	1.88989	-0.01972	-1.03202
H	2.56177	-0.01300	-1.81592	H	2.56241	-0.00795	-1.88745
C	2.76531	2.38526	-0.97223	C	3.45349	1.88710	-0.42017
C	2.83458	3.65441	-0.40545	C	3.82993	2.91036	0.44460
H	3.32386	2.14958	-1.86976	H	4.01115	1.69390	-1.32740
C	1.32989	2.89266	1.28465	C	1.99413	2.31127	1.84929
C	2.10266	3.91762	0.74886	C	3.08705	3.12991	1.60088
				H	4.69131	3.52666	0.21662

H	1.38628	2.44151	2.73671	H	1.34755	4.96056	-1.12736
H	3.34465	3.91566	2.29863	C	2.85820	-0.83756	0.19258
C	2.03572	-1.39321	-0.37993	C	4.50767	-2.01693	1.45909
C	3.00726	-3.58846	-0.30022	C	2.51976	-1.15576	2.48554
C	1.42894	-2.84422	1.32821	C	3.73419	-1.81579	2.60558
C	2.26268	-3.84379	0.84728	H	5.45074	-2.54625	1.52659
H	3.66934	-4.34302	-0.70762	H	1.86218	-1.00368	3.33274
H	0.82755	-2.99574	2.21678	H	4.06078	-2.17581	3.57226
H	2.32167	-4.79371	1.36193	C	2.06951	1.20160	-1.14413
C	2.34324	1.10782	-0.10493	C	4.06613	-1.53684	0.23142
C	2.89313	-2.34831	-0.92154	H	4.63986	-1.68418	-0.67451
H	3.46116	-2.12235	-1.81472	N	-1.12196	-1.02957	-0.96729
N	-0.55605	0.13123	-0.73317	N	1.19752	1.72753	-0.25468
N	1.62980	1.32154	1.01660	N	2.10377	-0.67887	1.30378
N	1.31721	-1.64602	0.73068	C	-3.26193	-1.75758	-1.62830
C	-2.03346	0.75959	-2.49386	H	-4.33416	-1.78503	-1.49997
H	-3.02640	1.00977	-2.83617	C	-3.04271	-0.10898	0.27690
C	-2.98115	0.13663	-0.25510	C	-4.39766	0.27944	0.19891
C	-4.23905	-0.13182	-0.84221	C	-2.27401	0.33615	1.39526
C	-2.90704	0.20239	1.17858	C	-5.00154	1.04710	1.17932
C	-5.39935	-0.28546	-0.10239	H	-4.98275	-0.01142	-0.66429
H	-4.30297	-0.25032	-1.91654	C	-2.91453	1.10473	2.39145
C	-4.11898	0.07338	1.90736	C	-4.24998	1.45240	2.29002
C	-5.33346	-0.16386	1.29198	H	-6.04107	1.33470	1.08113
H	-6.33773	-0.50248	-0.59835	H	-2.31822	1.41964	3.23985
H	-4.05042	0.15415	2.98679	H	-4.70927	2.05034	3.06959
H	-6.23092	-0.26874	1.89294	O	-0.99093	0.04740	1.56583
O	-1.79915	0.39135	1.85553	Mn	0.34125	-0.20932	0.22882
Mg	-0.00521	-0.05514	1.33337				

HL Mn (II)

$\Delta G = -2238.333752$

C	-2.48074	-0.96433	-0.77353
C	-2.67945	-2.53532	-2.62389
C	-1.28935	-2.56583	-2.79056
H	-3.31065	-3.13699	-3.26877
C	-0.60473	-1.77523	-1.89583
H	-0.80131	-3.16524	-3.54571
C	2.20913	-0.26771	-1.01107
H	2.41322	-0.79659	-1.93663
C	2.68906	1.99531	-2.11231
C	2.43362	3.36193	-2.10441
H	3.35865	1.54852	-2.83599
C	0.94382	3.04321	-0.25444
C	1.55927	3.89982	-1.15688
H	2.91273	4.00744	-2.83103
H	0.23030	3.40111	0.47814

HL Na (I)

$\Delta G = -1249.873668$

C	-1.84766	-0.73102	-1.02458
C	-0.90390	-1.77723	-2.98748
C	0.34481	-1.29969	-2.60178
H	-1.01256	-2.36405	-3.89285
C	0.43948	-0.56726	-1.41614
H	1.22568	-1.49365	-3.20136
C	1.82433	-0.05766	-0.99094
H	2.44719	-0.14242	-1.88138
C	2.41708	2.33995	-1.51152
C	2.44530	3.69023	-1.17837
H	2.82995	1.99647	-2.45231
C	1.36455	3.11637	0.86977
C	1.90870	4.09224	0.04136
H	2.88103	4.41323	-1.85823
H	0.93450	3.38732	1.82929
H	1.90967	5.13098	0.34708

C	2.48685	-0.95676	0.05455	C	3.34594	-3.29035	0.27172
C	4.33325	-2.34946	0.72496	C	1.42184	-2.57119	1.49543
C	2.42885	-1.98572	2.11586	C	2.44276	-3.49010	1.31373
C	3.66656	-2.59061	1.92271	H	4.15286	-3.99265	0.10217
H	5.29989	-2.79846	0.52794	H	0.69093	-2.68070	2.28732
H	1.87584	-2.14667	3.03628	H	2.51958	-4.34286	1.97475
H	4.08886	-3.22912	2.68844	C	2.19280	1.21628	-0.29814
C	1.84987	1.42448	-0.61801	C	3.20100	-2.17869	-0.55156
C	3.73621	-1.52276	-0.22129	H	3.88651	-1.99410	-1.36825
H	4.22909	-1.31940	-1.16423	N	-0.53201	-0.15542	-0.89547
N	-0.62322	-0.29640	-0.64844	N	1.52863	1.34711	0.86032
N	1.33119	1.81439	0.55510	N	1.28805	-1.49778	0.69526
N	1.84736	-1.18828	1.20976	C	-2.03946	0.11821	-2.71237
C	-2.00651	-1.49552	-2.19518	H	-3.05165	0.22340	-3.07551
H	-2.98592	-1.86830	-2.46539	C	-2.91120	-0.05575	-0.36323
C	-3.04002	-0.36529	-0.21990	C	-4.20304	-0.45979	-0.74902
C	-4.19128	0.05493	-0.90810	C	-2.70775	0.42038	0.96505
C	-3.06603	-0.47075	1.22269	C	-5.28196	-0.38044	0.11741
C	-5.37397	0.39598	-0.25925	H	-4.35651	-0.85981	-1.74423
H	-4.14574	0.13816	-1.98999	C	-3.82235	0.51858	1.82366
C	-4.30653	-0.12294	1.84961	C	-5.08485	0.12760	1.40740
C	-5.41772	0.29806	1.13861	H	-6.26255	-0.71154	-0.20157
H	-6.23478	0.73558	-0.82346	H	-3.65765	0.90161	2.82402
H	-4.34630	-0.20351	2.93209	H	-5.92054	0.20422	2.09450
H	-6.32886	0.55520	1.67177	O	-1.52039	0.81100	1.41979
O	-2.06271	-0.87501	1.92679	Ni	-0.09763	-0.21265	0.96915
Na	-0.11198	0.19909	1.72317				

HL V(II)

$\Delta G = -2031.393522$

HL Ni(II)

$\Delta G = -2595.691069$

C	-1.81019	-0.04967	-1.33722	C	-2.24791	0.75281	-1.21152
C	-0.97339	0.18746	-3.59197	C	-1.42338	1.39728	-3.38327
C	0.32986	0.12695	-3.10078	C	-0.08955	1.33642	-2.94750
H	-1.15104	0.31680	-4.65267	H	-1.63080	1.68952	-4.40746
C	0.51764	-0.03288	-1.73644	C	0.12743	0.94961	-1.61900
H	1.18382	0.21548	-3.75889	H	0.72192	1.59090	-3.61761
C	1.92124	-0.04553	-1.13489	C	3.17594	-1.11686	-0.32491
H	2.62699	-0.04720	-1.96291	H	4.05429	-1.59278	-0.74262
C	3.09560	2.17979	-0.74322	C	4.72682	0.69688	0.15950
C	3.31011	3.31085	0.04005	C	5.01410	1.92913	0.71663
H	3.61836	2.04652	-1.68196	H	5.50852	0.09208	-0.28126
C	1.73271	2.43794	1.60987	C	2.69028	2.14796	1.24259
C	2.61690	3.44528	1.23924	C	3.97759	2.66840	1.28810
H	4.00848	4.07354	-0.28316	H	6.02780	2.31018	0.71119
H	1.16960	2.49885	2.53415	H	1.85995	2.72015	1.64403
H	2.75578	4.30739	1.87884	H	4.14991	3.63432	1.74315
C	2.15431	-1.29331	-0.31168	C	2.03517	-1.96027	-0.25108
				C	1.15402	-4.21237	-0.48803

C	-0.17590	-2.41460	0.36822	C	5.09002	-2.92574	3.68552
C	-0.05664	-3.75678	0.04109	H	5.94997	-4.21937	2.17324
H	1.27891	-5.24950	-0.77340	H	4.10587	-1.42408	4.88522
H	-1.10587	-2.02239	0.75724	H	5.16049	-3.64887	4.48661
H	-0.89972	-4.41869	0.18632	C	5.02128	1.46412	0.96813
C	3.40365	0.19726	0.17533	C	5.48135	-2.29412	1.38905
C	2.19331	-3.31636	-0.63280	H	5.84131	-2.49577	0.38884
H	3.15092	-3.63639	-1.02226	N	1.30857	0.52469	2.67267
N	-0.94533	0.66740	-0.91738	N	4.48208	1.95597	2.14326
N	2.39295	0.95743	0.69790	N	4.43676	-0.76706	2.93959
N	0.82088	-1.52187	0.21730	C	-0.94382	0.27571	2.63994
C	-2.50765	1.12633	-2.53850	H	-1.93639	0.31081	3.06825
H	-3.51999	1.22845	-2.90603	C	0.41224	1.07145	4.75660
C	-3.14785	0.49109	-0.08898	C	-0.62456	1.26525	5.67744
C	-4.54083	0.42084	-0.26920	C	1.75804	1.29941	5.18637
C	-2.60509	0.33254	1.23097	C	-0.35709	1.67046	6.97823
C	-5.40408	0.20449	0.79263	H	-1.64856	1.09526	5.36858
H	-4.94616	0.53553	-1.26812	C	2.01269	1.70779	6.50075
C	-3.50713	0.11551	2.29323	C	0.96204	1.89150	7.38779
C	-4.87540	0.05319	2.08106	H	-1.17328	1.81370	7.67506
H	-6.47314	0.15248	0.62631	H	3.04007	1.87156	6.80018
H	-3.09390	0.00046	3.28871	H	1.16968	2.20669	8.40304
H	-5.53797	-0.11558	2.92299	O	2.84721	1.13699	4.38917
O	-1.30401	0.39152	1.52607	V	3.17500	0.64932	2.68924
V	0.32637	0.47710	0.48428				

HL Zn(II)

$\Delta G = -2866.763982$

HL V(III)

$\Delta G = -2031.169819$

C	0.18402	0.63359	3.38651	C	-1.94475	-0.63744	-0.76869
C	-0.77247	-0.14856	1.30564	C	-1.27179	-1.90409	-2.72145
C	0.47611	-0.24365	0.67392	C	0.06729	-1.67647	-2.40133
H	-1.65839	-0.42396	0.74511	H	-1.53009	-2.48391	-3.59975
C	1.56437	0.13284	1.47258	C	0.33834	-0.88290	-1.29790
H	0.57605	-0.58623	-0.34565	H	0.86887	-2.08375	-3.00302
C	5.10231	0.06579	0.76350	C	1.77988	-0.52584	-0.91902
H	5.40021	-0.23227	-0.23435	H	2.43248	-1.12717	-1.54842
C	5.51381	2.38100	0.00182	C	3.04127	1.29332	-2.17763
C	5.59736	3.71178	0.32097	C	3.27070	2.64169	-2.43516
H	5.85851	2.00229	-0.95128	H	3.59543	0.52518	-2.70107
C	4.59290	3.27670	2.46177	C	1.59880	3.17512	-0.81478
C	5.16364	4.16474	1.58963	C	2.53744	3.60133	-1.74317
H	6.00741	4.41709	-0.39074	H	4.01229	2.93735	-3.16735
H	4.18844	3.56893	3.42151	H	1.00219	3.88042	-0.25003
H	5.25332	5.20556	1.86953	H	2.68452	4.65929	-1.91508
C	4.99657	-0.99440	1.69401	C	2.11716	-0.87120	0.53099
C	5.54270	-3.23799	2.38095	C	3.36765	-2.11437	2.16146
C	4.52418	-1.70314	3.92777	C	1.74636	-0.47913	2.79487
				C	2.69227	-1.42484	3.16397

H	4.11258	-2.86024	2.41090	C	-2.66742	0.46006	0.36219
H	1.19179	0.08392	3.53517	C	-1.30260	-1.63407	-1.28763
H	2.88922	-1.61090	4.21143	H	-1.59130	-0.74013	-1.82179
C	2.08234	0.93823	-1.23310	N	0.77569	0.27533	0.62718
C	3.07729	-1.83447	0.82921	N	-2.30216	1.38528	-0.53834
H	3.58831	-2.35396	0.02894	N	-0.88448	-2.73188	0.80210
N	-0.63880	-0.37404	-0.52794	C	1.86337	1.84526	2.07572
N	1.37902	1.87303	-0.56752	H	2.74986	2.41615	2.32343
N	1.46727	-0.21009	1.50928	C	3.11302	0.79902	0.16900
C	-2.27243	-1.38505	-1.91893	C	4.27973	0.40592	0.83560
H	-3.30521	-1.54793	-2.18809	C	3.13153	1.04964	-1.25913
C	-2.98874	-0.17477	0.17595	C	5.48838	0.18954	0.17168
C	-4.22037	-0.87160	0.16844	H	4.23065	0.24210	1.90925
C	-2.84413	0.91496	1.10126	C	4.39201	0.79945	-1.90301
C	-5.29185	-0.52697	0.97292	C	5.52363	0.38750	-1.21528
H	-4.32883	-1.73546	-0.47445	H	6.36934	-0.13247	0.71513
C	-3.96923	1.26125	1.89367	H	4.43665	0.96494	-2.97627
C	-5.16232	0.56740	1.83742	H	6.44866	0.22084	-1.76153
H	-6.20842	-1.10315	0.93661	O	2.12087	1.49557	-1.91264
H	-3.84745	2.10107	2.56869	N	-0.14279	-4.92468	0.91388
H	-5.98883	0.86418	2.47455	H	-0.41487	-4.88073	1.88591
O	-1.76293	1.65472	1.27058	N	-2.81945	3.05536	-2.05658
Zn	0.00396	1.10734	0.80495	H	-1.83140	3.26516	-2.04204
				H	-0.23351	-5.84336	0.50522
				H	-3.41020	3.85354	-2.23744

HL-NH2

$\Delta G = -1198.346393$

C	1.87302	0.98604	0.96774
C	0.70793	1.95571	2.84369
C	-0.41193	1.21679	2.48521
H	0.68251	2.60960	3.70884
C	-0.33459	0.39026	1.35736
H	-1.32842	1.27520	3.06101
C	-1.57283	-0.42201	0.95959
H	-1.97900	-0.83215	1.88778
C	-3.99248	0.28115	0.75577
C	-4.97098	1.09625	0.17938
H	-4.25254	-0.46843	1.49256
C	-3.24400	2.16100	-1.09258
C	-4.60795	2.04791	-0.75632
H	-6.01110	0.98757	0.46637
H	-5.34332	2.69463	-1.21970
C	-1.23973	-1.64033	0.10255
C	-0.96995	-2.80789	-1.96925
C	-0.55923	-3.85238	0.14361
C	-0.58969	-3.93463	-1.26178
H	-1.00741	-2.83737	-3.05279
H	-0.32469	-4.85678	-1.76525

HL-NH2 Al (III)

$\Delta G = -1440.51567$

C	1.85971	-0.05368	1.47278
C	1.08015	-0.14758	3.76276
C	-0.25298	-0.11383	3.33766
H	1.30292	-0.19750	4.82151
C	-0.48238	-0.05651	1.98147
H	-1.07243	-0.13498	4.04253
C	-1.87555	-0.02599	1.33619
H	-2.61282	-0.04244	2.13369
C	-3.08125	2.16090	0.85713
C	-3.22618	3.31041	0.05150
H	-3.72490	1.98891	1.70808
C	-1.39283	2.57469	-1.32160
C	-2.40100	3.52140	-1.02244
H	-3.99580	4.03522	0.28675
H	-2.49788	4.40020	-1.64560
C	-2.12043	-1.26561	0.46463
C	-3.26717	-3.26861	-0.13582
C	-1.39974	-2.49709	-1.44130
C	-2.42663	-3.44108	-1.20486

H	-4.05127	-3.99186	0.05143	C	3.09980	3.29696	-0.26674
H	-2.52382	-4.28905	-1.86932	C	1.19056	2.38858	-1.41366
C	-2.10323	1.26208	0.53388	C	2.16668	3.40252	-1.27243
C	-3.11681	-2.16372	0.72922	H	3.85263	4.06766	-0.14992
H	-3.76896	-2.02621	1.58000	H	2.16547	4.24083	-1.95702
N	0.55148	-0.02771	1.10371	C	2.10606	-1.24635	0.42515
N	-1.27045	1.46235	-0.54761	C	3.08398	2.19692	0.60996
N	-1.27761	-1.42308	-0.61516	H	3.81160	2.09755	1.40347
C	2.12273	-0.12046	2.85160	N	-0.42864	-0.00021	1.11261
H	3.13558	-0.15436	3.21937	N	1.17767	-1.34038	-0.56120
C	2.91177	-0.01241	0.42926	N	1.17750	1.34062	-0.56080
C	4.26419	0.00509	0.83893	C	-1.97685	-0.00066	2.89600
C	2.66935	0.01151	-0.97709	H	-2.98952	-0.00082	3.26910
C	5.31653	0.03481	-0.05873	C	-2.76575	-0.00015	0.47179
H	4.50281	-0.00074	1.89250	C	-4.12656	-0.00014	0.84432
C	3.73960	0.03880	-1.87512	C	-2.45544	0.00003	-0.92247
C	5.05152	0.04915	-1.42969	C	-5.15094	0.00001	-0.08713
H	6.33545	0.04738	0.30715	H	-4.39311	-0.00023	1.89285
H	3.50532	0.05256	-2.93238	C	-3.51068	0.00017	-1.85408
H	5.86343	0.07067	-2.14701	C	-4.83502	0.00015	-1.45036
O	1.42747	0.00855	-1.55072	H	-6.18300	0.00002	0.24141
N	-0.55085	-2.62393	-2.47683	H	-3.24825	0.00029	-2.90578
H	0.27342	-2.04855	-2.57799	H	-5.62397	0.00026	-2.19428
N	-0.56371	2.73759	-2.36790	O	-1.20926	0.00009	-1.41228
H	0.24157	2.14785	-2.52244	N	0.26817	2.40789	-2.40475
H	-0.59957	-3.44318	-3.06204	H	-0.49042	1.73641	-2.38383
H	-0.60748	3.58586	-2.91067	N	0.26841	-2.40725	-2.40542
Al	-0.04336	0.01859	-0.67119	H	-0.49024	-1.73585	-2.38431
				H	0.15460	3.23936	-2.96127
				H	0.15499	-3.23852	-2.96224
				Be	0.05251	0.00005	-0.51446

HL-NH2 Be (II)

$\Delta G = -1213.012537$

C	-1.71905	-0.00035	1.51258
C	-0.92420	-0.00079	3.79658
C	0.39921	-0.00061	3.34473
H	-1.13074	-0.00103	4.86023
C	0.60230	-0.00032	1.97801
H	1.23396	-0.00070	4.03256
C	1.96991	-0.00011	1.29945
H	2.75265	-0.00018	2.05362
C	3.08430	-2.19676	0.60926
C	3.10025	-3.29653	-0.26778
H	3.81191	-2.09752	1.40278
C	1.19084	-2.38808	-1.41437
C	2.16712	-3.40192	-1.27348
H	3.85320	-4.06715	-0.15121
H	2.16601	-4.24003	-1.95831
C	2.10588	1.24642	0.42554

HL-NH2 B (III)

$\Delta G = -1222.878491$

C	-1.61106	0.00120	1.57232
C	-0.77955	0.00246	3.84198
C	0.53761	0.00187	3.37200
H	-0.97262	0.00317	4.90739
C	0.72863	0.00103	2.01080
H	1.38395	0.00207	4.04439
C	2.05665	0.00025	1.28462
H	2.88611	0.00039	1.98440
C	3.03928	-2.21306	0.48117
C	2.94507	-3.29430	-0.42158
H	3.82634	-2.15660	1.21937
C	0.99345	-2.27736	-1.42771
C	1.94632	-3.32714	-1.35539

H	3.66958	-4.09807	-0.37834
H	1.86244	-4.14126	-2.06269
C	2.10036	1.22952	0.39470
C	2.94693	3.29255	-0.42492
C	0.99472	2.27569	-1.43002
C	1.94818	3.32502	-1.35874
H	3.67188	4.09596	-0.38248
H	1.86474	4.13849	-2.06684
C	2.09966	-1.22997	0.39598
C	3.04055	2.21215	0.47889
H	3.82759	2.15598	1.21713
N	-0.31835	0.00077	1.14801
N	1.07597	-1.25433	-0.52552
N	1.07666	1.25353	-0.52679
C	-1.84102	0.00212	2.95365
H	-2.85230	0.00260	3.32908
C	-2.66182	0.00065	0.55721
C	-4.02898	0.00068	0.89454
C	-2.32335	0.00005	-0.80639
C	-5.00852	0.00023	-0.08477
H	-4.33100	0.00102	1.93304
C	-3.30211	-0.00037	-1.79544
C	-4.64320	-0.00026	-1.43373
H	-6.05327	0.00027	0.19869
H	-3.00111	-0.00079	-2.83582
H	-5.40379	-0.00059	-2.20508
O	-1.01573	-0.00017	-1.22981
N	0.04087	2.29017	-2.36819
H	-0.62392	1.53854	-2.45738
N	0.03954	-2.29224	-2.36582
H	-0.62475	-1.54027	-2.45581
H	0.01106	3.04751	-3.03201
H	0.00930	-3.05020	-3.02891
B	0.10120	-0.00005	-0.36330

HL-NH2 Ca (II)

$\Delta G = -1875.874369$

C	-1.96864	0.04572	1.30570
C	-1.11269	0.08773	3.56529
C	0.17525	-0.04025	3.05193
H	-1.27167	0.16475	4.63470
C	0.33790	-0.11406	1.67096
H	1.03644	-0.06006	3.70735
C	1.76330	-0.12714	1.10914
H	2.41150	-0.07151	1.98192
C	3.37571	-2.01540	0.79890
C	3.79219	-3.17991	0.14810

H	3.96323	-1.58821	1.60035
C	1.80708	-3.06422	-1.18964
C	3.00750	-3.71745	-0.84965
H	4.71608	-3.66730	0.43714
H	3.28643	-4.63207	-1.35780
C	2.06711	1.14670	0.31134
C	3.33988	3.14288	-0.03734
C	1.38784	2.64621	-1.33493
C	2.46315	3.50754	-1.04024
H	4.16976	3.79206	0.21753
H	2.57360	4.44314	-1.57417
C	2.19066	-1.41238	0.39629
C	3.13311	1.95675	0.67750
H	3.78011	1.68101	1.49956
N	-0.71029	-0.10799	0.82777
N	1.42518	-1.91218	-0.59820
N	1.24689	1.46264	-0.70711
C	-2.18442	0.15704	2.69208
H	-3.18308	0.32246	3.07131
C	-3.12430	0.13312	0.37701
C	-4.36552	-0.37720	0.80808
C	-3.05425	0.79176	-0.90046
C	-5.52995	-0.23995	0.06648
H	-4.40952	-0.91456	1.74893
C	-4.27233	0.95416	-1.61419
C	-5.47594	0.45079	-1.15098
H	-6.46110	-0.66165	0.42579
H	-4.22129	1.47863	-2.56266
H	-6.37665	0.58402	-1.74188
O	-1.93209	1.23096	-1.42149
N	0.44203	2.95024	-2.28653
H	-0.49314	2.58459	-2.11466
N	1.00621	-3.57651	-2.18661
H	0.01388	-3.40590	-2.11905
H	0.45270	3.89442	-2.64351
H	1.21971	-4.51631	-2.48711
Ca	-0.28866	-0.27771	-1.58748

HL-NH2 Co (II)

$\Delta G = -2580.921115$

C	1.87922	-0.36894	1.43399
C	1.13051	-0.44466	3.73253
C	-0.18910	-0.35612	3.29230
H	1.35071	-0.49152	4.79229
C	-0.42508	-0.28312	1.92783
H	-1.01472	-0.32289	3.99065
C	-1.83611	-0.09001	1.38190

H	-2.51812	-0.11458	2.22922	C	-0.47968	-0.00030	1.93758
C	-2.89250	2.21084	1.17712	H	-1.07497	-0.00068	3.98686
C	-2.97602	3.43899	0.50567	C	-1.91071	-0.00013	1.41940
H	-3.51500	1.99512	2.03490	H	-2.57941	-0.00022	2.27573
C	-1.23515	2.70507	-0.98070	C	-3.16573	2.14887	0.86790
C	-2.15202	3.69641	-0.56894	C	-3.30804	3.24914	0.00483
H	-3.67995	4.19255	0.83912	H	-3.80602	2.01545	1.72844
H	-2.18627	4.64425	-1.09115	C	-1.44527	2.44898	-1.29993
C	-2.24488	-1.19954	0.43058	C	-2.46067	3.40418	-1.06578
C	-3.69258	-2.96863	-0.25768	H	-4.08047	3.98552	0.18983
C	-1.79281	-2.30758	-1.57875	H	-2.54117	4.25331	-1.73186
C	-2.91951	-3.13372	-1.38479	C	-2.17654	-1.23777	0.58557
H	-4.55613	-3.60252	-0.09513	C	-3.30845	-3.24880	0.00384
H	-3.15237	-3.89137	-2.12192	C	-1.44544	-2.44858	-1.30055
C	-1.98699	1.27641	0.70928	C	-2.46101	-3.40370	-1.06673
C	-3.35383	-1.98388	0.67893	H	-4.08101	-3.98512	0.18859
H	-3.94094	-1.83207	1.57408	H	-2.54155	-4.25266	-1.73303
N	0.58428	-0.32928	1.03365	C	-2.17638	1.23779	0.58594
N	-1.19373	1.50842	-0.35830	C	-3.16604	-2.14879	0.86722
N	-1.47646	-1.34904	-0.67606	H	-3.80635	-2.01552	1.72777
C	2.16168	-0.42945	2.80941	N	0.54152	-0.00017	1.03666
H	3.18781	-0.43127	3.14706	N	-1.35069	1.37416	-0.47729
C	2.95791	-0.29041	0.43075	N	-1.35082	-1.37396	-0.47766
C	4.23225	-0.80798	0.73798	C	2.10075	-0.00063	2.82783
C	2.77711	0.37148	-0.82169	H	3.11625	-0.00079	3.18655
C	5.31380	-0.66176	-0.11571	C	2.98364	-0.00010	0.49633
H	4.37035	-1.35211	1.66450	C	4.31642	-0.00009	0.95871
C	3.89865	0.53706	-1.66301	C	2.80575	0.00008	-0.91327
C	5.14194	0.03356	-1.31903	C	5.39448	0.00005	0.08892
H	6.27654	-1.08255	0.14739	H	4.53333	-0.00018	2.01572
H	3.74932	1.06222	-2.59949	C	3.90155	0.00021	-1.79321
H	5.97956	0.16786	-1.99494	C	5.18987	0.00019	-1.29624
O	1.60974	0.85694	-1.23157	H	6.39968	0.00005	0.49119
N	-1.03382	-2.43389	-2.70815	H	3.69839	0.00034	-2.85656
H	-0.07927	-2.10872	-2.70673	H	6.03420	0.00030	-1.97473
N	-0.38795	2.89698	-2.03580	O	1.59256	0.00012	-1.45128
H	0.46411	2.34342	-2.03888	N	-0.59311	-2.56866	-2.34696
H	-1.18110	-3.26137	-3.26650	H	0.28336	-2.06647	-2.35892
H	-0.28399	3.84304	-2.37053	N	-0.59309	2.56914	-2.34646
Co	0.06024	-0.08628	-0.83025	H	0.28332	2.06686	-2.35864
				H	-0.59836	-3.43347	-2.86588
				H	-0.59830	3.43406	-2.86520
				Co	-0.01824	0.00007	-0.75284

HL-NH2 Co (III)

$\Delta G = -2580.701621$

C	1.85148	-0.00029	1.44132
C	1.07509	-0.00077	3.74702
C	-0.24193	-0.00058	3.29764
H	1.29543	-0.00102	4.80695

HL-NH2 Cr (II)

$\Delta G = -2242.635701$

C	-1.86986	-0.44346	1.39430
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C	-1.09025	-0.57400	3.68869	HL-NH2 Cr (III)			
C	0.22002	-0.43424	3.23257	$\Delta G = -2242.495839$			
H	-1.29929	-0.66456	4.74744	C	-1.86913	0.76462	1.26688
C	0.44202	-0.29206	1.87367	C	-1.09389	1.33131	3.49181
H	1.05470	-0.40416	3.92105	C	0.21097	1.01648	3.11449
C	1.83901	0.00281	1.34177	H	-1.30570	1.65725	4.50264
H	2.50503	0.04161	2.20125	C	0.43554	0.59068	1.82021
C	3.54110	-1.75316	0.72753	H	1.03313	1.08355	3.81371
C	4.01350	-2.71784	-0.17168	C	1.82193	0.16255	1.36182
H	4.07501	-1.52779	1.64048	H	2.47927	0.23579	2.22404
C	2.11030	-2.27466	-1.57480	C	2.66131	-2.21933	1.47994
C	3.30486	-2.98109	-1.32173	C	2.60755	-3.54349	1.00788
H	4.92950	-3.25769	0.03705	H	3.34340	-1.93065	2.26719
H	3.63986	-3.72525	-2.03295	C	0.83656	-2.91088	-0.49946
C	1.87941	1.38168	0.68431	C	1.70701	-3.89121	0.03381
C	2.71769	3.61038	0.49365	H	3.26633	-4.29395	1.42748
C	0.94730	2.81038	-0.92531	H	1.62616	-4.90861	-0.32570
C	1.81759	3.84477	-0.52413	C	2.39329	1.07443	0.28603
H	3.38987	4.39813	0.81291	C	4.03006	2.62038	-0.50155
H	1.75760	4.80904	-1.01277	C	2.20673	1.89418	-1.90457
C	2.37582	-1.08061	0.41713	C	3.37991	2.66584	-1.70580
C	2.74901	2.36023	1.12689	H	4.92515	3.20982	-0.34438
H	3.42976	2.16057	1.94336	H	3.74146	3.28223	-2.51854
N	-0.57139	-0.34558	0.96542	C	1.82234	-1.29121	0.91579
N	1.66631	-1.32509	-0.71544	C	3.53043	1.80417	0.52843
N	1.01653	1.58858	-0.34074	H	4.02440	1.74506	1.48798
C	-2.12717	-0.54690	2.76857	N	-0.57501	0.50243	0.92060
H	-3.14911	-0.58462	3.11667	N	0.94443	-1.61932	-0.07631
C	-2.97914	-0.41037	0.41666	N	1.72557	1.10529	-0.90444
C	-4.22406	-0.97550	0.76734	C	-2.12391	1.18696	2.58257
C	-2.87203	0.22182	-0.85873	H	-3.14042	1.36625	2.89683
C	-5.33627	-0.89444	-0.05519	C	-2.97505	0.54918	0.31672
H	-4.31501	-1.50875	1.70542	C	-4.23190	1.14511	0.55397
C	-4.02069	0.31765	-1.67175	C	-2.85609	-0.31230	-0.80515
C	-5.23305	-0.22502	-1.28045	C	-5.33280	0.87080	-0.23919
H	-6.27097	-1.34975	0.24916	H	-4.34436	1.85086	1.36607
H	-3.91728	0.82299	-2.62534	C	-3.98381	-0.60929	-1.58511
H	-6.09542	-0.14258	-1.93306	C	-5.20964	-0.02830	-1.30410
O	-1.73147	0.73399	-1.32177	H	-6.28031	1.35248	-0.03267
N	0.03826	2.98368	-1.92772	H	-3.86095	-1.28920	-2.41924
H	-0.77639	2.37502	-1.93109	H	-6.06777	-0.26085	-1.92410
N	1.41420	-2.51605	-2.72675	O	-1.68524	-0.86328	-1.16195
H	0.42902	-2.30872	-2.77935	N	1.59610	1.94897	-3.10818
H	-0.12390	3.92880	-2.24040	H	0.71902	1.51019	-3.32670
H	1.68297	-3.33185	-3.25609	N	-0.07987	-3.22775	-1.43828
Cr	-0.05300	-0.08247	-0.91953	H	-0.88372	-2.62512	-1.58279
				H	1.94890	2.58941	-3.80121
				H	-0.19574	-4.20094	-1.67524

Cr -0.02622 -0.06911 -0.90775

H -0.29854 -2.09446 -2.40609

H 0.98683 3.76719 -2.73713

H 0.48758 -3.52319 -2.90416

HL-NH2 Cu(II)

Cu -0.05179 0.21047 -0.81213

$\Delta G = -2838.629298$

C -1.90166 0.02013 1.49066

HL-NH2 Fe(II)

$\Delta G = -2461.86347$

C -1.13010 -0.30803 3.75718

C -1.90037 -0.20421 1.44799

C 0.19046 -0.24288 3.31188

C -1.13287 -0.10932 3.74351

H -1.34086 -0.47298 4.80707

C 0.18967 -0.09536 3.29397

C 0.41512 -0.04660 1.95712

H -1.34752 -0.06192 4.80458

H 1.02094 -0.36401 3.99461

C 0.42035 -0.13819 1.93040

C 1.82956 -0.06721 1.37179

H 1.01672 -0.02932 3.98905

H 2.51847 -0.12927 2.21132

C 1.83853 -0.03190 1.35927

C 3.00018 -2.26725 0.86931

H 2.51997 -0.02269 2.20863

C 3.14284 -3.39377 0.04547

C 3.31119 -2.01706 0.78415

H 3.60330 -2.14187 1.75836

C 3.61185 -3.08225 -0.07548

C 1.39127 -2.54612 -1.36104

H 3.92140 -1.81198 1.65327

C 2.34261 -3.54668 -1.06696

C 1.71204 -2.48652 -1.41793

H 3.87484 -4.15423 0.29135

C 2.81911 -3.32299 -1.17607

H 2.42280 -4.41827 -1.70420

H 4.46459 -3.71973 0.12582

C 2.17766 1.20076 0.60493

H 3.02863 -4.14216 -1.85234

C 3.53425 3.13030 0.22098

C 2.04989 1.29074 0.60303

C 1.67659 2.60498 -1.20943

C 3.12451 3.39710 0.27051

C 2.76074 3.44283 -0.87374

C 1.33235 2.66761 -1.15169

H 4.36561 3.76898 0.49455

C 2.29651 3.63818 -0.80359

H 2.96037 4.31964 -1.47605

H 3.86482 4.13511 0.55645

C 2.05819 -1.31912 0.51183

H 2.36407 4.55866 -1.36996

C 3.24383 1.99099 0.98465

C 2.21507 -1.22917 0.49479

H 3.83733 1.72931 1.84961

C 2.99824 2.20931 1.00855

N -0.61175 0.11288 1.10270

H 3.62346 2.01960 1.87078

N 1.29244 -1.44721 -0.59053

N -0.60292 -0.22605 1.04811

N 1.41202 1.50130 -0.47443

N 1.43082 -1.45654 -0.58944

C -2.17367 -0.19815 2.85310

N 1.25904 1.50476 -0.47319

H -3.19341 -0.30608 3.19288

C -2.16852 -0.14353 2.82938

C -2.97626 0.11386 0.47981

H -3.19075 -0.09073 3.17379

C -4.26750 0.50225 0.89273

C -2.98195 -0.19835 0.44652

C -2.78265 -0.22305 -0.89626

C -4.27722 -0.60883 0.83115

C -5.34777 0.53260 0.02647

C -2.80241 0.26743 -0.89020

H -4.41994 0.80588 1.92092

C -5.35966 -0.53631 -0.02577

C -3.90221 -0.21438 -1.75511

H -4.43052 -1.01678 1.82225

C -5.15929 0.15495 -1.30746

C -3.91995 0.36609 -1.73687

H -6.32148 0.84751 0.38099

C -5.17810 -0.02741 -1.31606

H -3.73950 -0.49499 -2.78921

H -6.33535 -0.87224 0.30193

H -5.99333 0.16180 -2.00070

H -3.75783 0.74699 -2.73803

O -1.61170 -0.57308 -1.43126

H -6.01929 0.04803 -1.99557

N 0.90204 2.86224 -2.29993

O -1.61279 0.62618 -1.39697

H -0.01415 2.44530 -2.37037

N 0.56316 -2.62745 -2.44630

N	0.46270	2.83770	-2.18735	H	-3.71435	-0.08602	-2.85984
H	-0.39668	2.29796	-2.18100	H	-6.04971	-0.17661	-1.98547
N	0.91417	-2.66520	-2.51126	O	-1.61695	0.01848	-1.47921
H	-0.00157	-2.24266	-2.53888	N	0.75859	2.68076	-2.40768
H	0.40973	3.74582	-2.62062	H	-0.10432	2.17410	-2.53809
H	1.02227	-3.50471	-3.05782	N	0.55879	-2.57642	-2.40540
Fe	-0.04962	-0.10153	-0.79546	H	-0.31697	-2.07394	-2.42853

HL-NH2 Fe(III)

$\Delta G = -2461.659596$

C	-1.88408	0.02877	1.44968
C	-1.10223	0.06163	3.75009
C	0.21406	0.03564	3.29649
H	-1.31783	0.08093	4.81088
C	0.44116	0.02409	1.93439
H	1.04897	0.02788	3.98349
C	1.86149	0.00066	1.38899
H	2.54162	-0.02439	2.23637
C	3.11503	-2.13794	0.81472
C	3.27582	-3.23241	-0.05442
H	3.76179	-1.99606	1.66916
C	1.40609	-2.45453	-1.35792
C	2.43614	-3.39548	-1.12898
H	4.06200	-3.95486	0.12764
H	2.53640	-4.23632	-1.80262
C	2.15962	1.25426	0.58052
C	3.38290	3.23293	0.06487
C	1.54662	2.51376	-1.32146
C	2.58514	3.43165	-1.03428
H	4.17472	3.93705	0.28957
H	2.72743	4.28148	-1.68882
C	2.10946	-1.24197	0.54608
C	3.17502	2.12049	0.90072
H	3.79291	1.94373	1.76980
N	-0.57981	0.03264	1.03856
N	1.28221	-1.39233	-0.52222
N	1.36246	1.44432	-0.50490
C	-2.13376	0.05648	2.83535
H	-3.14765	0.07229	3.19896
C	-3.00622	-0.01748	0.49233
C	-4.33945	-0.07484	0.94994
C	-2.82411	-0.02617	-0.91756
C	-5.41622	-0.13014	0.08005
H	-4.55552	-0.08358	2.00724
C	-3.91970	-0.08289	-1.79685
C	-5.20864	-0.13283	-1.30430
H	-6.42091	-0.17420	0.48134

H	-3.71435	-0.08602	-2.85984
H	-6.04971	-0.17661	-1.98547
O	-1.61695	0.01848	-1.47921
N	0.75859	2.68076	-2.40768
H	-0.10432	2.17410	-2.53809
N	0.55879	-2.57642	-2.40540
H	-0.31697	-2.07394	-2.42853
H	0.84651	3.53275	-2.93951
H	0.58932	-3.42265	-2.95282
Fe	-0.00228	0.05633	-0.77489

HL-NH2 K(I)

$\Delta G = -1798.254357$

C	-2.05662	0.24060	1.35134
C	-1.15934	1.28215	3.33395
C	0.11591	1.03174	2.84263
H	-1.29508	1.77641	4.28963
C	0.24545	0.39893	1.60267
H	0.99682	1.31234	3.40769
C	1.65681	0.09034	1.09247
H	2.26751	-0.03013	1.99089
C	1.87809	-2.41835	1.11407
C	1.96111	-3.63717	0.43815
H	1.91517	-2.37607	2.19536
C	1.81294	-2.43246	-1.62437
C	1.93097	-3.65903	-0.94502
H	2.06185	-4.56355	0.99258
H	2.00646	-4.58804	-1.49703
C	2.29446	1.24728	0.32325
C	4.23404	2.51791	-0.28156
C	2.04692	3.06774	-1.08202
C	3.42664	3.34182	-1.04568
H	5.30016	2.70703	-0.22355
H	3.83423	4.18249	-1.59399
C	1.74957	-1.25139	0.36310
C	3.66863	1.45469	0.42574
H	4.27892	0.80705	1.04260
N	-0.81147	0.02668	0.86892
N	1.71285	-1.25925	-0.97764
N	1.50223	2.03453	-0.41932
C	-2.25738	0.87770	2.58486
H	-3.26518	1.05033	2.94105
C	-3.23029	-0.26399	0.58689
C	-4.09596	-1.16196	1.22495
C	-3.51063	0.18957	-0.75395
C	-5.22603	-1.68490	0.59667
H	-3.86306	-1.47356	2.23969

C	-4.67814	-0.37183	-1.36455
C	-5.50387	-1.27694	-0.71400
H	-5.86664	-2.39206	1.11085
H	-4.91093	-0.05030	-2.37586
H	-6.37693	-1.66862	-1.22899
O	-2.78198	1.06233	-1.36649
N	1.18572	3.82778	-1.85234
H	0.21814	3.81266	-1.56120
N	1.74309	-2.38400	-3.00461
H	2.01383	-1.50464	-3.42197
H	1.50964	4.74516	-2.12252
H	2.08803	-3.19008	-3.50512
K	-0.37429	0.48894	-2.00265

HL-NH2 Li (I)

$\Delta G = -1205.868101$

C	1.87933	-0.03314	1.36257
C	1.09064	-0.37765	3.62301
C	-0.22230	-0.25463	3.16631
H	1.28737	-0.56607	4.67259
C	-0.41910	-0.04381	1.80429
H	-1.06302	-0.34173	3.84317
C	-1.83633	-0.00622	1.21935
H	-2.52859	-0.03677	2.06018
C	-3.13401	2.13467	0.91211
C	-3.39484	3.30284	0.18817
H	-3.68953	1.89883	1.81034
C	-1.67555	2.66187	-1.35308
C	-2.66902	3.57893	-0.95364
H	-4.16264	3.99149	0.52236
H	-2.84779	4.47538	-1.53464
C	-2.09937	-1.25991	0.37951
C	-3.26786	-3.29018	-0.09473
C	-1.38570	-2.57810	-1.39676
C	-2.40055	-3.52470	-1.14636
H	-4.05499	-4.00356	0.12287
H	-2.48496	-4.41351	-1.75962
C	-2.13916	1.28004	0.45005
C	-3.12216	-2.14538	0.69969
H	-3.77845	-1.95876	1.53975
N	0.60102	0.08213	0.94716
N	-1.42481	1.53822	-0.66173
N	-1.27287	-1.46652	-0.65456
C	2.14273	-0.28690	2.72539
H	3.15725	-0.43261	3.07002
C	2.97440	0.09751	0.37303
C	4.23059	0.55110	0.82448

C	2.81739	-0.24770	-1.02597
C	5.33946	0.65788	-0.00289
H	4.33254	0.85409	1.86089
C	3.99219	-0.15550	-1.83524
C	5.20922	0.28492	-1.34847
H	6.28130	1.02775	0.38509
H	3.88642	-0.43689	-2.87859
H	6.06343	0.34953	-2.01606
O	1.70264	-0.63822	-1.56404
N	-0.47969	-2.71289	-2.42324
H	0.38005	-2.17848	-2.31582
N	-0.95285	2.86594	-2.50848
H	-0.07984	2.36513	-2.58894
H	-0.36623	-3.63361	-2.82014
H	-0.92072	3.80804	-2.86875
Li	0.07061	0.03797	-0.97042

HL-NH2 Mg (II)

$\Delta G = -1398.337895$

C	-1.92918	0.13708	1.37531
C	-1.13157	0.43705	3.63900
C	0.17793	0.26223	3.19066
H	-1.32659	0.63144	4.68722
C	0.37706	0.04516	1.83452
H	1.01720	0.31547	3.87163
C	1.79334	-0.05635	1.25854
H	2.47094	-0.03819	2.10940
C	3.03878	-2.22086	1.04374
C	3.31343	-3.41476	0.36400
H	3.56463	-1.96395	1.95302
C	1.65894	-2.80414	-1.26895
C	2.63086	-3.71164	-0.79144
H	4.05809	-4.10196	0.74809
H	2.81802	-4.62644	-1.33919
C	2.13453	1.17685	0.41626
C	3.43155	3.13123	-0.03563
C	1.52023	2.55886	-1.36854
C	2.59682	3.42777	-1.09190
H	4.26045	3.78946	0.19741
H	2.74292	4.31493	-1.69474
C	2.07867	-1.37072	0.52811
C	3.19609	1.99580	0.75373
H	3.82132	1.76723	1.60601
N	-0.64846	-0.03242	0.96842
N	1.39215	-1.65157	-0.61333
N	1.33648	1.43572	-0.64417
C	-2.18114	0.39172	2.73676

H	-3.18959	0.57793	3.07685	N	-1.49200	1.47766	-0.58107
C	-3.03344	0.07244	0.38933	N	-1.22457	-1.53503	-0.49051
C	-4.31245	-0.31271	0.84388	C	2.17758	0.14018	2.81059
C	-2.87789	0.42133	-0.99606	H	3.20014	0.09989	3.15640
C	-5.42512	-0.33438	0.01771	C	3.00486	0.24397	0.44281
H	-4.42978	-0.62630	1.87440	C	4.26928	0.72940	0.83454
C	-4.03997	0.42290	-1.80699	C	2.86089	-0.27760	-0.88044
C	-5.28168	0.05332	-1.32024	C	5.37563	0.67753	0.00140
H	-6.38646	-0.65053	0.40438	H	4.38077	1.17368	1.81606
H	-3.91505	0.71189	-2.84502	C	4.00894	-0.35434	-1.69857
H	-6.14073	0.05374	-1.98326	C	5.24135	0.11162	-1.27154
O	-1.72450	0.75260	-1.54565	H	6.32773	1.07175	0.33518
N	0.64302	2.79692	-2.38998	H	3.88642	-0.77647	-2.68965
H	-0.27884	2.37702	-2.32771	H	6.09763	0.04975	-1.93453
N	1.01366	-3.07910	-2.44134	O	1.70530	-0.69709	-1.38933
H	0.13809	-2.63847	-2.67475	N	-0.43724	-2.83583	-2.24043
H	0.66601	3.70844	-2.82116	H	0.41044	-2.27785	-2.23122
H	1.11380	-4.01173	-2.81167	N	-1.10458	2.84051	-2.46061
Mg	-0.06379	-0.11267	-1.05433	H	-0.11578	2.63975	-2.47027

HL-NH2 Mn (II)

$\Delta G = -2349.155382$

C	1.90747	0.22124	1.43480
C	1.13943	0.06710	3.72428
C	-0.17591	0.03409	3.26682
H	1.35157	0.00314	4.78474
C	-0.40396	0.10509	1.90036
H	-1.00678	-0.06281	3.95298
C	-1.82160	-0.02371	1.34564
H	-2.48984	-0.05704	2.20370
C	-3.39422	1.87303	0.83847
C	-3.78076	2.94587	0.02877
H	-3.97210	1.58943	1.70747
C	-1.85319	2.53375	-1.35198
C	-3.01187	3.28074	-1.06453
H	-4.67179	3.51599	0.26295
H	-3.27537	4.11359	-1.70406
C	-2.00976	-1.34458	0.58992
C	-3.03445	-3.47621	0.26806
C	-1.28437	-2.69340	-1.17717
C	-2.21530	-3.69229	-0.81990
H	-3.75050	-4.23486	0.56195
H	-2.26551	-4.61125	-1.39020
C	-2.25073	1.17068	0.50428
C	-2.93122	-2.28750	1.00649
H	-3.54966	-2.11148	1.87620
N	0.61360	0.23188	1.01860

Mn	0.08273	0.17345	-0.90796
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HL-NH2 Na (I)

$\Delta G = -1360.620042$

C	-1.95242	0.10915	1.33816
C	-1.09271	0.40412	3.57500
C	0.19462	0.24073	3.06920
H	-1.24700	0.58921	4.63233
C	0.34799	0.02000	1.69863
H	1.05950	0.29777	3.71869
C	1.76883	-0.07096	1.12527
H	2.43117	-0.06299	1.99075
C	3.00197	-2.25122	0.98725
C	3.30868	-3.44600	0.33022
H	3.46591	-2.00392	1.93312
C	1.78929	-2.80128	-1.40442
C	2.70525	-3.73365	-0.87735
H	4.01598	-4.14318	0.76516
H	2.92119	-4.64868	-1.41529
C	2.13580	1.18509	0.32488
C	3.55748	3.06612	-0.09075
C	1.50907	2.73452	-1.28402
C	2.66304	3.50826	-1.05015
H	4.45276	3.64161	0.11724
H	2.83162	4.42754	-1.59803
C	2.08635	-1.38096	0.39959

C	3.29555	1.89481	0.62876	H	-4.21208	-3.90069	-0.00990
H	3.96834	1.55482	1.40566	H	-2.67352	-4.20797	-1.93223
N	-0.69920	-0.06813	0.86916	C	-2.10422	1.20387	0.62478
N	1.48926	-1.65202	-0.77606	C	-3.18110	-2.15174	0.72463
N	1.28825	1.58587	-0.62926	H	-3.83091	-1.99104	1.57365
C	-2.17272	0.35607	2.70618	N	0.61753	-0.25531	1.07288
H	-3.17771	0.52542	3.07048	N	-1.41101	1.42291	-0.50876
C	-3.10085	0.04092	0.39828	N	-1.27956	-1.46809	-0.56139
C	-4.25772	-0.63800	0.81902	C	2.18096	-0.10113	2.85207
C	-3.08625	0.69596	-0.89519	H	3.20425	-0.02497	3.19121
C	-5.40826	-0.72211	0.04178	C	2.96927	-0.10791	0.46208
H	-4.24196	-1.13536	1.78433	C	4.27253	-0.54476	0.76095
C	-4.29885	0.60256	-1.65165	C	2.71592	0.47684	-0.81317
C	-5.41610	-0.08322	-1.20576	C	5.31561	-0.40026	-0.14097
H	-6.27306	-1.27227	0.39408	H	4.46328	-1.02155	1.71517
H	-4.31109	1.09949	-2.61742	C	3.79249	0.63581	-1.70839
H	-6.30305	-0.12653	-1.83176	C	5.06883	0.20745	-1.37755
O	-2.06963	1.34568	-1.36309	H	6.30658	-0.75787	0.11020
N	0.55430	3.08870	-2.21638	H	3.58990	1.09797	-2.66749
H	-0.37056	2.69973	-2.05129	H	5.87563	0.33451	-2.09111
N	1.20465	-3.02731	-2.63419	O	1.51152	0.91443	-1.18378
H	0.35224	-2.52579	-2.83350	N	-0.63400	-2.62059	-2.49613
H	0.55285	4.05054	-2.52237	H	0.28444	-2.20293	-2.47260
H	1.19777	-3.98104	-2.96454	N	-0.82077	2.74499	-2.31741
Na	-0.27519	-0.03519	-1.48730	H	0.05640	2.23834	-2.34529
				H	-0.68421	-3.48015	-3.02176
				H	-0.77600	3.67915	-2.69666
				Ni	0.10105	-0.14462	-0.76410

HL-NH2 Ni (II)

$\Delta G = -2706.439821$

C	1.90759	-0.17717	1.47784
C	1.13945	-0.08162	3.76478
C	-0.17843	-0.09368	3.31042
H	1.34879	-0.02308	4.82604
C	-0.40968	-0.16566	1.94424
H	-1.01030	-0.03318	3.99932
C	-1.82627	-0.11069	1.37589
H	-2.51161	-0.14779	2.22013
C	-3.03663	2.10607	1.10886
C	-3.25019	3.28424	0.37959
H	-3.58158	1.90428	2.02123
C	-1.57743	2.57110	-1.18788
C	-2.52504	3.52923	-0.76810
H	-3.97815	4.00977	0.72363
H	-2.66258	4.43911	-1.33890
C	-2.11775	-1.30331	0.48935
C	-3.38859	-3.21394	-0.16492
C	-1.46670	-2.49622	-1.42327
C	-2.53982	-3.39073	-1.23521

HL-NH2 V (II)

$\Delta G = -2142.16889$

C	1.86745	-0.06257	1.45671
C	1.02165	-0.28661	3.72738
C	-0.28677	-0.19934	3.24292
H	1.20870	-0.41060	4.78645
C	-0.47960	-0.07204	1.88317
H	-1.13660	-0.24805	3.91261
C	-1.87441	-0.04517	1.25732
H	-2.58805	-0.08557	2.07829
C	-3.20941	2.08229	0.91334
C	-3.43284	3.28256	0.22320
H	-3.83978	1.79444	1.74412
C	-1.56120	2.77605	-1.19134
C	-2.61182	3.63729	-0.82544
H	-4.24749	3.93401	0.51613
H	-2.75998	4.56202	-1.36873
C	-2.12175	-1.31178	0.42140

C	-3.29385	-3.34113	-0.06186	H	-4.39991	3.78350	-0.02402
C	-1.36378	-2.69362	-1.33578	H	-3.02843	4.09029	-2.06416
C	-2.39824	-3.60941	-1.07785	C	-2.03999	-1.25089	0.69631
H	-4.09854	-4.03653	0.14470	C	-3.16994	-3.34478	0.49871
H	-2.47820	-4.50955	-1.67417	C	-1.32285	-2.79464	-0.93884
C	-2.16627	1.27160	0.51693	C	-2.32804	-3.69754	-0.52847
C	-3.15516	-2.17930	0.71126	H	-3.94058	-4.03274	0.82470
H	-3.83718	-1.96768	1.52408	H	-2.40899	-4.65724	-1.02189
N	0.56876	-0.00207	1.00664	C	-2.19223	1.26618	0.38597
N	-1.35997	1.60815	-0.53517	C	-3.02585	-2.10046	1.13792
N	-1.25931	-1.55337	-0.60923	H	-3.67201	-1.81229	1.95524
C	2.08009	-0.22909	2.83321	N	0.61320	0.20817	1.00128
H	3.08629	-0.32843	3.21122	N	-1.43407	1.42082	-0.74668
C	2.98366	0.03976	0.49141	N	-1.21645	-1.57678	-0.34168
C	4.29714	0.23805	0.97758	C	2.15905	0.44347	2.79986
C	2.84268	-0.04682	-0.92437	H	3.17760	0.47125	3.15651
C	5.40181	0.31085	0.14907	C	3.01546	0.21813	0.45687
H	4.45692	0.35959	2.03983	C	4.30658	0.66568	0.79360
C	3.96975	0.01952	-1.75588	C	2.85250	-0.34071	-0.83018
C	5.23930	0.19072	-1.23351	C	5.37283	0.53856	-0.08504
H	6.38459	0.46816	0.57593	H	4.47739	1.14325	1.74883
H	3.80808	-0.06393	-2.82389	C	3.92268	-0.48769	-1.71347
H	6.09565	0.24260	-1.89549	C	5.18480	-0.05033	-1.33843
O	1.64834	-0.19559	-1.55767	H	6.35021	0.90425	0.20434
N	-0.45364	-2.88019	-2.33397	H	3.74001	-0.93434	-2.68266
H	0.41654	-2.36547	-2.31942	H	6.01664	-0.15501	-2.02444
N	-0.73344	3.06729	-2.23475	O	1.62068	-0.74836	-1.23343
H	0.13674	2.57194	-2.35183	N	-0.45973	-3.10038	-1.93659
H	-0.43382	-3.76637	-2.81266	H	0.42178	-2.61223	-2.01333
H	-0.78671	3.97579	-2.66613	N	-0.96950	2.60970	-2.71629
V	-0.01745	0.04908	-0.85250	H	-0.12318	2.09858	-2.90405
				H	-0.47585	-4.03488	-2.31520
				H	-1.17326	3.37949	-3.33358
				V	0.02252	-0.07642	-0.92666

HL-NH2 V(III)

$\Delta G = -2141.996018$

C	1.90512	0.30241	1.42791
C	1.11494	0.52302	3.70391
C	-0.19609	0.43470	3.24223
H	1.31764	0.63657	4.76144
C	-0.41111	0.26031	1.88608
H	-1.03685	0.48525	3.92097
C	-1.82332	0.12101	1.32785
H	-2.50456	0.18697	2.17245
C	-3.24966	2.09062	0.67565
C	-3.56427	3.12458	-0.22632
H	-3.82928	1.93940	1.57541
C	-1.71944	2.43436	-1.61026
C	-2.81213	3.29963	-1.35791

HL-NH2 Zn(II)

$\Delta G = -2977.513327$

C	-1.88443	0.09970	1.48198
C	-1.10221	0.52669	3.73135
C	0.21751	0.40048	3.29390
H	-1.30949	0.74903	4.77155
C	0.42913	0.14858	1.94671
H	1.05035	0.51872	3.97446
C	1.83992	0.09931	1.34856
H	2.53891	0.17352	2.17871
C	3.17049	-2.02403	1.12141
C	3.45722	-3.21874	0.44533

H	3.72713	-1.73302	2.00142	H	0.815120000	-1.344319000	1.492745000
C	1.71011	-2.70340	-1.12279	N	0.225135000	-1.878071000	-0.429515000
C	2.73677	-3.56393	-0.67335	C	-0.483361000	-0.598246000	-0.529778000
H	4.24500	-3.87026	0.80447	H	-1.043423000	-0.585180000	-1.469205000
H	2.93695	-4.47982	-1.21433	H	-1.229406000	-0.481005000	0.269696000
C	2.08629	1.32111	0.45683	C	-0.350752000	-2.964383000	-1.212608000
C	3.19592	3.36420	-0.08695	H	-0.391517000	-2.653927000	-2.263118000
C	1.35794	2.55354	-1.40122	H	0.341518000	-3.810361000	-1.178382000
C	2.34570	3.53170	-1.15901	C	-1.766618000	-3.520233000	-0.865892000
H	3.95661	4.10864	0.11707	O	-2.128012000	-4.502230000	-1.576867000
H	2.41268	4.39940	-1.80260	O	-2.436306000	-2.979155000	0.049482000
C	2.15828	-1.21839	0.63892	C	-1.766618000	3.208435000	1.143156000
C	3.06679	2.24827	0.75469	O	-1.847097000	3.699685000	2.306332000
H	3.70815	2.11810	1.61567	O	-2.574973000	3.404929000	0.201722000
N	-0.59535	-0.01039	1.09259	C	-0.558290000	2.253827000	0.939874000
N	1.43712	-1.55384	-0.46590	H	0.303746000	2.694183000	1.461002000
N	1.27436	1.46235	-0.61452	H	-0.815120000	1.344319000	1.492745000
C	-2.14898	0.39556	2.83331	N	-0.225135000	1.878071000	-0.429515000
H	-3.16408	0.54360	3.17147	C	0.483361000	0.598246000	-0.529778000
C	-2.97331	-0.08091	0.49159	H	1.043423000	0.585180000	-1.469205000
C	-4.23912	-0.47665	0.97784	H	1.229406000	0.481005000	0.269696000
C	-2.83604	0.14791	-0.92048	C	0.350752000	2.964383000	-1.212608000
C	-5.35116	-0.61015	0.16326	H	0.391517000	2.653927000	-2.263118000
H	-4.34514	-0.70860	2.03039	H	-0.341518000	3.810361000	-1.178382000
C	-3.99718	0.03565	-1.72241	C	1.766618000	3.520233000	-0.865892000
C	-5.22512	-0.33311	-1.20299	O	2.128012000	4.502230000	-1.576867000
H	-6.29843	-0.92874	0.58118	O	2.436306000	2.979155000	0.049482000
H	-3.88089	0.23582	-2.78181				
H	-6.08326	-0.42078	-1.86099				
O	-1.70947	0.48320	-1.53861				
N	0.47812	2.64796	-2.43985				
H	-0.38932	2.12509	-2.37445				
N	1.01319	-3.00820	-2.25172				
H	0.13607	-2.55737	-2.46039				
H	0.41101	3.53416	-2.91667				
H	1.11601	-3.93525	-2.63390				
Zn	-0.01439	-0.14544	-0.88385				

EDTA Al (III)

$\Delta G = -1342.623362$

EDTA-4H

$\Delta G = -1100.357742$

C	1.766618000	-3.208435000	1.143156000	C	-1.452641000	2.267944000	0.800801000
O	1.847097000	-3.699685000	2.306332000	O	-0.676602000	1.510414000	1.525453000
O	2.574973000	-3.404929000	0.201722000	O	-2.240399000	3.094593000	1.239352000
C	0.558290000	-2.253827000	0.939874000	C	-1.305796000	2.074756000	-0.733249000
H	-0.303746000	-2.694183000	1.461002000	H	-2.119236000	1.436563000	-1.081261000
				H	-1.380391000	3.039065000	-1.240968000
				N	0.000000000	1.412269000	-0.965332000
				C	0.249019000	0.722682000	-2.264541000
				H	-0.199540000	1.269030000	-3.098677000
				H	1.328426000	0.732984000	-2.418005000
				C	1.110584000	2.367071000	-0.689960000
				H	1.505075000	2.798159000	-1.611389000
				H	0.747280000	3.193329000	-0.077422000
				C	2.213125000	1.669071000	0.104356000
				O	3.330433000	2.167319000	0.191157000
				O	1.834894000	0.566809000	0.666296000
				C	1.452641000	-2.267944000	0.800801000
				O	0.676602000	-1.510414000	1.525453000

O	2.240399000	-3.094593000	1.239352000	O	4.762152000	-0.923813000	-0.039338000
C	1.305796000	-2.074756000	-0.733249000	O	2.694145000	-1.792873000	0.114360000
H	2.119236000	-1.436563000	-1.081261000	Be	-1.266367000	0.395529000	0.794144000
H	1.380391000	-3.039065000	-1.240968000				
N	0.000000000	-1.412269000	-0.965332000				
C	-0.249019000	-0.722682000	-2.264541000				
H	0.199540000	-1.269030000	-3.098677000				
H	-1.328426000	-0.732984000	-2.418005000				
C	-1.110584000	-2.367071000	-0.689960000				
H	-1.505075000	-2.798159000	-1.611389000				
H	-0.747280000	-3.193329000	-0.077422000				
C	-2.213125000	-1.669071000	0.104356000				
O	-3.330433000	-2.167319000	0.191157000				
O	-1.834894000	-0.566809000	0.666296000				
Al	0.000000000	0.000000000	0.615776000				

EDTA Be (II)

$\Delta G = -1115.033923$

C	-0.888592000	-2.024787000	1.223534000
O	-1.241350000	-0.905024000	1.774078000
O	-0.805149000	-3.106009000	1.802771000
C	-0.515180000	-1.888953000	-0.254367000
H	0.576896000	-1.820769000	-0.280680000
H	-0.833892000	-2.765147000	-0.825304000
N	-1.107212000	-0.628860000	-0.769761000
C	-0.416235000	-0.076895000	-1.973898000
H	-0.613649000	-0.725667000	-2.835589000
H	-0.894391000	0.881855000	-2.189796000
C	-2.558881000	-0.796247000	-1.084561000
H	-2.734415000	-0.863560000	-2.159639000
H	-2.925445000	-1.723882000	-0.638489000
C	-3.378418000	0.345395000	-0.473441000
O	-4.525093000	0.568344000	-0.854739000
O	-2.755839000	0.976729000	0.466853000
C	0.510671000	2.409541000	0.908343000
O	-0.356501000	1.563263000	1.357200000
O	0.853528000	3.421652000	1.523756000
C	1.100114000	2.111169000	-0.476287000
H	0.310418000	2.337543000	-1.199268000
H	1.913637000	2.819299000	-0.672863000
N	1.529401000	0.719515000	-0.616002000
C	1.100295000	0.084072000	-1.854930000
H	1.430791000	0.637728000	-2.753743000
H	1.575001000	-0.895705000	-1.899331000
C	2.962800000	0.575146000	-0.359995000
H	3.565088000	0.998209000	-1.182703000
H	3.207195000	1.165665000	0.528433000
C	3.504388000	-0.851847000	-0.075531000

EDTA B (III)

$\Delta G = -1124.913382$

C	-0.694813000	-2.204090000	0.892591000
O	-1.375338000	-1.227260000	1.499642000
O	-0.498086000	-3.289519000	1.380914000
C	-0.185614000	-1.749455000	-0.465309000
H	0.884159000	-1.524172000	-0.358991000
H	-0.320110000	-2.512886000	-1.229683000
N	-0.961307000	-0.504707000	-0.770705000
C	-0.255006000	0.510966000	-1.652127000
H	-0.409470000	0.201142000	-2.686475000
H	-0.794280000	1.451840000	-1.523718000
C	-2.313374000	-0.808383000	-1.365675000
H	-2.343308000	-0.588619000	-2.430450000
H	-2.552890000	-1.863665000	-1.227704000
C	-3.327992000	0.023294000	-0.593319000
O	-4.470851000	0.205352000	-0.930556000
O	-2.781299000	0.508424000	0.518587000
C	-0.190431000	2.200723000	0.903204000
O	-0.557367000	0.981313000	1.347086000
O	-0.895058000	3.176466000	0.995841000
C	1.241651000	2.249209000	0.385029000
H	1.308092000	3.080551000	-0.334064000
H	1.846328000	2.536339000	1.251344000
N	1.728349000	0.980021000	-0.127471000
C	1.253429000	0.680918000	-1.473791000
H	1.530215000	1.475929000	-2.191319000
H	1.754268000	-0.227654000	-1.804521000
C	3.184314000	0.844030000	-0.030211000
H	3.708237000	1.452502000	-0.785902000
H	3.496776000	1.225783000	0.945096000
C	3.743383000	-0.602313000	-0.124854000
O	4.998845000	-0.668652000	-0.142925000
O	2.936754000	-1.567051000	-0.158344000
B	-1.414281000	0.028746000	0.745689000

EDTA Ca (II)

$\Delta G = -1777.944127$

C	-0.195087000	3.138674000	0.446157000
O	-0.043987000	2.382880000	1.456799000
O	-0.516273000	4.343572000	0.465770000
C	0.000000000	2.488892000	-0.946404000
H	-0.999891000	2.239308000	-1.311523000
H	0.414299000	3.235143000	-1.638413000

N	0.817298000	1.268386000	-0.892491000	O	2.324376000	-3.108983000	1.230673000
C	0.654475000	0.394140000	-2.071641000	C	1.315938000	-2.064600000	-0.684249000
H	0.717788000	0.970287000	-3.007947000	H	2.109647000	-1.393207000	-1.013228000
H	1.498759000	-0.299156000	-2.081531000	H	1.412526000	-3.016492000	-1.217088000
C	2.238216000	1.596917000	-0.683778000	N	0.000000000	-1.426078000	-0.910174000
H	2.753332000	1.792569000	-1.633184000	C	-0.252817000	-0.720979000	-2.204046000
H	2.302521000	2.516894000	-0.095949000	H	0.184691000	-1.268118000	-3.046361000
C	3.020595000	0.535714000	0.119891000	H	-1.334041000	-0.724617000	-2.346868000
O	4.257950000	0.504388000	-0.033570000	C	-1.089982000	-2.413275000	-0.675356000
O	2.343350000	-0.187557000	0.915719000	H	-1.333763000	-2.939144000	-1.603167000
C	0.195087000	-3.138674000	0.446157000	H	-0.744522000	-3.160927000	0.039637000
O	0.043987000	-2.382880000	1.456799000	C	-2.349685000	-1.768228000	-0.069648000
O	0.516273000	-4.343572000	0.465770000	O	-3.413894000	-2.416083000	-0.141931000
C	0.000000000	-2.488892000	-0.946404000	O	-2.175451000	-0.644204000	0.485740000
H	0.999891000	-2.239308000	-1.311523000	Co	0.000000000	0.000000000	0.508012000
H	-0.414299000	-3.235143000	-1.638413000				
N	-0.817298000	-1.268386000	-0.892491000	EDTA Co(III)			
C	-0.654475000	-0.394140000	-2.071641000	$\Delta G = -2482.822977$			
H	-0.717788000	-0.970287000	-3.007947000	C	-0.803201000	2.503143000	1.083008000
H	-1.498759000	0.299156000	-2.081531000	O	-0.210773000	1.489871000	1.635941000
C	-2.238216000	-1.596917000	-0.683778000	O	-1.221410000	3.487067000	1.685709000
H	-2.753332000	-1.792569000	-1.633184000	C	-0.975771000	2.402938000	-0.447768000
H	-2.302521000	-2.516894000	-0.095949000	H	-1.987552000	2.055838000	-0.651604000
C	-3.020595000	-0.535714000	0.119891000	H	-0.831555000	3.375121000	-0.921737000
O	-4.257950000	-0.504388000	-0.033570000	N	0.000000000	1.396868000	-0.949692000
O	-2.343350000	0.187557000	0.915719000	C	-0.355795000	0.678591000	-2.215388000
Ca	0.000000000	0.000000000	1.239290000	H	-1.437699000	0.552642000	-2.237141000
				H	-0.071293000	1.266665000	-3.090996000
EDTA Co(II)				C	1.377988000	1.989671000	-1.010540000
$\Delta G = -2482.948385$				H	1.690497000	2.120602000	-2.047520000
C	-1.481875000	2.285615000	0.846467000	H	1.363145000	2.979019000	-0.552788000
O	-0.716975000	1.584573000	1.603157000	C	2.402471000	1.148344000	-0.254830000
O	-2.324376000	3.108983000	1.230673000	O	3.595350000	1.429185000	-0.311687000
C	-1.315938000	2.064600000	-0.684249000	O	1.903263000	0.169021000	0.425184000
H	-2.109647000	1.393207000	-1.013228000	C	0.803201000	-2.503143000	1.083008000
H	-1.412526000	3.016492000	-1.217088000	O	0.210773000	-1.489871000	1.635941000
N	0.000000000	1.426078000	-0.910174000	O	1.221410000	-3.487067000	1.685709000
C	0.252817000	0.720979000	-2.204046000	C	0.975771000	-2.402938000	-0.447768000
H	-0.184691000	1.268118000	-3.046361000	H	1.987552000	-2.055838000	-0.651604000
H	1.334041000	0.724617000	-2.346868000	H	0.831555000	-3.375121000	-0.921737000
C	1.089982000	2.413275000	-0.675356000	N	0.000000000	-1.396868000	-0.949692000
H	1.333763000	2.939144000	-1.603167000	C	0.355795000	-0.678591000	-2.215388000
H	0.744522000	3.160927000	0.039637000	H	1.437699000	-0.552642000	-2.237141000
C	2.349685000	1.768228000	-0.069648000	H	0.071293000	-1.266665000	-3.090996000
O	3.413894000	2.416083000	-0.141931000	C	-1.377988000	-1.989671000	-1.010540000
O	2.175451000	0.644204000	0.485740000	H	-1.690497000	-2.120602000	-2.047520000
C	1.481875000	-2.285615000	0.846467000	H	-1.363145000	-2.979019000	-0.552788000
O	0.716975000	-1.584573000	1.603157000	C	-2.402471000	-1.148344000	-0.254830000

O	-3.595350000	-1.429185000	-0.311687000	N	0.000000000	1.438107000	-0.950717000
O	-1.903263000	-0.169021000	0.425184000	C	0.265017000	0.714724000	-2.239752000
Co	0.000000000	0.000000000	0.425301000	H	-0.154860000	1.266727000	-3.085468000
				H	1.347325000	0.702973000	-2.369026000
EDTA Cr(II)				C	1.121559000	2.389597000	-0.690656000
$\Delta G = -2144.673999$				H	1.460476000	2.855226000	-1.618268000
C	-0.296469000	2.883306000	0.665401000	H	0.778217000	3.185426000	-0.029351000
O	0.000000000	1.985912000	1.523298000	C	2.266300000	1.670136000	0.020801000
O	-0.668853000	4.044133000	0.913682000	O	3.388232000	2.163037000	0.057039000
C	-0.190248000	2.464951000	-0.826800000	O	1.917695000	0.554496000	0.580917000
H	-1.193505000	2.204275000	-1.171926000	C	1.477832000	-2.359038000	0.766000000
H	0.165679000	3.310349000	-1.426955000	O	0.709132000	-1.639298000	1.528320000
N	0.688935000	1.285127000	-0.939342000	O	2.291079000	-3.188422000	1.158266000
C	0.590856000	0.484400000	-2.192025000	C	1.303323000	-2.121830000	-0.757556000
H	0.532132000	1.129638000	-3.078196000	H	2.115694000	-1.482239000	-1.104503000
H	1.520941000	-0.081245000	-2.274686000	H	1.350309000	-3.070214000	-1.298710000
C	2.101879000	1.650942000	-0.680771000	N	0.000000000	-1.438107000	-0.950717000
H	2.637435000	1.882067000	-1.607229000	C	-0.265017000	-0.714724000	-2.239752000
H	2.132984000	2.547567000	-0.059198000	H	0.154860000	-1.266727000	-3.085468000
C	2.828675000	0.548074000	0.101101000	H	-1.347325000	-0.702973000	-2.369026000
O	4.069416000	0.550524000	0.126206000	C	-1.121559000	-2.389597000	-0.690656000
O	2.067131000	-0.283081000	0.704833000	H	-1.460476000	-2.855226000	-1.618268000
C	0.296469000	-2.883306000	0.665401000	H	-0.778217000	-3.185426000	-0.029351000
O	0.000000000	-1.985912000	1.523298000	C	-2.266300000	-1.670136000	0.020801000
O	0.668853000	-4.044133000	0.913682000	O	-3.388232000	-2.163037000	0.057039000
C	0.190248000	-2.464951000	-0.826800000	O	-1.917695000	-0.554496000	0.580917000
H	1.193505000	-2.204275000	-1.171926000	Cr	0.000000000	0.000000000	0.580917000
H	-0.165679000	-3.310349000	-1.426955000				
N	-0.688935000	-1.285127000	-0.939342000	EDTA Cu(II)			
C	-0.590856000	-0.484400000	-2.192025000	$\Delta G = -2740.670145$			
H	-0.532132000	-1.129638000	-3.078196000	C	-0.225914000	2.873470000	0.376440000
H	-1.520941000	0.081245000	-2.274686000	O	-0.094584000	1.995823000	1.294569000
C	-2.101879000	-1.650942000	-0.680771000	O	-0.534688000	4.063040000	0.566018000
H	-2.637435000	-1.882067000	-1.607229000	C	0.000000000	2.408850000	-1.077894000
H	-2.132984000	-2.547567000	-0.059198000	H	-0.988391000	2.190711000	-1.491704000
C	-2.828675000	-0.548074000	0.101101000	H	0.408787000	3.251230000	-1.653661000
O	-4.069416000	-0.550524000	0.126206000	N	0.835191000	1.214967000	-1.152540000
O	-2.067131000	0.283081000	0.704833000	C	0.656478000	0.394735000	-2.355135000
Cr	0.000000000	0.000000000	0.637333000	H	0.697497000	0.996742000	-3.277048000
				H	1.497790000	-0.299878000	-2.403599000
EDTA Cr(III)				C	2.236888000	1.478545000	-0.820840000
$\Delta G = -2144.591144$				H	2.893415000	1.320335000	-1.682863000
C	-1.477832000	2.359038000	0.766000000	H	2.364681000	2.528421000	-0.538846000
O	-0.709132000	1.639298000	1.528320000	C	2.800159000	0.654071000	0.353198000
O	-2.291079000	3.188422000	1.158266000	O	4.027953000	0.704948000	0.541404000
C	-1.303323000	2.121830000	-0.757556000	O	1.986638000	-0.015745000	1.076150000
H	-2.115694000	1.482239000	-1.104503000	C	0.225914000	-2.873470000	0.376440000
H	-1.350309000	3.070214000	-1.298710000	O	0.094584000	-1.995823000	1.294569000

O	0.534688000	-4.063040000	0.566018000	O	4.185226000	1.337817000	-0.296363000
C	0.000000000	-2.408850000	-1.077894000	O	2.217719000	2.158416000	0.419462000
H	0.988391000	-2.190711000	-1.491704000	Fe	-0.351537000	-0.369143000	-0.583891000
H	-0.408787000	-3.251230000	-1.653661000				
N	-0.835191000	-1.214967000	-1.152540000	EDTA Fe(III)			
C	-0.656478000	-0.394735000	-2.355135000	$\Delta G = -2363.750482$			
H	-0.697497000	-0.996742000	-3.277048000	C	-1.454624000	2.304328000	0.764023000
H	-1.497790000	0.299878000	-2.403599000	O	-0.676279000	1.567054000	1.496159000
C	-2.236888000	-1.478545000	-0.820840000	O	-2.246933000	3.138676000	1.188713000
H	-2.893415000	-1.320335000	-1.682863000	C	-1.308910000	2.075244000	-0.760300000
H	-2.364681000	-2.528421000	-0.538846000	H	-2.119225000	1.430395000	-1.099916000
C	-2.800159000	-0.654071000	0.353198000	H	-1.357646000	3.021819000	-1.303298000
O	-4.027953000	-0.704948000	0.541404000	N	0.000000000	1.397932000	-0.958141000
O	-1.986638000	0.015745000	1.076150000	C	0.267278000	0.709896000	-2.264239000
Cu	0.000000000	0.000000000	0.857639000	H	-0.154581000	1.281207000	-3.095292000
				H	1.349376000	0.698493000	-2.393512000
EDTA Fe(II)				C	1.109956000	2.364576000	-0.689585000
$\Delta G = -2363.901456$				H	1.462517000	2.815532000	-1.618517000
C	-0.806342000	2.419850000	-1.012091000	H	0.751469000	3.168462000	-0.047482000
O	-0.564087000	1.369057000	-1.708592000	C	2.234485000	1.652318000	0.050806000
O	-0.917603000	3.572041000	-1.454515000	O	3.357648000	2.140768000	0.123570000
C	-0.907778000	2.199795000	0.509774000	O	1.869104000	0.538557000	0.597597000
H	0.089011000	2.406586000	0.900482000	C	1.454624000	-2.304328000	0.764023000
H	-1.625262000	2.892108000	0.958873000	O	0.676279000	-1.567054000	1.496159000
N	-1.257144000	0.786754000	0.798749000	O	2.246933000	-3.138676000	1.188713000
C	-0.738422000	0.259979000	2.097879000	C	1.308910000	-2.075244000	-0.760300000
H	-1.003350000	0.929000000	2.925340000	H	2.119225000	-1.430395000	-1.099916000
H	-1.249487000	-0.689190000	2.274180000	H	1.357646000	-3.021819000	-1.303298000
C	-2.724258000	0.568185000	0.697156000	N	0.000000000	-1.397932000	-0.958141000
H	-3.221424000	0.733771000	1.657127000	C	-0.267278000	-0.709896000	-2.264239000
H	-3.135004000	1.291925000	-0.011061000	H	0.154581000	-1.281207000	-3.095292000
C	-3.055829000	-0.824459000	0.142321000	H	-1.349376000	-0.698493000	-2.393512000
O	-4.192067000	-1.282579000	0.305212000	C	-1.109956000	-2.364576000	-0.689585000
O	-2.101954000	-1.391419000	-0.505558000	H	-1.462517000	-2.815532000	-1.618517000
C	1.116418000	-2.643763000	-0.631819000	H	-0.751469000	-3.168462000	-0.047482000
O	0.586851000	-1.861861000	-1.509057000	C	-2.234485000	-1.652318000	0.050806000
O	1.566310000	-3.772230000	-0.852765000	O	-3.357648000	-2.140768000	0.123570000
C	1.141072000	-2.090088000	0.815250000	O	-1.869104000	-0.538557000	0.597597000
H	0.216528000	-2.401974000	1.309055000	Fe	0.000000000	0.000000000	0.493266000
H	1.979599000	-2.523914000	1.369855000				
N	1.210663000	-0.598819000	0.791084000	EDTA K(I)			
C	0.777219000	0.051160000	2.064742000	$\Delta G = -1700.279805$			
H	1.085859000	-0.540635000	2.934340000	C	3.392361000	-0.867552000	-0.794682000
H	1.283489000	1.011909000	2.108347000	O	2.755068000	-0.453995000	-1.798094000
C	2.620340000	-0.244773000	0.434809000	O	4.570322000	-1.317305000	-0.790264000
H	3.278916000	-0.606087000	1.236773000	C	2.664765000	-0.908552000	0.576821000
H	2.880090000	-0.810041000	-0.460171000	H	2.235047000	-1.912881000	0.647992000
C	3.018113000	1.229912000	0.159743000	H	3.426741000	-0.835396000	1.370957000

N	1.584649000	0.063462000	0.755940000	O	3.555082000	-1.602023000	1.333739000
C	0.687426000	-0.338679000	1.847475000	C	1.960760000	-1.138076000	-0.396049000
H	0.553615000	-1.419939000	1.791492000	H	2.216559000	-0.126476000	-0.723180000
H	1.152222000	-0.131797000	2.830903000	H	2.555413000	-1.848224000	-0.989097000
C	2.122099000	1.415379000	0.941568000	N	0.514210000	-1.345987000	-0.572501000
H	2.383767000	1.595803000	1.997056000	C	0.000000000	-0.767385000	-1.824668000
H	3.055318000	1.488374000	0.373619000	H	0.577896000	-1.112040000	-2.699879000
C	1.270073000	2.614002000	0.439376000	H	-1.016699000	-1.139083000	-1.948173000
O	1.410406000	3.685197000	1.090896000	C	0.208589000	-2.779574000	-0.477918000
O	0.572081000	2.458263000	-0.595398000	H	0.636114000	-3.328503000	-1.333106000
C	-3.392351000	0.867571000	-0.794682000	H	0.706659000	-3.171324000	0.414829000
O	-2.755060000	0.454011000	-1.798094000	C	-1.280419000	-3.194699000	-0.349128000
O	-4.570305000	1.317340000	-0.790264000	O	-1.482529000	-4.431780000	-0.499230000
C	-2.664759000	0.908553000	0.576825000	O	-2.142124000	-2.320902000	-0.088587000
H	-2.235036000	1.912879000	0.648008000	Li	0.000000000	0.000000000	1.057774000
H	-3.426739000	0.835393000	1.370957000				
N	-1.584650000	-0.063469000	0.755938000	EDTA Mg (II)			
C	-0.687427000	0.338656000	1.847480000	$\Delta G = -1300.400923$			
H	-0.553616000	1.419917000	1.791512000	C	-1.755553000	2.314459000	0.580830000
H	-1.152224000	0.131761000	2.830904000	O	-1.099980000	1.695484000	1.480550000
C	-2.122109000	-1.415384000	0.941552000	O	-2.685615000	3.119171000	0.769079000
H	-2.383795000	-1.595812000	1.997035000	C	-1.357747000	2.012630000	-0.886441000
H	-3.055321000	-1.488371000	0.373588000	H	-2.075329000	1.282241000	-1.270135000
C	-1.270083000	-2.614008000	0.439366000	H	-1.468997000	2.922932000	-1.488963000
O	-1.410417000	-3.685202000	1.090887000	N	0.000000000	1.453738000	-0.954677000
O	-0.572087000	-2.458271000	-0.595406000	C	0.312027000	0.697577000	-2.183435000
K	0.000000000	-0.000005000	-1.644625000	H	-0.006856000	1.235818000	-3.087413000
				H	1.399360000	0.610170000	-2.240387000
				C	1.022975000	2.479707000	-0.676605000
EDTA Li (I)				H	1.480581000	2.856588000	-1.597461000
$\Delta G = -1107.883008$				H	0.552524000	3.338164000	-0.190655000
C	-2.395817000	1.201730000	1.087010000	C	2.124365000	1.997229000	0.287569000
O	-1.548372000	0.785611000	1.937073000	O	3.172918000	2.666007000	0.341883000
O	-3.555082000	1.602023000	1.333739000	O	1.854806000	0.966566000	0.983007000
C	-1.960760000	1.138076000	-0.396049000	C	1.755553000	-2.314459000	0.580830000
H	-2.216559000	0.126476000	-0.723180000	O	1.099980000	-1.695484000	1.480550000
H	-2.555413000	1.848224000	-0.989097000	O	2.685615000	-3.119171000	0.769079000
N	-0.514210000	1.345987000	-0.572501000	C	1.357747000	-2.012630000	-0.886441000
C	0.000000000	0.767385000	-1.824668000	H	2.075329000	-1.282241000	-1.270135000
H	-0.577896000	1.112040000	-2.699879000	H	1.468997000	-2.922932000	-1.488963000
H	1.016699000	1.139083000	-1.948173000	N	0.000000000	-1.453738000	-0.954677000
C	-0.208589000	2.779574000	-0.477918000	C	-0.312027000	-0.697577000	-2.183435000
H	-0.636114000	3.328503000	-1.333106000	H	0.006856000	-1.235818000	-3.087413000
H	-0.706659000	3.171324000	0.414829000	H	-1.399360000	-0.610170000	-2.240387000
C	1.280419000	3.194699000	-0.349128000	C	-1.022975000	-2.479707000	-0.676605000
O	1.482529000	4.431780000	-0.499230000	H	-1.480581000	-2.856588000	-1.597461000
O	2.142124000	2.320902000	-0.088587000	H	-0.552524000	-3.338164000	-0.190655000
C	2.395817000	-1.201730000	1.087010000	C	-2.124365000	-1.997229000	0.287569000
O	1.548372000	-0.785611000	1.937073000				

O	-3.172918000	-2.666007000	0.341883000	N	0.822430000	1.292283000	-0.802749000
O	-1.854806000	-0.966566000	0.983007000	C	0.653203000	0.401595000	-1.956676000
Mg	0.000000000	0.000000000	0.871684000	H	0.708493000	0.957754000	-2.910725000
				H	1.500506000	-0.288942000	-1.962264000
EDTA Mn (II)				C	2.229383000	1.633792000	-0.593474000
$\Delta G = -2251.190128$				H	2.740999000	1.865915000	-1.540863000
C	-1.529869000	2.357161000	0.919424000	H	2.277065000	2.541006000	0.016089000
O	-0.884544000	1.576279000	1.707300000	C	3.060669000	0.579600000	0.181659000
O	-2.269975000	3.293911000	1.232872000	O	4.301080000	0.589140000	-0.042124000
C	-1.340172000	2.056478000	-0.603481000	O	2.453144000	-0.154224000	1.004019000
H	-2.109499000	1.332711000	-0.880063000	C	0.223763000	-3.167909000	0.538721000
H	-1.464685000	2.979041000	-1.185155000	O	0.000000000	-2.491859000	1.576611000
N	0.000000000	1.454695000	-0.804493000	O	0.636917000	-4.357540000	0.492917000
C	0.255261000	0.723692000	-2.073527000	C	0.021687000	-2.483138000	-0.841381000
H	-0.180839000	1.256669000	-2.933825000	H	1.021754000	-2.204685000	-1.185397000
H	1.337307000	0.720554000	-2.210476000	H	-0.352172000	-3.238051000	-1.553364000
C	1.056939000	2.478575000	-0.610002000	N	-0.822430000	-1.292283000	-0.802749000
H	1.138311000	3.121153000	-1.497559000	C	-0.653203000	-0.401595000	-1.956676000
H	0.770457000	3.107877000	0.234443000	H	-0.708493000	-0.957754000	-2.910725000
C	2.433709000	1.846465000	-0.273712000	H	-1.500506000	0.288942000	-1.962264000
O	3.438412000	2.536367000	-0.533426000	C	-2.229383000	-1.633792000	-0.593474000
O	2.365148000	0.698167000	0.245558000	H	-2.740999000	-1.865915000	-1.540863000
C	1.529869000	-2.357161000	0.919424000	H	-2.277065000	-2.541006000	0.016089000
O	0.884544000	-1.576279000	1.707300000	C	-3.060669000	-0.579600000	0.181659000
O	2.269975000	-3.293911000	1.232872000	O	-4.301080000	-0.589140000	-0.042124000
C	1.340172000	-2.056478000	-0.603481000	O	-2.453144000	0.154224000	1.004019000
H	2.109499000	-1.332711000	-0.880063000	Na	0.000000000	0.000000000	1.187508000
H	1.464685000	-2.979041000	-1.185155000				
N	0.000000000	-1.454695000	-0.804493000	EDTA Ni (II)			
C	-0.255261000	-0.723692000	-2.073527000	$\Delta G = -2608.484744$			
H	0.180839000	-1.256669000	-2.933825000	C	-0.926894000	2.415074000	1.336422000
H	-1.337307000	-0.720554000	-2.210476000	O	-0.313992000	1.417187000	1.895749000
C	-1.056939000	-2.478575000	-0.610002000	O	-1.400834000	3.376620000	1.940374000
H	-1.138311000	-3.121153000	-1.497559000	C	-1.067009000	2.304127000	-0.190737000
H	-0.770457000	-3.107877000	0.234443000	H	-2.035595000	1.847940000	-0.396401000
C	-2.433709000	-1.846465000	-0.273712000	H	-1.014227000	3.287654000	-0.664287000
O	-3.438412000	-2.536367000	-0.533426000	N	0.000000000	1.385545000	-0.688285000
O	-2.365148000	-0.698167000	0.245558000	C	-0.321616000	0.694407000	-1.981567000
Mn	0.000000000	0.000000000	0.698675000	H	-1.403137000	0.613362000	-2.049824000
				H	0.035970000	1.283365000	-2.831103000
EDTA Na (I)				C	1.276617000	2.169437000	-0.777554000
$\Delta G = -1262.648833$				H	1.205686000	2.828547000	-1.646989000
C	-0.223763000	3.167909000	0.538721000	H	1.329526000	2.803883000	0.110409000
O	0.000000000	2.491859000	1.576611000	C	2.626333000	1.405843000	-0.819958000
O	-0.636917000	4.357540000	0.492917000	O	3.539118000	2.003775000	-1.439567000
C	-0.021687000	2.483138000	-0.841381000	O	2.710184000	0.322301000	-0.192076000
H	-1.021754000	2.204685000	-1.185397000	C	0.926894000	-2.415074000	1.336422000
H	0.352172000	3.238051000	-1.553364000	O	0.313992000	-1.417187000	1.895749000

O	1.400834000	-3.376620000	1.940374000	O	-4.128188000	-0.510581000	0.167995000
C	1.067009000	-2.304127000	-0.190737000	O	-2.116245000	0.241514000	0.822639000
H	2.035595000	-1.847940000	-0.396401000	V	0.000000000	0.000000000	0.750194000
H	1.014227000	-3.287654000	-0.664287000				
N	0.000000000	-1.385545000	-0.688285000	EDTA V(III)			
C	0.321616000	-0.694407000	-1.981567000	$\Delta G = -2044.090265$			
H	1.403137000	-0.613362000	-2.049824000	C	-2.123270000	1.875022000	-0.559059000
H	-0.035970000	-1.283365000	-2.831103000	O	-1.526600000	1.052757000	-1.381704000
C	-1.276617000	-2.169437000	-0.777554000	O	-2.785718000	2.845401000	-0.892407000
H	-1.205686000	-2.828547000	-1.646989000	C	-1.908404000	1.513491000	0.917295000
H	-1.329526000	-2.803883000	0.110409000	H	-1.163456000	2.194352000	1.333105000
C	-2.626333000	-1.405843000	-0.819958000	H	-2.835458000	1.641681000	1.484051000
O	-3.539118000	-2.003775000	-1.439567000	N	-1.406455000	0.119688000	0.961690000
O	-2.710184000	-0.322301000	-0.192076000	C	-0.710177000	-0.259332000	2.222718000
Ni	0.000000000	0.000000000	0.661480000	H	-1.256200000	0.110764000	3.096386000
				H	-0.714782000	-1.348686000	2.278528000
EDTA V(II)				C	-2.530117000	-0.834560000	0.713381000
$\Delta G = -2044.230718$				H	-2.950662000	-1.194153000	1.654622000
C	-0.233302000	2.936012000	0.580076000	H	-3.329332000	-0.319158000	0.177897000
O	0.000000000	2.051859000	1.472105000	C	-2.087831000	-2.001354000	-0.172068000
O	-0.576529000	4.112550000	0.785175000	O	-2.747877000	-3.041548000	-0.188353000
C	-0.086465000	2.467593000	-0.889955000	O	-1.050752000	-1.755147000	-0.892540000
H	-1.086657000	2.230058000	-1.260742000	C	2.123263000	-1.875028000	-0.559058000
H	0.310923000	3.284403000	-1.504158000	O	1.526589000	-1.052763000	-1.381704000
N	0.758196000	1.259752000	-0.945233000	O	2.785705000	-2.845409000	-0.892407000
C	0.627289000	0.434189000	-2.173514000	C	1.908408000	-1.513489000	0.917297000
H	0.636603000	1.057688000	-3.077441000	H	1.163460000	-2.194346000	1.333112000
H	1.512249000	-0.203630000	-2.222296000	H	2.835466000	-1.641681000	1.484046000
C	2.179971000	1.594251000	-0.698201000	N	1.406465000	-0.119685000	0.961689000
H	2.726230000	1.755128000	-1.633515000	C	0.710191000	0.259347000	2.222714000
H	2.234730000	2.527268000	-0.133280000	H	1.256214000	-0.110740000	3.096386000
C	2.885784000	0.527470000	0.154515000	H	0.714797000	1.348702000	2.278514000
O	4.128188000	0.510581000	0.167995000	C	2.530126000	0.834560000	0.713367000
O	2.116245000	-0.241514000	0.822639000	H	2.950685000	1.194150000	1.654603000
C	0.233302000	-2.936012000	0.580076000	H	3.329332000	0.319155000	0.177872000
O	0.000000000	-2.051859000	1.472105000	C	2.087831000	2.001354000	-0.172077000
O	0.576529000	-4.112550000	0.785175000	O	2.747870000	3.041552000	-0.188361000
C	0.086465000	-2.467593000	-0.889955000	O	1.050752000	1.755142000	-0.892547000
H	1.086657000	-2.230058000	-1.260742000	V	-0.000001000	0.000000000	-0.752158000
H	-0.310923000	-3.284403000	-1.504158000				
N	-0.758196000	-1.259752000	-0.945233000	EDTA Zn(II)			
C	-0.627289000	-0.434189000	-2.173514000	$\Delta G = -2879.561167$			
H	-0.636603000	-1.057688000	-3.077441000	C	2.884977000	-0.982581000	1.085463000
H	-1.512249000	0.203630000	-2.222296000	O	2.239743000	-1.506826000	0.115758000
C	-2.179971000	-1.594251000	-0.698201000	O	3.916429000	-1.412205000	1.613972000
H	-2.726230000	-1.755128000	-1.633515000	C	2.267589000	0.302767000	1.703836000
H	-2.234730000	-2.527268000	-0.133280000	H	1.720511000	-0.029356000	2.591294000
C	-2.885784000	-0.527470000	0.154515000	H	3.081740000	0.948082000	2.057587000

N	1.348600000	1.014303000	0.809548000	H	0.879533000	1.912597000	1.086058000
C	0.138623000	1.530880000	1.472195000	H	-1.138599000	2.423262000	-0.241590000
H	0.384353000	2.027430000	2.425277000	H	-2.175794000	1.785144000	1.013468000
H	-0.314870000	2.286280000	0.829122000	H	1.788141000	-0.405331000	1.641051000
C	2.020788000	1.975114000	-0.078842000	H	1.812485000	-0.009135000	-1.401907000
H	1.842893000	3.009979000	0.236298000	H	2.375336000	1.194401000	-0.264641000
H	3.100616000	1.809561000	-0.023646000	H	1.259703000	-1.566981000	0.436739000
C	1.669598000	1.872000000	-1.592071000	H	-1.830510000	-1.519206000	-0.657778000
O	2.050610000	2.806863000	-2.299740000	H	-0.572603000	-2.577745000	-0.049909000
O	1.059714000	0.816058000	-1.986227000	H	-0.617136000	-1.278988000	2.149424000
C	-3.502757000	1.078583000	0.444777000	H	-1.894231000	-0.281027000	1.475814000
O	-4.577610000	1.385861000	-0.293160000				
O	-3.390383000	2.104674000	1.300242000				
C	-2.258216000	0.634935000	-0.315108000				
H	-2.563543000	0.057459000	-1.189905000				
H	-1.707764000	1.514280000	-0.687253000				
N	-1.291935000	-0.222235000	0.460963000				
C	-0.883159000	0.418171000	1.729799000				
H	-1.744066000	0.835166000	2.262360000				
H	-0.431768000	-0.354099000	2.360574000				
C	-1.831522000	-1.589728000	0.617517000				
H	-1.382243000	-2.053913000	1.501745000				
H	-2.914616000	-1.571256000	0.766915000				
C	-1.489974000	-2.520128000	-0.580133000				
O	-2.161176000	-3.546182000	-0.705294000				
O	-0.503073000	-2.162668000	-1.323004000				
Zn	0.578747000	-0.607626000	-0.677630000				
NTP							
$\Delta G = -856.858734$							
O	-2.385782000	4.270424000	1.428849000				
O	3.854655000	-1.661436000	-0.033913000				
O	-3.339688000	-2.438816000	1.644167000				
C	-1.003363000	-0.847586000	1.206990000				
C	-1.426350000	-1.970025000	0.257806000				
C	-2.514987000	-2.915577000	0.817777000				
C	1.337363000	-0.498428000	0.635845000				
C	3.685357000	-0.496032000	-0.483871000				
C	-0.052164000	1.388585000	1.297924000				
C	-1.213245000	2.273523000	0.842936000				
C	-1.271673000	3.677416000	1.489085000				
N	-0.018110000	0.078407000	0.623616000				
O	4.572219000	0.221787000	-1.026547000				
O	-0.215492000	4.142522000	1.996507000				
O	-2.513992000	-4.098309000	0.374255000				
C	2.267018000	0.116926000	-0.411075000				
H	-0.086337000	1.257151000	2.394905000				
NTP Al (III)							
$\Delta G = -1099.072397$							
H	-2.563543000	0.057459000	-1.189905000	Al	0.122183000	-0.185893000	-0.894401000
H	-1.707764000	1.514280000	-0.687253000	O	-0.411880000	1.417531000	-1.383907000
N	-1.291935000	-0.222235000	0.460963000	O	1.781233000	-0.554987000	-1.332485000
C	-0.883159000	0.418171000	1.729799000	O	-1.005148000	-1.486647000	-1.257385000
H	-1.744066000	0.835166000	2.262360000	C	-0.970821000	-0.965043000	1.656453000
H	-0.431768000	-0.354099000	2.360574000	C	-2.234383000	-1.167455000	0.805046000
C	-1.831522000	-1.589728000	0.617517000	C	-2.034729000	-1.898475000	-0.520117000
H	-1.382243000	-2.053913000	1.501745000	C	1.467233000	-0.607801000	1.574675000
H	-2.914616000	-1.571256000	0.766915000	C	2.890120000	-0.486400000	-0.599622000
C	-1.489974000	-2.520128000	-0.580133000	C	-0.022189000	1.359451000	1.510696000
O	-2.161176000	-3.546182000	-0.705294000	C	-1.110873000	2.181628000	0.812752000
O	-0.503073000	-2.162668000	-1.323004000	C	-0.931866000	2.421820000	-0.684742000
Zn	0.578747000	-0.607626000	-0.677630000	N	0.128113000	-0.084945000	1.070245000
				O	3.982851000	-0.716690000	-1.070981000
				O	-1.271879000	3.459923000	-1.211012000
				O	-2.776063000	-2.782315000	-0.892130000
				C	2.711339000	-0.069637000	0.858170000
				H	-0.205812000	1.355889000	2.587057000
				H	0.938226000	1.846722000	1.348914000
				H	-2.103056000	1.747206000	0.961240000
				H	-1.139394000	3.157273000	1.299564000
				H	1.534247000	-0.375660000	2.640126000
				H	2.763519000	1.023182000	0.892486000
				H	3.581845000	-0.424489000	1.411088000
				H	1.440003000	-1.692620000	1.475518000
				H	-2.931720000	-1.751837000	1.406063000
				H	-2.740768000	-0.223100000	0.588003000
				H	-0.525023000	-1.941084000	1.842052000
				H	-1.251888000	-0.546783000	2.624190000
NTP Be (II)							
$\Delta G = -871.529719$							
				Be	0.118668000	-0.174950000	-0.717336000
				O	-0.584340000	1.167640000	-1.283168000

O	1.627064000	-0.297429000	-1.253679000	H	1.167705000	1.795433000	1.103064000
O	-0.708496000	-1.499922000	-1.120608000	H	-1.872944000	2.041671000	1.373853000
C	-1.046827000	-0.798575000	1.668233000	H	-0.714502000	3.316966000	1.086807000
C	-2.204833000	-1.070368000	0.698468000	H	1.352980000	-0.728214000	2.614131000
C	-1.795453000	-1.885856000	-0.527684000	H	2.972269000	0.598645000	1.343358000
C	1.392720000	-0.725703000	1.555099000	H	3.397129000	-1.079755000	1.134461000
C	2.749068000	-0.290905000	-0.610595000	H	1.129164000	-1.848393000	1.266835000
C	0.121119000	1.374755000	1.461956000	H	-2.912419000	-1.769045000	1.143494000
C	-1.033902000	2.175580000	0.864587000	H	-2.719479000	-0.297654000	0.203598000
C	-1.106995000	2.177162000	-0.665329000	H	-0.793456000	-1.538145000	2.236130000
N	0.131146000	-0.069673000	1.070756000	H	-1.580958000	0.021626000	2.364722000
O	3.849549000	-0.324359000	-1.165213000				
O	-1.670232000	3.109661000	-1.242507000	NTP Ca(II)			
O	-2.477647000	-2.838903000	-0.907653000	$\Delta G = -1534.405089$			
C	2.680942000	-0.208390000	0.916243000	Ca	0.188943000	-0.293071000	-1.537647000
H	0.100682000	1.448770000	2.555469000	O	-0.799160000	1.738000000	-1.320203000
H	1.058449000	1.815178000	1.123338000	O	2.395905000	-0.612004000	-1.144740000
H	-1.999255000	1.825644000	1.243674000	O	-1.271631000	-1.966682000	-1.045634000
H	-0.943661000	3.210970000	1.198553000	C	-0.995974000	-0.722849000	1.700645000
H	1.454971000	-0.621790000	2.644745000	C	-2.272446000	-0.905675000	0.856020000
H	2.885199000	0.829383000	1.196674000	C	-2.184863000	-2.062869000	-0.151772000
H	3.512357000	-0.789308000	1.320854000	C	1.401830000	-0.699092000	1.586659000
H	1.292096000	-1.789410000	1.332970000	C	3.255906000	-0.290074000	-0.256210000
H	-2.984510000	-1.609180000	1.238846000	C	0.195047000	1.405806000	1.375635000
H	-2.650596000	-0.137292000	0.342601000	C	-1.044208000	2.236941000	1.033871000
H	-0.684752000	-1.755908000	2.044377000	C	-1.392460000	2.460764000	-0.448993000
H	-1.409111000	-0.238056000	2.533885000	N	0.166408000	-0.046507000	1.047574000
				O	4.463993000	-0.087423000	-0.476940000
				O	-2.242467000	3.332099000	-0.708270000
				O	-2.981124000	-3.013711000	-0.052067000
				C	2.769327000	-0.131057000	1.194179000
				H	0.381739000	1.519113000	2.456385000
				H	1.049185000	1.845883000	0.859176000
				H	-1.939349000	1.848035000	1.527810000
				H	-0.891538000	3.228047000	1.471692000
				H	1.351948000	-0.678079000	2.687255000
				H	2.858006000	0.927834000	1.453366000
				H	3.507028000	-0.634756000	1.826145000
				H	1.357905000	-1.749153000	1.287687000
				H	-3.099197000	-1.106480000	1.540478000
				H	-2.518719000	0.009433000	0.312090000
				H	-0.666252000	-1.714224000	2.018551000
				H	-1.251577000	-0.182275000	2.621915000
				NTP Co(II)			
				$\Delta G = -2239.423535$			
				Co	0.133854000	-0.276550000	-0.944932000
				O	-0.546707000	1.637212000	-1.116555000
NTP B(III)							
$\Delta G = -881.410107$							
B	0.070017000	-0.111478000	-0.570820000				
O	-0.813407000	0.912263000	-1.127370000				
O	1.395077000	0.084144000	-1.142987000				
O	-0.406500000	-1.434507000	-0.963549000				
C	-1.139258000	-0.681278000	1.662048000				
C	-2.178932000	-1.142897000	0.636939000				
C	-1.561801000	-1.931236000	-0.500073000				
C	1.315592000	-0.807270000	1.527181000				
C	2.590013000	-0.145983000	-0.595523000				
C	0.211101000	1.420170000	1.460810000				
C	-0.918552000	2.265271000	0.886111000				
C	-1.144743000	2.096038000	-0.603963000				
N	0.103788000	-0.029452000	1.046022000				
O	3.593425000	-0.126910000	-1.272910000				
O	-1.671548000	2.946947000	-1.284698000				
O	-2.040060000	-2.939350000	-0.967430000				
C	2.626027000	-0.342532000	0.906823000				
H	0.217689000	1.463688000	2.550491000				

O	2.022653000	-0.033422000	-1.206869000	H	1.512348000	1.072469000	1.320982000
O	-1.523364000	-1.197678000	-1.253446000	H	-1.405250000	1.749563000	1.928859000
C	-0.999901000	-1.044523000	1.671802000	H	-0.017793000	2.791741000	1.987327000
C	-2.350679000	-0.839465000	0.973448000	H	1.283446000	-1.849828000	2.215524000
C	-2.471932000	-1.462754000	-0.417610000	H	3.094157000	-0.350986000	1.620814000
C	1.398680000	-1.202570000	1.437235000	H	3.379451000	-1.888853000	0.863030000
C	3.028834000	-0.313876000	-0.446064000	H	1.064939000	-2.390988000	0.557824000
C	0.385921000	1.022421000	1.590030000	H	-3.190802000	-1.209546000	1.570640000
C	-0.700957000	2.051537000	1.278900000	H	-2.584796000	0.349281000	1.075715000
C	-0.958955000	2.424934000	-0.194245000	H	-0.960959000	-2.236868000	1.409347000
N	0.200618000	-0.371690000	1.070813000	H	-1.049862000	-0.975942000	2.632954000
O	4.200401000	-0.268506000	-0.836065000				
O	-1.570466000	3.486092000	-0.407274000	NTP Cr(II)			
O	-3.457009000	-2.153067000	-0.702513000	$\Delta G = -1901.138845$			
C	2.769813000	-0.664844000	1.024959000	Cr	0.121480000	-0.286493000	-1.082600000
H	0.510603000	0.963477000	2.679339000	O	-0.458638000	1.709706000	-1.096503000
H	1.321610000	1.392178000	1.175028000	O	2.095015000	-0.060904000	-1.223796000
H	-1.658126000	1.784226000	1.732661000	O	-1.654619000	-1.142190000	-1.290702000
H	-0.401003000	2.973901000	1.783922000	C	-1.005439000	-1.093785000	1.625844000
H	1.403853000	-1.344605000	2.525706000	C	-2.375008000	-0.828967000	0.979867000
H	3.037577000	0.221899000	1.607204000	C	-2.577616000	-1.401214000	-0.425063000
H	3.504363000	-1.422786000	1.307218000	C	1.386115000	-1.272927000	1.386499000
H	1.240198000	-2.183276000	0.984311000	C	3.078171000	-0.352965000	-0.442938000
H	-3.115197000	-1.284307000	1.613061000	C	0.405775000	0.955299000	1.599457000
H	-2.600345000	0.218239000	0.876954000	C	-0.651500000	2.022319000	1.312167000
H	-0.788126000	-2.115018000	1.686062000	C	-0.882337000	2.460292000	-0.147943000
H	-1.082806000	-0.725462000	2.717053000	N	0.198863000	-0.417347000	1.036760000
				O	4.265313000	-0.296552000	-0.788741000
				O	-1.481337000	3.535141000	-0.324758000
				O	-3.600349000	-2.045633000	-0.686000000
				C	2.774230000	-0.744655000	1.011598000
				H	0.520894000	0.865472000	2.688905000
				H	1.353150000	1.318539000	1.204912000
				H	-1.621108000	1.766324000	1.744978000
				H	-0.334376000	2.918272000	1.853647000
				H	1.381987000	-1.451592000	2.470693000
				H	3.045555000	0.117761000	1.627886000
				H	3.488987000	-1.524246000	1.287140000
				H	1.221675000	-2.237955000	0.902424000
				H	-3.127383000	-1.271434000	1.635686000
				H	-2.597249000	0.237939000	0.927512000
				H	-0.817305000	-2.168120000	1.579055000
				H	-1.059818000	-0.830620000	2.689300000
				NTP Cr(III)			
				$\Delta G = -1901.030028$			
				Cr	0.083660000	-0.253277000	-1.035576000
				O	-0.427837000	1.546705000	-0.969278000

O	1.981465000	0.009005000	-1.184346000	H	1.145823000	1.627301000	1.115345000
O	-1.661344000	-0.987828000	-1.286550000	H	-1.867005000	1.772045000	1.631044000
C	-1.041004000	-1.178134000	1.555575000	H	-0.728975000	3.074437000	1.611529000
C	-2.412623000	-0.797872000	0.990276000	H	1.495496000	-0.943575000	2.683397000
C	-2.660708000	-1.187030000	-0.463378000	H	2.949333000	0.667599000	1.500145000
C	1.352195000	-1.443769000	1.240127000	H	3.584469000	-0.949432000	1.504264000
C	3.017885000	-0.362087000	-0.478138000	H	1.385396000	-1.962955000	1.249448000
C	0.474892000	0.823963000	1.659498000	H	-3.035861000	-1.421583000	1.604543000
C	-0.521411000	1.953887000	1.427344000	H	-2.614107000	0.063643000	0.776314000
C	-0.712456000	2.407737000	-0.016851000	H	-0.649750000	-2.013450000	1.880360000
N	0.190688000	-0.495943000	0.986800000	H	-1.136830000	-0.574624000	2.760304000
O	4.167797000	-0.236136000	-0.875876000				
O	-1.129302000	3.526293000	-0.270410000	NTP Fe(II)			
O	-3.738490000	-1.634942000	-0.826517000	$\Delta G = -2120.369928$			
C	2.753897000	-0.929803000	0.917472000	Fe	0.139783000	-0.236832000	-0.915757000
H	0.557782000	0.628259000	2.732734000	O	-0.642763000	1.597003000	-1.247352000
H	1.449524000	1.156747000	1.311365000	O	2.079364000	-0.326023000	-1.216684000
H	-1.505139000	1.736824000	1.847893000	O	-1.265793000	-1.601464000	-1.122739000
H	-0.156217000	2.818955000	1.985154000	C	-0.999256000	-0.831396000	1.721917000
H	1.317664000	-1.723659000	2.297169000	C	-2.304697000	-0.900537000	0.920543000
H	3.078911000	-0.172870000	1.635995000	C	-2.246535000	-1.811329000	-0.308664000
H	3.436938000	-1.770613000	1.058514000	C	1.413223000	-0.870087000	1.552396000
H	1.142354000	-2.347710000	0.664434000	C	3.075508000	-0.325298000	-0.397169000
H	-3.158332000	-1.304903000	1.604777000	C	0.262092000	1.295180000	1.471080000
H	-2.621581000	0.269120000	1.080948000	C	-0.918214000	2.185156000	1.089852000
H	-0.894385000	-2.247872000	1.405763000	C	-1.177231000	2.413304000	-0.409067000
H	-1.032498000	-0.998167000	2.633751000	N	0.179707000	-0.149542000	1.066489000
				O	4.257901000	-0.301224000	-0.757141000
				O	-1.895478000	3.369596000	-0.732525000
				O	-3.119583000	-2.667781000	-0.488211000
				C	2.766978000	-0.323360000	1.104092000
				H	0.399644000	1.333795000	2.558653000
				H	1.161307000	1.705015000	1.013454000
				H	-1.850668000	1.843419000	1.546931000
				H	-0.730141000	3.167185000	1.531925000
				H	1.390153000	-0.876482000	2.648818000
				H	2.934477000	0.693819000	1.469733000
				H	3.531758000	-0.931658000	1.593193000
				H	1.312740000	-1.904571000	1.218859000
				H	-3.078396000	-1.275218000	1.593327000
				H	-2.628233000	0.087722000	0.586459000
				H	-0.690243000	-1.852169000	1.949910000
				H	-1.185111000	-0.337087000	2.680346000
				NTP Fe(III)			
				$\Delta G = -2120.186371$			
				Fe	0.074797000	-0.219388000	-0.903351000
				O	-0.408047000	1.541614000	-1.040971000
NTP Cu(II)							
$\Delta G = -2497.136548$							
Cu	0.174503000	-0.268772000	-0.885018000				
O	-0.571261000	1.675956000	-1.207919000				
O	2.031598000	-0.054157000	-1.214781000				
O	-1.342626000	-1.357823000	-1.211962000				
C	-0.958552000	-0.974581000	1.755840000				
C	-2.278824000	-0.956269000	0.971183000				
C	-2.267729000	-1.694875000	-0.368297000				
C	1.466251000	-0.927948000	1.586116000				
C	3.040816000	-0.231766000	-0.421853000				
C	0.245571000	1.205027000	1.557470000				
C	-0.933860000	2.096499000	1.165411000				
C	-1.204839000	2.359452000	-0.333792000				
N	0.202475000	-0.239844000	1.158855000				
O	4.205284000	-0.270245000	-0.825687000				
O	-2.035162000	3.248991000	-0.595115000				
O	-3.129969000	-2.538583000	-0.621035000				
C	2.785305000	-0.332597000	1.088019000				
H	0.366336000	1.243129000	2.648242000				

O	1.899372000	-0.100500000	-1.192728000	H	0.874579000	1.869742000	0.940341000
O	-1.549276000	-1.013213000	-1.272334000	H	-2.135135000	1.628721000	1.412065000
C	-1.092628000	-1.033345000	1.637272000	H	-1.218013000	3.075712000	1.699457000
C	-2.427237000	-0.737377000	0.950128000	H	1.315857000	-0.729008000	2.678338000
C	-2.547365000	-1.294795000	-0.460663000	H	2.712248000	1.042149000	1.439046000
C	1.297283000	-1.366279000	1.345808000	H	3.444698000	-0.464737000	1.882076000
C	2.941033000	-0.449962000	-0.466524000	H	1.359865000	-1.703383000	1.198914000
C	0.456844000	0.936571000	1.649410000	H	-3.115945000	-1.270465000	1.260531000
C	-0.540984000	2.046815000	1.347328000	H	-2.401616000	-0.210036000	0.036226000
C	-0.691808000	2.442588000	-0.117078000	H	-0.693891000	-1.791853000	1.981788000
N	0.159434000	-0.411175000	1.045593000	H	-1.428284000	-0.299795000	2.540671000
O	4.075790000	-0.391944000	-0.910930000				
O	-1.080767000	3.553392000	-0.432018000	NTP Li (I)			
O	-3.519850000	-1.931404000	-0.829763000	$\Delta G = -864.376645$			
C	2.698207000	-0.896137000	0.971881000	Li	0.155086000	-0.144506000	-1.073810000
H	0.532619000	0.799100000	2.731946000	O	-0.625312000	1.587054000	-1.405866000
H	1.434837000	1.244745000	1.288196000	O	2.031409000	-0.355924000	-1.372510000
H	-1.535681000	1.831217000	1.743958000	O	-0.924555000	-1.719111000	-1.368221000
H	-0.204993000	2.937794000	1.881459000	C	-1.004431000	-0.859469000	1.578798000
H	1.269348000	-1.583182000	2.417468000	C	-2.162696000	-1.144919000	0.601386000
H	3.040439000	-0.085943000	1.620976000	C	-1.796076000	-2.119063000	-0.534252000
H	3.377747000	-1.728070000	1.169312000	C	1.409852000	-0.669355000	1.482006000
H	1.059824000	-2.293920000	0.822470000	C	3.005398000	-0.198624000	-0.576851000
H	-3.209244000	-1.189403000	1.561618000	C	0.047256000	1.352614000	1.398754000
H	-2.645735000	0.330888000	0.904189000	C	-1.178925000	2.116936000	0.891741000
H	-0.935329000	-2.111421000	1.628074000	C	-1.338152000	2.297385000	-0.634753000
H	-1.142435000	-0.721526000	2.682903000	N	0.128948000	-0.074976000	1.027921000
				O	4.210658000	-0.116558000	-0.915887000
				O	-2.185336000	3.144881000	-1.006201000
				O	-2.371816000	-3.233152000	-0.567245000
				C	2.708115000	-0.064961000	0.931904000
				H	0.083895000	1.453095000	2.499038000
				H	0.935479000	1.850232000	1.007761000
				H	-2.106379000	1.675868000	1.270188000
				H	-1.142900000	3.119189000	1.329822000
				H	1.467666000	-0.629072000	2.584709000
				H	2.788550000	0.998122000	1.181225000
				H	3.533104000	-0.543316000	1.467445000
				H	1.380937000	-1.727314000	1.208713000
				H	-2.987429000	-1.570259000	1.178478000
				H	-2.518084000	-0.213394000	0.154673000
				H	-0.617610000	-1.819804000	1.929861000
				H	-1.407559000	-0.355780000	2.469120000
				NTP Mg (II)			
				$\Delta G = -1056.867946$			
				Mg	0.183655000	-0.150163000	-1.142281000
				O	-0.945811000	1.443574000	-1.390774000
NTP K (I)							
$\Delta G = -1456.764343$							
K	0.139517000	-0.235488000	-1.754900000				
O	-0.696003000	2.178144000	-1.267036000				
O	2.585406000	-0.743410000	-1.107014000				
O	-1.643897000	-2.150550000	-1.422458000				
C	-1.052906000	-0.817342000	1.639855000				
C	-2.216574000	-1.085500000	0.661446000				
C	-1.989091000	-2.352739000	-0.221643000				
C	1.354406000	-0.674229000	1.567660000				
C	3.302633000	-0.192207000	-0.228193000				
C	0.040059000	1.375030000	1.438958000				
C	-1.234066000	2.161075000	1.094381000				
C	-1.466471000	2.634829000	-0.378104000				
N	0.094315000	-0.056620000	1.089749000				
O	4.470023000	0.242767000	-0.351707000				
O	-2.413052000	3.440981000	-0.522613000				
O	-2.160745000	-3.454229000	0.349675000				
C	2.700597000	-0.026134000	1.205543000				
H	0.209223000	1.477238000	2.535212000				

O	2.134047000	-0.278422000	-1.287546000	H	0.356646000	2.354210000	0.853156000
O	-0.776941000	-1.875701000	-1.189574000	H	-2.494624000	1.347350000	1.337636000
C	-0.909509000	-0.867416000	1.674093000	H	-1.985527000	2.994194000	1.118818000
C	-2.066573000	-1.307131000	0.756453000	H	1.541483000	0.595807000	2.700701000
C	-1.661744000	-2.292780000	-0.348793000	H	2.377695000	1.888497000	0.580068000
C	1.473208000	-0.395030000	1.587538000	H	3.537935000	0.982633000	1.519089000
C	3.090073000	-0.045466000	-0.455738000	H	1.802905000	-0.872914000	1.765345000
C	-0.114347000	1.453830000	1.407899000	H	-2.469943000	-1.909356000	1.731929000
C	-1.424234000	2.066377000	0.904066000	H	-2.444134000	-0.660763000	0.498978000
C	-1.605562000	2.229943000	-0.614341000	H	-0.035455000	-1.526875000	2.176209000
N	0.132839000	0.021976000	1.061433000	H	-1.121318000	-0.255962000	2.698908000
O	4.288573000	-0.053600000	-0.763640000				
O	-2.395469000	3.094350000	-1.015650000	NTP Na (I)			
O	-2.187651000	-3.412087000	-0.394744000	$\Delta G = -1019.130644$			
C	2.710928000	0.291725000	0.994630000	Na	0.174696000	-0.120978000	-1.500385000
H	-0.081348000	1.561031000	2.501644000	O	-0.296427000	2.110850000	-1.270186000
H	0.712459000	2.039640000	1.004561000	O	2.290995000	-0.913451000	-1.257120000
H	-2.290871000	1.513351000	1.279315000	O	-1.512670000	-1.667848000	-1.570543000
H	-1.507300000	3.062028000	1.346237000	C	-1.140258000	-0.777085000	1.576046000
H	1.488179000	-0.241432000	2.675876000	C	-2.302343000	-0.918154000	0.572862000
H	2.637752000	1.381746000	1.064246000	C	-2.042992000	-2.021071000	-0.473342000
H	3.560306000	0.017854000	1.624025000	C	1.268148000	-0.928007000	1.475872000
H	1.557722000	-1.470136000	1.416301000	C	3.052734000	-0.363489000	-0.409441000
H	-2.819708000	-1.784532000	1.385665000	C	0.206591000	1.271179000	1.453865000
H	-2.542133000	-0.443265000	0.284530000	C	-0.949656000	2.192991000	1.061150000
H	-0.409089000	-1.766378000	2.038175000	C	-1.163700000	2.506613000	-0.438077000
H	-1.327122000	-0.371015000	2.557338000	N	0.088363000	-0.141410000	1.037960000
				O	4.143263000	0.206456000	-0.665817000
				O	-2.196853000	3.167057000	-0.715397000
				O	-2.352898000	-3.197910000	-0.158627000
				C	2.655224000	-0.412536000	1.083563000
				H	0.325389000	1.326985000	2.552811000
				H	1.119025000	1.675004000	1.014765000
				H	-1.901231000	1.846936000	1.472280000
				H	-0.766691000	3.158798000	1.547488000
				H	1.259777000	-1.020779000	2.577766000
				H	2.860450000	0.567608000	1.519900000
				H	3.378333000	-1.086599000	1.559274000
				H	1.143314000	-1.936096000	1.073081000
				H	-3.197771000	-1.186276000	1.141605000
				H	-2.491225000	0.033790000	0.073577000
				H	-0.886241000	-1.778802000	1.932930000
				H	-1.489108000	-0.223822000	2.459569000
				NTP Ni (II)			
				$\Delta G = -2364.937718$			
				Ni	0.255064000	-0.425342000	-0.887668000
				O	-0.601524000	1.814438000	-1.193758000
NTP Mn (II)							
$\Delta G = -2007.66298$							
Mn	0.232416000	-0.087413000	-0.952540000				
O	-1.354600000	1.010451000	-1.378613000				
O	2.173826000	-0.444984000	-1.088776000				
O	-0.521679000	-2.029065000	-0.910889000				
C	-0.693786000	-0.737520000	1.812912000				
C	-1.827064000	-1.401948000	1.010174000				
C	-1.375860000	-2.432409000	-0.038128000				
C	1.559480000	0.186402000	1.683062000				
C	3.102092000	0.117457000	-0.386038000				
C	-0.343490000	1.665784000	1.328094000				
C	-1.754627000	1.968188000	0.823478000				
C	-2.036747000	1.858439000	-0.682215000				
N	0.174481000	0.276313000	1.104248000				
O	4.301070000	0.085435000	-0.686810000				
O	-2.935060000	2.560878000	-1.160243000				
O	-1.856477000	-3.575718000	-0.007421000				
C	2.663496000	0.873762000	0.875030000				
H	-0.315034000	1.869406000	2.406732000				

O	2.005614000	0.061756000	-1.183987000	H	1.371438000	1.388525000	1.135486000
O	-1.359101000	-1.250926000	-1.161383000	H	-1.595338000	1.863644000	1.696970000
C	-0.848023000	-1.045089000	1.700462000	H	-0.309333000	3.025439000	1.751025000
C	-2.230633000	-0.944565000	1.055873000	H	1.340925000	-1.363515000	2.504616000
C	-2.345023000	-1.501614000	-0.358678000	H	3.032679000	0.172839000	1.621015000
C	1.557362000	-0.989379000	1.492403000	H	3.458726000	-1.492315000	1.387018000
C	3.062222000	-0.067332000	-0.444672000	H	1.178584000	-2.179080000	0.951449000
C	0.345338000	1.147940000	1.443626000	H	-3.154182000	-1.084993000	1.659136000
C	-0.880835000	2.022744000	1.196877000	H	-2.578786000	0.325638000	0.795662000
C	-1.353684000	2.225744000	-0.263676000	H	-0.849521000	-2.038355000	1.689888000
N	0.286982000	-0.307866000	1.042874000	H	-1.099690000	-0.623455000	2.695462000
O	4.203492000	0.078238000	-0.884925000				
O	-2.449540000	2.818655000	-0.402948000	NTP V(III)			
O	-3.349670000	-2.122292000	-0.708988000	ΔG = -1800.530723			
C	2.866468000	-0.344654000	1.047143000	V	0.097783000	-0.011387000	-1.029691000
H	0.582195000	1.167788000	2.514572000	O	-0.809598000	1.577872000	-1.181670000
H	1.185641000	1.580015000	0.906793000	O	1.989474000	0.267457000	-1.106606000
H	-1.730112000	1.730579000	1.815874000	O	-0.071338000	-1.864169000	-1.053846000
H	-0.600400000	3.017966000	1.561623000	C	-1.098871000	-1.147210000	1.607860000
H	1.544777000	-1.029096000	2.587922000	C	-1.842191000	-1.970812000	0.547648000
H	3.038547000	0.602803000	1.566023000	C	-0.927946000	-2.675690000	-0.437257000
H	3.677511000	-1.002799000	1.366378000	C	1.208517000	-0.353374000	1.692233000
H	1.503976000	-2.014394000	1.124528000	C	2.870566000	0.482996000	-0.151196000
H	-2.924890000	-1.496662000	1.692383000	C	-0.626509000	1.278331000	1.597424000
H	-2.595703000	0.082817000	1.023087000	C	-1.908434000	1.794797000	0.946214000
H	-0.558570000	-2.096383000	1.728870000	C	-1.754802000	2.231205000	-0.501982000
H	-0.906951000	-0.699715000	2.738284000	N	-0.152733000	-0.063335000	1.102453000
				O	4.056497000	0.649675000	-0.395064000
				O	-2.430714000	3.096443000	-1.012766000
				O	-0.965401000	-3.867395000	-0.664328000
				C	2.360133000	0.567701000	1.285753000
NTP V(II)				H	-0.772988000	1.204932000	2.679251000
ΔG = -1800.685837				H	0.168481000	2.001378000	1.427547000
V	0.111201000	-0.304990000	-1.129177000	H	-2.710412000	1.049711000	0.980797000
O	-0.540206000	1.626673000	-1.131753000	H	-2.268575000	2.653926000	1.514184000
O	2.148155000	-0.153752000	-1.235374000	H	1.114070000	-0.323761000	2.783619000
O	-1.699600000	-1.248326000	-1.278377000	H	2.129703000	1.618776000	1.483173000
C	-1.028394000	-0.961947000	1.654272000	H	3.203047000	0.328776000	1.936679000
C	-2.386435000	-0.734835000	0.966219000	H	1.453781000	-1.380236000	1.417937000
C	-2.589067000	-1.458981000	-0.370086000	H	-2.440484000	-2.720116000	1.067431000
C	1.359138000	-1.206980000	1.416889000	H	-2.535956000	-1.346210000	-0.024765000
C	3.108364000	-0.420722000	-0.420739000	H	-0.516845000	-1.824823000	2.232436000
C	0.426748000	1.047289000	1.556470000	H	-1.837849000	-0.683847000	2.261484000
C	-0.629492000	2.109179000	1.247806000				
C	-0.873813000	2.474931000	-0.225228000	NTP Zn(II)			
N	0.191808000	-0.336250000	1.039331000	ΔG = -2635.899421			
O	4.305948000	-0.416406000	-0.740853000	Zn	0.018624000	-0.248619000	-0.860741000
O	-1.399179000	3.572791000	-0.468790000	O	0.118982000	1.673343000	-1.291553000
O	-3.584863000	-2.179784000	-0.529726000				
C	2.764028000	-0.719545000	1.047738000				
H	0.555713000	0.994259000	2.646947000				

O	1.799817000	-1.074419000	-1.102640000	H	1.950587000	-2.120730000	-0.639306000
O	-3.488177000	-1.656507000	-0.997632000	H	2.147699000	2.591604000	-0.815086000
C	-1.121821000	-0.906959000	1.860205000	H	-0.185226000	3.381236000	-0.523226000
C	-2.434813000	-0.893006000	1.068373000	N	-3.083432000	-0.693120000	0.105360000
C	-2.402993000	-1.734983000	-0.192180000	O	-2.242385000	1.904669000	-0.158972000
C	1.300134000	-0.617462000	1.803897000	O	-4.990339000	1.504963000	0.540678000
C	2.799072000	-0.921762000	-0.295674000	H	-4.149540000	1.039060000	0.342015000
C	-0.118630000	1.364314000	1.702356000	H	-4.743297000	2.440492000	0.472456000
C	-0.938218000	2.300416000	0.799427000	O	-3.626616000	4.112723000	0.116180000
C	-0.320132000	2.647151000	-0.560164000	H	-2.945609000	3.393169000	0.005456000
N	-0.003193000	-0.075571000	1.295633000	H	-3.329685000	4.646231000	0.860343000
O	3.936488000	-1.338659000	-0.541676000	O	2.935658000	0.067988000	-0.873046000
O	-0.275743000	3.829271000	-0.918444000	S	4.077038000	0.173047000	0.278916000
O	-1.375335000	-1.627476000	-1.068211000	O	3.511329000	-0.777193000	1.461808000
C	2.545871000	-0.173835000	1.020860000	O	4.178652000	1.532546000	0.774702000
H	-0.535502000	1.400532000	2.715474000	O	5.218457000	-0.519017000	-0.269392000
H	0.891948000	1.768133000	1.770446000	H	2.912376000	-0.285906000	2.049446000
H	-1.938461000	1.899945000	0.617748000				
H	-1.075741000	3.234862000	1.346180000				
H	1.415682000	-0.330957000	2.856607000				
H	2.508568000	0.897137000	0.794435000				
H	3.418189000	-0.321132000	1.658825000				
H	1.235683000	-1.705719000	1.775526000				
H	-3.218083000	-1.288239000	1.722693000				
H	-2.744456000	0.131883000	0.820036000				
H	-0.766521000	-1.938156000	1.900892000				
H	-1.306756000	-0.588404000	2.892561000				
				10-HBQS A1 (III)			
				$\Delta G = -1724.498528$			
				C	-3.494051000	2.883755000	0.174152000
				C	-2.182145000	3.271695000	-0.010707000
				C	-1.162677000	2.315947000	-0.156005000
				C	-1.483848000	0.929831000	-0.112836000
				C	-3.769645000	1.529803000	0.213436000
				C	0.189321000	2.735509000	-0.350338000
				C	-0.431463000	-0.057411000	-0.264795000
				C	0.908995000	0.423988000	-0.444856000
				C	1.182558000	1.827533000	-0.489986000
				C	1.952866000	-0.509604000	-0.592170000
				C	1.734042000	-1.868669000	-0.594383000
				C	0.437960000	-2.345112000	-0.416970000
				C	-0.628126000	-1.474163000	-0.251695000
				H	0.396736000	3.797747000	-0.386095000
				H	-4.295663000	3.599491000	0.288089000
				H	-1.920611000	4.322613000	-0.046150000
				H	-4.784754000	1.180950000	0.359955000
				H	2.200351000	2.153333000	-0.649284000
				H	2.557860000	-2.555986000	-0.733056000
				H	0.234984000	-3.407945000	-0.411074000
				N	-2.814245000	0.582846000	0.078236000
				O	-1.845392000	-2.035688000	-0.090278000
				H	-4.960022000	-2.234496000	1.794545000
				H	-4.097872000	-1.137509000	2.536243000
				H	-5.494394000	-1.643315000	-1.142248000
				H	-4.265230000	-2.282158000	-1.908834000
				O	-4.289242000	-1.540997000	1.672182000
				O	-4.535199000	-1.796238000	-1.110841000
10-HBQS							
$\Delta G = -1482.392923$							
C	-3.707604000	-3.020999000	0.225199000				
C	-2.395583000	-3.394560000	0.025846000				
C	-1.403337000	-2.410953000	-0.138102000				
C	-1.779410000	-1.028216000	-0.099917000				
C	-3.989918000	-1.648916000	0.258491000				
C	-0.037478000	-2.778726000	-0.339526000				
C	-0.761854000	-0.001981000	-0.276383000				
C	0.596028000	-0.432559000	-0.451047000				
C	0.920055000	-1.831531000	-0.485746000				
C	1.610810000	0.529143000	-0.617527000				
C	1.341477000	1.884927000	-0.657936000				
C	0.038202000	2.320525000	-0.493947000				
C	-1.061841000	1.433537000	-0.296794000				
H	0.217669000	-3.832770000	-0.373256000				
H	-4.498108000	-3.749695000	0.355352000				
H	-2.110403000	-4.441075000	-0.006024000				
H	-5.010380000	-1.310108000	0.420345000				

Al	-3.323074000	-1.221353000	0.142532000	C	-3.930161000	2.404009000	0.272396000
O	3.247370000	-0.012873000	-0.841663000	C	-2.682138000	2.964672000	0.051720000
S	4.368899000	0.013178000	0.356497000	C	-1.556659000	2.144644000	-0.122511000
O	4.801791000	-1.533346000	0.475019000	C	-1.727032000	0.740170000	-0.070303000
O	3.735307000	0.322617000	1.615641000	C	-4.053698000	1.028196000	0.306859000
O	5.449467000	0.797530000	-0.191028000	C	-0.244355000	2.673901000	-0.347989000
H	5.390356000	-1.792560000	-0.255956000	C	-0.606559000	-0.129008000	-0.214654000
				C	0.683420000	0.431808000	-0.428802000
10-HBQS Be (II)				C	0.828210000	1.854619000	-0.501557000
$\Delta G = -1497.006004$				C	1.761565000	-0.464453000	-0.555434000
C	-3.816219000	2.571772000	-0.191981000	C	1.592921000	-1.832933000	-0.486739000
C	-2.534953000	3.061799000	-0.030256000	C	0.323102000	-2.375076000	-0.257517000
C	-1.454690000	2.177655000	0.123887000	C	-0.755058000	-1.526196000	-0.123594000
C	-1.703395000	0.776055000	0.106176000	H	-0.127999000	3.749284000	-0.394059000
C	-3.995626000	1.193513000	-0.205978000	H	-4.809466000	3.015258000	0.417049000
C	-0.118417000	2.657467000	0.303409000	H	-2.565252000	4.041213000	0.016418000
C	-0.612170000	-0.152596000	0.283090000	H	-5.008323000	0.552422000	0.483174000
C	0.705296000	0.377637000	0.451914000	H	1.809928000	2.270614000	-0.680529000
C	0.916589000	1.796111000	0.458242000	H	2.445373000	-2.487950000	-0.608219000
C	1.769205000	-0.523285000	0.636913000	H	0.178467000	-3.445186000	-0.192767000
C	1.576200000	-1.889183000	0.694019000	N	-2.985876000	0.212973000	0.132481000
C	0.295835000	-2.407479000	0.529424000	O	-1.992528000	-2.054456000	0.111007000
C	-0.807179000	-1.572822000	0.317438000	H	-4.542283000	-2.555943000	1.232351000
H	0.046431000	3.728386000	0.317217000	H	-3.743865000	-1.568276000	2.191893000
H	-4.668633000	3.227093000	-0.306926000	H	-4.773503000	-1.307892000	-1.459976000
H	-2.348964000	4.129699000	-0.017114000	H	-3.563284000	-2.310839000	-1.769099000
H	-4.983365000	0.765559000	-0.323996000	O	-4.086274000	-1.695759000	1.287949000
H	1.921020000	2.170073000	0.598674000	O	-4.022742000	-1.797662000	-1.080954000
H	2.418411000	-2.547475000	0.863874000	B	-3.150938000	-1.305724000	0.116782000
H	0.126968000	-3.476389000	0.566887000	O	3.023322000	0.078941000	-0.847624000
N	-2.985336000	0.322908000	-0.070659000	S	4.185232000	0.154841000	0.313805000
O	-1.998550000	-2.122855000	0.164983000	O	4.731989000	-1.357367000	0.362264000
H	-5.118700000	-2.511901000	0.661298000	O	3.573136000	0.376983000	1.600908000
H	-4.602955000	-1.534639000	1.766805000	O	5.182963000	1.032927000	-0.246432000
H	-4.535248000	-1.495383000	-2.197182000	H	5.312045000	-1.547323000	-0.396578000
H	-3.214527000	-2.337778000	-2.222513000				
O	-4.632453000	-1.689682000	0.812633000	10-HBQS Ca (I)			
O	-3.858040000	-1.906859000	-1.644263000	$\Delta G = -2159.907469$			
Be	-3.281268000	-1.346385000	-0.145650000	C	-2.907773000	3.487885000	-0.293612000
O	3.053413000	0.019173000	0.879986000	C	-1.561265000	3.719997000	-0.124374000
S	4.219973000	-0.061551000	-0.258460000	C	-0.682777000	2.641001000	0.072935000
O	3.626487000	0.857022000	-1.447234000	C	-1.198098000	1.304510000	0.102956000
O	4.364686000	-1.422315000	-0.733804000	C	-3.336582000	2.160006000	-0.277338000
O	5.319655000	0.674367000	0.310700000	C	0.715463000	2.885558000	0.237343000
H	3.137986000	0.322091000	-2.096246000	C	-0.279634000	0.196895000	0.342059000
				C	1.118070000	0.505764000	0.477344000
10-HBQS B (III)				C	1.580478000	1.862335000	0.421471000
$\Delta G = -1506.824275$				C	2.038368000	-0.534238000	0.704519000

C	1.644553000	-1.848541000	0.855694000	N	-2.468410000	0.842507000	-0.200800000
C	0.300305000	-2.161919000	0.741020000	O	-1.662208000	-1.767753000	-0.437008000
C	-0.694202000	-1.190139000	0.476751000	H	-5.862874000	-0.603863000	-0.132346000
H	1.066758000	3.911029000	0.209401000	H	-5.366678000	-0.296423000	1.304710000
H	-3.618281000	4.289999000	-0.444398000	H	-4.678705000	-3.152148000	-0.285909000
H	-1.160860000	4.727757000	-0.140999000	H	-3.145028000	-3.366175000	-0.101989000
H	-4.393551000	1.955138000	-0.422257000	O	-5.113603000	-0.259743000	0.372260000
H	2.636684000	2.055961000	0.543534000	O	-3.896419000	-2.817745000	0.172375000
H	2.380201000	-2.616716000	1.059357000	Co	-3.256067000	-0.928253000	-0.063037000
H	-0.032577000	-3.186629000	0.855628000	O	3.475969000	-0.255915000	0.920902000
N	-2.539204000	1.105937000	-0.095020000	S	4.712994000	-0.283854000	-0.142909000
O	-1.923158000	-1.583587000	0.382506000	O	4.344126000	0.913544000	-1.163028000
H	-4.185044000	-2.181172000	2.442062000	O	4.727172000	-1.539043000	-0.866292000
H	-5.663929000	-1.947319000	2.055526000	O	5.845023000	0.175784000	0.620448000
H	-4.105990000	-2.655477000	-3.008388000	H	3.837936000	0.584386000	-1.925328000
H	-2.722302000	-2.976631000	-2.401110000				
O	-4.758250000	-1.855234000	1.738526000	10-HBQS Co (III)			
O	-3.518780000	-2.448713000	-2.272266000	$\Delta G = -2864.674486$			
Ca	-3.883297000	-1.023400000	-0.358245000	C	-3.401812000	3.018408000	-0.040533000
O	3.402723000	-0.186328000	0.901401000	C	-2.109710000	3.483313000	-0.080369000
S	4.506802000	-0.489255000	-0.256174000	C	-1.036773000	2.570316000	-0.131039000
O	4.070812000	0.504367000	-1.456187000	C	-1.316653000	1.171878000	-0.154778000
O	4.399001000	-1.860705000	-0.713265000	C	-3.613275000	1.637519000	-0.018237000
O	5.737610000	0.045804000	0.270562000	C	0.313215000	3.024162000	-0.150776000
H	3.429311000	0.079071000	-2.050337000	C	-0.230362000	0.244063000	-0.258507000
				C	1.098758000	0.741406000	-0.258416000
10-HBQS Co (II)				C	1.349062000	2.143903000	-0.198587000
$\Delta G = -2864.921469$				C	2.172327000	-0.188149000	-0.330096000
C	-2.927356000	3.196109000	-0.428709000	C	1.971370000	-1.561572000	-0.392443000
C	-1.620445000	3.495179000	-0.112328000	C	0.676897000	-2.047522000	-0.394817000
C	-0.703865000	2.457399000	0.117390000	C	-0.426057000	-1.170611000	-0.365534000
C	-1.135167000	1.100020000	0.017468000	H	0.497264000	4.090933000	-0.119300000
C	-3.309888000	1.858942000	-0.442772000	H	-4.252516000	3.684361000	-0.001937000
C	0.655110000	2.755412000	0.451165000	H	-1.899772000	4.545899000	-0.068648000
C	-0.155817000	0.040330000	0.134264000	H	-4.617550000	1.240897000	0.058814000
C	1.200496000	0.395821000	0.436990000	H	2.370842000	2.494731000	-0.200351000
C	1.564124000	1.768676000	0.628210000	H	2.808190000	-2.242655000	-0.457543000
C	2.166523000	-0.622029000	0.523782000	H	0.480594000	-3.109376000	-0.463352000
C	1.857034000	-1.952061000	0.320023000	N	-2.618589000	0.747487000	-0.069425000
C	0.554528000	-2.301201000	-0.006713000	O	-1.607935000	-1.709396000	-0.498125000
C	-0.464740000	-1.339907000	-0.105313000	H	-4.674168000	-1.711865000	1.802330000
H	0.938306000	3.795870000	0.559955000	H	-3.913369000	-0.428594000	2.274906000
H	-3.661111000	3.964010000	-0.632806000	H	-4.548056000	-3.078769000	-0.915945000
H	-1.283116000	4.522930000	-0.043124000	H	-3.237264000	-3.586206000	-0.249419000
H	-4.338746000	1.589609000	-0.625115000	O	-4.284165000	-0.876688000	1.500393000
H	2.585753000	2.005468000	0.889195000	O	-3.925240000	-2.906140000	-0.194067000
H	2.624842000	-2.709354000	0.410812000	Co	-3.194238000	-1.065886000	-0.091962000
H	0.290504000	-3.336507000	-0.181912000	O	3.423827000	0.385092000	-0.396957000

S	4.769191000	-0.220686000	0.364577000	C	-0.966287000	2.589793000	-0.113096000
O	5.174384000	-1.443017000	-0.588518000	C	-1.292569000	1.198738000	-0.112720000
O	4.374183000	-0.817578000	1.613176000	C	-3.562776000	1.756536000	0.019617000
O	5.716135000	0.856645000	0.255299000	C	0.388459000	3.013000000	-0.158530000
H	5.601872000	-1.135912000	-1.408664000	C	-0.220867000	0.239778000	-0.211832000
				C	1.116999000	0.716138000	-0.253235000
10-HBQS Cr (II)				C	1.403660000	2.107943000	-0.214965000
$\Delta G = -2526.630837$				C	2.193231000	-0.220975000	-0.346016000
C	-2.990500000	-3.293850000	0.396345000	C	1.989506000	-1.594377000	-0.429558000
C	-1.669231000	-3.574759000	0.092320000	C	0.697415000	-2.066156000	-0.408616000
C	-0.763342000	-2.518008000	-0.089648000	C	-0.421726000	-1.190744000	-0.295654000
C	-1.207992000	-1.165914000	0.031068000	H	0.598009000	4.075669000	-0.146414000
C	-3.378323000	-1.967960000	0.485363000	H	-4.134699000	3.828502000	0.017708000
C	0.606846000	-2.791516000	-0.398876000	H	-1.748390000	4.599921000	-0.073307000
C	-0.254091000	-0.083885000	-0.115754000	H	-4.580656000	1.399937000	0.097090000
C	1.112913000	-0.420961000	-0.404336000	H	2.432568000	2.434952000	-0.243654000
C	1.504110000	-1.790941000	-0.557671000	H	2.823250000	-2.276006000	-0.524622000
C	2.059386000	0.609919000	-0.542729000	H	0.487762000	-3.125254000	-0.481216000
C	1.725905000	1.944152000	-0.432171000	N	-2.612844000	0.819669000	-0.020956000
C	0.412006000	2.281528000	-0.139155000	O	-1.577995000	-1.749941000	-0.283060000
C	-0.583534000	1.308823000	0.030223000	H	-6.091782000	-0.862223000	0.181360000
H	0.910379000	-3.826777000	-0.505168000	H	-5.559194000	-0.795776000	1.644442000
H	-3.719683000	-4.076497000	0.559517000	H	-4.764326000	-3.509507000	-0.281501000
H	-1.320347000	-4.596215000	-0.001202000	H	-3.237123000	-3.785345000	-0.457290000
H	-4.407309000	-1.717791000	0.720875000	O	-5.305794000	-0.691330000	0.717389000
H	2.534280000	-2.013734000	-0.796704000	O	-3.882256000	-3.165755000	-0.092005000
H	2.478784000	2.709374000	-0.567858000	Cr	-3.334511000	-1.150248000	0.081043000
H	0.121545000	3.319585000	-0.036309000	O	3.446520000	0.345338000	-0.421095000
N	-2.543325000	-0.920324000	0.291569000	S	4.782964000	-0.256607000	0.362296000
O	-1.792389000	1.752253000	0.334068000	O	5.195849000	-1.488627000	-0.574792000
H	-4.150456000	1.720006000	-2.037767000	O	4.371353000	-0.840937000	1.611476000
H	-3.596526000	0.275530000	-2.265735000	O	5.734105000	0.817157000	0.254160000
H	-5.113045000	2.977489000	0.966770000	H	5.630508000	-1.189760000	-1.394204000
H	-3.688974000	3.486344000	0.632792000				
O	-3.965296000	0.875613000	-1.605357000	10-HBQS Cu (II)			
O	-4.339050000	2.804516000	0.415187000	$\Delta G = -3122.634709$			
Cr	-3.417958000	0.856565000	0.361580000	C	-2.882206000	3.232100000	-0.391777000
O	3.380137000	0.247025000	-0.908626000	C	-1.555570000	3.524776000	-0.159418000
S	4.603661000	0.352757000	0.163820000	C	-0.632664000	2.490176000	0.060278000
O	4.246212000	-0.798696000	1.239343000	C	-1.074397000	1.131372000	0.035284000
O	4.587039000	1.642252000	0.824338000	C	-3.268004000	1.897557000	-0.361397000
O	5.753010000	-0.122470000	-0.563570000	C	0.741531000	2.794615000	0.311162000
H	3.724805000	-0.440424000	1.977848000	C	-0.104787000	0.064464000	0.191370000
				C	1.264033000	0.430595000	0.427507000
10-HBQS Cr (III)				C	1.647752000	1.809340000	0.503763000
$\Delta G = -2526.490067$				C	2.226457000	-0.581967000	0.583413000
C	-3.308229000	3.131998000	-0.013905000	C	1.902324000	-1.921863000	0.526571000
C	-2.003388000	3.546934000	-0.066499000	C	0.589045000	-2.287413000	0.271602000

C	-0.426030000	-1.333207000	0.093254000	H	-5.770580000	0.985091000	-0.789642000
H	1.037439000	3.836379000	0.347815000	H	-5.178994000	-0.372976000	-1.238237000
H	-3.619408000	4.000984000	-0.577991000	H	-4.793034000	3.019510000	0.876538000
H	-1.206910000	4.550981000	-0.146146000	H	-3.328851000	3.403133000	0.488643000
H	-4.303251000	1.624498000	-0.514476000	O	-5.119014000	0.309917000	-0.556526000
H	2.681806000	2.049896000	0.704551000	O	-4.057423000	2.795697000	0.291034000
H	2.666043000	-2.674451000	0.673178000	Fe	-3.300775000	0.940899000	0.087611000
H	0.312114000	-3.332047000	0.209460000	O	3.487985000	0.213436000	-0.913549000
N	-2.412420000	0.888887000	-0.141810000	S	4.703634000	0.308051000	0.171984000
O	-1.626831000	-1.803704000	-0.170678000	O	4.319770000	-0.835704000	1.245751000
H	-5.743523000	-1.046145000	0.611480000	O	4.693657000	1.599948000	0.827321000
H	-5.183010000	0.182045000	1.367948000	O	5.852692000	-0.183082000	-0.544393000
H	-4.650054000	-2.847525000	-1.230813000	H	3.805640000	-0.466819000	1.984258000
H	-3.365822000	-3.358749000	-0.525860000				
O	-5.109052000	-0.319249000	0.544057000				
O	-4.101253000	-2.734058000	-0.442500000				
Cu	-3.241938000	-0.894314000	-0.058232000				
O	3.547279000	-0.191263000	0.908454000				
S	4.755563000	-0.329031000	-0.180776000				
O	4.358671000	0.765555000	-1.300099000				
O	4.746295000	-1.648363000	-0.779064000				
O	5.907909000	0.196692000	0.505146000				
H	3.839664000	0.363390000	-2.017534000				
				10-HBQS Fe(III)			
				$\Delta G = -2745.638817$			
				C	-3.353222000	-3.046169000	0.085854000
				C	-2.050224000	-3.487959000	0.106422000
				C	-0.992196000	-2.559349000	0.145055000
				C	-1.291682000	-1.166670000	0.169353000
				C	-3.586240000	-1.673176000	0.051799000
				C	0.364888000	-2.997501000	0.163824000
				C	-0.218435000	-0.220649000	0.303272000
				C	1.120220000	-0.705757000	0.317517000
				C	1.386928000	-2.105364000	0.230054000
				C	2.178904000	0.226414000	0.453460000
				C	1.962264000	1.584347000	0.602683000
				C	0.658749000	2.058793000	0.607140000
				C	-0.427470000	1.183308000	0.467920000
				H	0.561508000	-4.061850000	0.124584000
				H	-4.191904000	-3.728018000	0.068215000
				H	-1.822608000	-4.547088000	0.096497000
				H	-4.597143000	-1.292078000	-0.004379000
				H	2.413328000	-2.442730000	0.240646000
				H	2.792954000	2.265987000	0.725175000
				H	0.451448000	3.112983000	0.735079000
				N	-2.601535000	-0.763661000	0.075072000
				O	-1.627858000	1.728181000	0.539675000
				H	-5.263507000	1.484282000	-1.570168000
				H	-4.567172000	0.181372000	-2.072868000
				H	-4.624336000	3.244902000	0.473355000
				H	-3.096821000	3.579023000	0.450319000
				O	-4.671649000	0.764609000	-1.306775000
				O	-3.776864000	2.999973000	0.074667000
				Fe	-3.170351000	1.091865000	-0.042405000
				O	3.456215000	-0.322223000	0.515412000
				S	4.694104000	0.201824000	-0.441732000
				O	5.190818000	1.515738000	0.336613000

10-HBQS Fe(II)

$\Delta G = -2745.870268$

C	-2.936917000	-3.193932000	0.444114000
C	-1.622168000	-3.496847000	0.162039000
C	-0.700750000	-2.466349000	-0.083304000
C	-1.135126000	-1.106931000	-0.039521000
C	-3.316478000	-1.857493000	0.416416000
C	0.665813000	-2.775507000	-0.369645000
C	-0.159690000	-0.046357000	-0.186866000
C	1.204092000	-0.414135000	-0.440978000
C	1.576554000	-1.792818000	-0.558416000
C	2.170919000	0.599331000	-0.567909000
C	1.854749000	1.937682000	-0.457885000
C	0.543136000	2.300554000	-0.184439000
C	-0.475354000	1.346392000	-0.045665000
H	0.953569000	-3.818440000	-0.430862000
H	-3.671189000	-3.957491000	0.661299000
H	-1.281329000	-4.525419000	0.135072000
H	-4.344976000	-1.583036000	0.607527000
H	2.605524000	-2.036215000	-0.781168000
H	2.622559000	2.690641000	-0.578590000
H	0.271961000	3.343862000	-0.084079000
N	-2.469895000	-0.847557000	0.157003000
O	-1.684129000	1.806953000	0.211980000

O	4.166798000	0.677180000	-1.695336000	C	-3.783473000	2.074255000	-0.298869000
O	5.672179000	-0.850599000	-0.338153000	C	0.241972000	2.859559000	0.362402000
H	5.686419000	1.286685000	1.143339000	C	-0.699244000	0.148781000	0.231271000
				C	0.685874000	0.471400000	0.435635000
10-HBQS K (I)				C	1.118376000	1.838373000	0.507150000
$\Delta G = -2082.298144$				C	1.622213000	-0.567103000	0.593674000
C	-2.591321000	-3.925840000	-0.002468000	C	1.252757000	-1.896890000	0.595369000
C	-1.231955000	-4.032874000	0.195542000	C	-0.078736000	-2.225063000	0.399101000
C	-0.445178000	-2.871440000	0.302704000	C	-1.092667000	-1.253929000	0.207625000
C	-1.078737000	-1.588882000	0.220973000	H	0.576782000	3.889506000	0.419587000
C	-3.125268000	-2.635643000	-0.112987000	H	-4.108775000	4.206200000	-0.377589000
C	0.969595000	-2.967112000	0.476101000	H	-1.676152000	4.686386000	0.023694000
C	-0.277016000	-0.380059000	0.374079000	H	-4.828646000	1.830094000	-0.468170000
C	1.144650000	-0.541366000	0.502192000	H	2.165144000	2.041577000	0.684140000
C	1.732018000	-1.850584000	0.552127000	H	1.998162000	-2.667875000	0.746279000
C	1.965733000	0.595936000	0.613607000	H	-0.380935000	-3.265826000	0.396111000
C	1.447001000	1.874266000	0.657658000	N	-2.959036000	1.039616000	-0.149028000
C	0.075650000	2.048773000	0.572758000	O	-2.311799000	-1.656926000	0.030396000
C	-0.840146000	0.969084000	0.435280000	H	-4.845379000	-3.000715000	-0.255846000
H	1.421311000	-3.951502000	0.536705000	H	-6.157475000	-2.201472000	0.050258000
H	-3.230190000	-4.795892000	-0.087545000	H	-3.126535000	-4.635628000	-0.679066000
H	-0.751369000	-5.003058000	0.266233000	H	-2.836308000	-3.264537000	0.027836000
H	-4.191004000	-2.517268000	-0.298750000	O	-5.309776000	-2.146116000	-0.401945000
H	2.802779000	-1.934343000	0.678900000	O	-3.429815000	-4.064136000	0.034431000
H	2.107670000	2.726442000	0.765827000	Li	-3.896089000	-0.757246000	-0.214690000
H	-0.342611000	3.047599000	0.618597000	O	2.970279000	-0.214543000	0.878760000
N	-2.418543000	-1.516468000	-0.014057000	S	4.125181000	-0.373358000	-0.256627000
O	-2.103693000	1.221976000	0.388930000	O	3.704569000	0.719597000	-1.372792000
H	-4.714433000	3.202218000	0.183008000	O	4.078431000	-1.696061000	-0.848464000
H	-5.805207000	3.552839000	-0.870652000	O	5.318819000	0.140597000	0.368318000
H	-3.307988000	3.515569000	2.067688000	H	3.095739000	0.336757000	-2.027169000
H	-2.713798000	2.655211000	0.889502000				
O	-5.413969000	2.815690000	-0.391439000	10-HBQS Mg (II)			
O	-3.230709000	3.488551000	1.108185000	$\Delta G = -1682.354643$			
O	3.366277000	0.411352000	0.789417000	C	-3.279300000	3.057366000	-0.357094000
S	4.371853000	0.536279000	-0.487280000	C	-1.955375000	3.393998000	-0.176845000
O	4.453930000	2.131390000	-0.741510000	C	-0.993918000	2.392654000	0.037920000
O	3.758847000	0.008692000	-1.685449000	C	-1.394802000	1.019479000	0.073975000
O	5.644656000	0.052543000	0.002761000	C	-3.608712000	1.706092000	-0.313459000
H	4.989371000	2.565163000	-0.054969000	C	0.376975000	2.752703000	0.219113000
K	-4.081959000	0.513934000	-1.120644000	C	-0.389892000	-0.012569000	0.297023000
				C	0.975644000	0.413525000	0.450376000
10-HBQS Li (I)				C	1.321047000	1.804788000	0.414931000
$\Delta G = -1489.900444$				C	1.980499000	-0.547166000	0.662863000
C	-3.384386000	3.412421000	-0.248275000	C	1.703187000	-1.895101000	0.768214000
C	-2.048253000	3.668781000	-0.028025000	C	0.393782000	-2.321571000	0.622121000
C	-1.144768000	2.603480000	0.132857000	C	-0.675563000	-1.433109000	0.379685000
C	-1.630110000	1.258335000	0.067350000	H	0.641334000	3.803700000	0.196800000

H	-4.046571000	3.800825000	-0.526211000	H	-4.824936000	-3.202509000	-0.771908000
H	-1.636512000	4.430163000	-0.198574000	H	-3.308025000	-3.469536000	-0.487644000
H	-4.640320000	1.399335000	-0.447707000	O	-5.289706000	-0.299965000	0.337828000
H	2.355152000	2.086052000	0.553939000	O	-4.049836000	-2.877120000	-0.298379000
H	2.500648000	-2.602151000	0.958407000	Mn	-3.357608000	-0.953236000	-0.074935000
H	0.150694000	-3.374605000	0.694783000	O	3.500922000	-0.208692000	0.907246000
N	-2.723348000	0.723209000	-0.106327000	S	4.686699000	-0.316880000	-0.207934000
O	-1.863385000	-1.947951000	0.249541000	O	4.235870000	0.760179000	-1.324700000
H	-6.181896000	-1.420948000	0.722926000	O	4.703181000	-1.639222000	-0.800189000
H	-5.495705000	-0.387622000	1.655267000	O	5.840952000	0.244129000	0.446939000
H	-5.033873000	-2.665828000	-1.964310000	H	3.693505000	0.345235000	-2.017133000
H	-3.718317000	-3.420614000	-1.623205000				
O	-5.408023000	-0.850753000	0.812544000	10-HBQS Na (I)			
O	-4.307731000	-2.714435000	-1.330753000	$\Delta G = -1644.661552$			
Mg	-3.588122000	-1.212380000	-0.107749000	C	-2.941814000	-3.727424000	0.262370000
O	3.304382000	-0.084728000	0.883846000	C	-1.587176000	-3.890918000	0.075058000
S	4.449621000	-0.280643000	-0.258712000	C	-0.762638000	-2.765566000	-0.101971000
O	3.917758000	0.643603000	-1.474056000	C	-1.346161000	-1.456118000	-0.084320000
O	4.495331000	-1.661317000	-0.697009000	C	-3.436029000	-2.418709000	0.261753000
O	5.607569000	0.390963000	0.275457000	C	0.641707000	-2.930651000	-0.302664000
H	3.343680000	0.138494000	-2.074970000	C	-0.490261000	-0.286955000	-0.262816000
				C	0.917087000	-0.520654000	-0.445294000
10-HBQS Mn (II)				C	1.445516000	-1.855149000	-0.469233000
$\Delta G = -2633.170148$				C	1.788043000	0.570008000	-0.626823000
C	-2.910098000	3.232453000	-0.410398000	C	1.334486000	1.872688000	-0.675848000
C	-1.590747000	3.518271000	-0.135394000	C	-0.015396000	2.119135000	-0.495438000
C	-0.682216000	2.475709000	0.106769000	C	-0.974062000	1.093252000	-0.270330000
C	-1.132133000	1.119031000	0.070074000	H	1.049083000	-3.935698000	-0.322129000
C	-3.301698000	1.899040000	-0.384447000	H	-3.609719000	-4.567732000	0.403175000
C	0.688345000	2.776658000	0.379818000	H	-1.139284000	-4.878930000	0.060955000
C	-0.162788000	0.047610000	0.225957000	H	-4.501986000	-2.258710000	0.402836000
C	1.207585000	0.411783000	0.462708000	H	2.506493000	-1.988289000	-0.626898000
C	1.592716000	1.788460000	0.563684000	H	2.029924000	2.685164000	-0.847588000
C	2.175398000	-0.600000000	0.594135000	H	-0.381443000	3.138680000	-0.527773000
C	1.857549000	-1.940334000	0.516851000	N	-2.691951000	-1.329209000	0.097211000
C	0.543192000	-2.303392000	0.266745000	O	-2.206802000	1.428660000	-0.091000000
C	-0.481390000	-1.353000000	0.112032000	H	-4.780702000	3.202055000	0.273562000
H	0.984560000	3.817830000	0.432823000	H	-6.234248000	2.843486000	-0.163329000
H	-3.636711000	4.004914000	-0.622653000	H	-2.780244000	4.368633000	0.805179000
H	-1.234796000	4.541904000	-0.111605000	H	-2.671733000	3.014574000	0.009739000
H	-4.334035000	1.636999000	-0.572873000	O	-5.500431000	2.538975000	0.379962000
H	2.625810000	2.025133000	0.774071000	O	-3.158028000	3.889512000	0.059973000
H	2.626334000	-2.691614000	0.643060000	Na	-4.241116000	0.560553000	0.113502000
H	0.268285000	-3.347934000	0.190080000	O	3.162202000	0.295596000	-0.879923000
N	-2.471006000	0.875893000	-0.129181000	S	4.280416000	0.576293000	0.267439000
O	-1.682751000	-1.821942000	-0.136026000	O	3.892589000	-0.475627000	1.434671000
H	-6.030338000	-0.919826000	0.333218000	O	4.151493000	1.924640000	0.784998000
H	-5.470953000	0.336455000	1.042164000	O	5.515503000	0.095231000	-0.301451000

H	3.231105000	-0.099057000	2.039739000	C	-0.216419000	0.140735000	-0.384955000
				C	1.150570000	0.536607000	-0.485552000
10-HBQS Ni (II)				C	1.502239000	1.922460000	-0.440104000
$\Delta G = -2990.453579$				C	2.130128000	-0.468252000	-0.644270000
C	-2.944437000	3.164874000	-0.463920000	C	1.819795000	-1.807299000	-0.732013000
C	-1.644760000	3.482332000	-0.134095000	C	0.483549000	-2.201007000	-0.646423000
C	-0.716576000	2.457156000	0.105808000	C	-0.502428000	-1.244556000	-0.479039000
C	-1.133218000	1.097245000	0.003180000	H	0.812018000	3.921339000	-0.257524000
C	-3.315062000	1.824020000	-0.474262000	H	-3.914135000	3.887641000	0.323577000
C	0.638719000	2.762285000	0.450073000	H	-1.510313000	4.555830000	0.055801000
C	-0.148416000	0.049190000	0.116801000	H	-4.491933000	1.502233000	0.269200000
C	1.200445000	0.406134000	0.435666000	H	2.540719000	2.203943000	-0.542652000
C	1.553126000	1.780602000	0.635152000	H	2.600476000	-2.542928000	-0.871667000
C	2.163635000	-0.615064000	0.521911000	H	0.202850000	-3.243122000	-0.719400000
C	1.851807000	-1.941857000	0.302756000	N	-2.556535000	0.828906000	-0.049175000
C	0.551412000	-2.288572000	-0.044118000	O	-1.786065000	-1.665560000	-0.427780000
C	-0.456707000	-1.320844000	-0.150061000	H	-3.549361000	-2.094428000	2.348091000
H	0.914820000	3.804319000	0.560794000	H	-3.183195000	-0.576442000	2.501467000
H	-3.685517000	3.922768000	-0.678102000	H	-5.753227000	-2.318770000	0.445785000
H	-1.323202000	4.514946000	-0.063655000	H	-5.531580000	-2.383573000	-1.106993000
H	-4.339428000	1.544742000	-0.663393000	O	-3.475711000	-1.253350000	1.874661000
H	2.570771000	2.023794000	0.905946000	O	-5.119973000	-2.142678000	-0.264614000
H	2.616722000	-2.701767000	0.395253000	V	-3.372890000	-1.073308000	-0.132497000
H	0.290369000	-3.321331000	-0.236816000	O	3.460261000	-0.047729000	-0.809419000
N	-2.460455000	0.822882000	-0.217233000	S	4.543270000	-0.199887000	0.417224000
O	-1.652000000	-1.727606000	-0.533945000	O	4.924954000	-1.761424000	0.358296000
H	-5.752088000	-0.601611000	0.066519000	O	3.873958000	-0.021726000	1.682486000
H	-5.130553000	-0.378732000	1.473523000	O	5.662393000	0.607350000	-0.002783000
H	-4.628131000	-3.073361000	-0.282339000	H	5.532389000	-1.948319000	-0.379473000
H	-3.097559000	-3.327692000	-0.126834000				
O	-4.965577000	-0.275434000	0.525744000	10-HBQS V (III)			
O	-3.832423000	-2.772025000	0.177573000	$\Delta G = -2425.986245$			
Ni	-3.200115000	-0.924216000	-0.063273000	C	-2.944267000	3.300964000	-0.384542000
O	3.468830000	-0.254010000	0.931149000	C	-1.615193000	3.569904000	-0.128825000
S	4.714255000	-0.275761000	-0.125213000	C	-0.711531000	2.510693000	0.053024000
O	4.344574000	0.920589000	-1.145122000	C	-1.170611000	1.159529000	-0.034815000
O	4.737131000	-1.530396000	-0.848843000	C	-3.337343000	1.970462000	-0.444351000
O	5.837947000	0.187702000	0.647460000	C	0.662518000	2.789271000	0.333578000
H	3.854474000	0.588427000	-1.916679000	C	-0.218933000	0.073410000	0.135865000
				C	1.151914000	0.416711000	0.399237000
10-HBQS V (II)				C	1.554846000	1.787904000	0.506676000
$\Delta G = -2426.183701$				C	2.099039000	-0.609872000	0.566851000
C	-3.131815000	3.156246000	0.174863000	C	1.762009000	-1.945885000	0.505340000
C	-1.810965000	3.515377000	0.028397000	C	0.444802000	-2.290139000	0.238812000
C	-0.833280000	2.520826000	-0.151568000	C	-0.557230000	-1.324952000	0.050163000
C	-1.229188000	1.154313000	-0.196636000	H	0.971133000	3.825658000	0.408361000
C	-3.457847000	1.803047000	0.136904000	H	-3.673605000	4.086281000	-0.531571000
C	0.546771000	2.871414000	-0.285757000	H	-1.253672000	4.589555000	-0.063118000

H	-4.378026000	1.731235000	-0.633202000	O	-4.984493000	-0.986113000	1.107875000
H	2.589349000	2.010137000	0.725822000	O	-4.300536000	-1.960572000	-1.511937000
H	2.514990000	-2.707286000	0.661778000	Zn	-3.246016000	-0.906209000	-0.006479000
H	0.151560000	-3.330927000	0.180387000	O	3.589297000	-0.149105000	0.891785000
N	-2.506068000	0.925889000	-0.278927000	S	4.767288000	-0.363091000	-0.214874000
O	-1.771368000	-1.773617000	-0.196582000	O	4.277498000	0.557773000	-1.449331000
H	-5.195604000	-1.247913000	1.711079000	O	4.812852000	-1.747197000	-0.641250000
H	-4.525217000	0.133793000	1.966329000	O	5.914226000	0.301040000	0.350488000
H	-5.071332000	-3.190187000	-1.008488000	H	3.711598000	0.056140000	-2.061065000
H	-3.718572000	-3.634677000	-0.395605000				
O	-4.715412000	-0.525019000	1.286240000				
O	-4.371468000	-2.922161000	-0.399515000				
V	-3.470921000	-0.933419000	-0.374016000				
O	3.420762000	-0.236950000	0.918877000				
S	4.644292000	-0.372869000	-0.149954000				
O	4.288178000	0.750066000	-1.255952000				
O	4.626252000	-1.679440000	-0.776040000				
O	5.793927000	0.120552000	0.564845000				
H	3.766890000	0.372202000	-1.984710000				

10-HBQS Zn(II)

$\Delta G = -3261.512847$

C	-2.834633000	3.307211000	-0.288732000
C	-1.490648000	3.566604000	-0.132670000
C	-0.580678000	2.512535000	0.049025000
C	-1.046908000	1.159224000	0.059360000
C	-3.239418000	1.978899000	-0.250005000
C	0.804389000	2.805675000	0.236957000
C	-0.089350000	0.069718000	0.232475000
C	1.291916000	0.437601000	0.422987000
C	1.699293000	1.812082000	0.427657000
C	2.260090000	-0.562555000	0.620106000
C	1.940325000	-1.903918000	0.656453000
C	0.624157000	-2.276945000	0.448510000
C	-0.409731000	-1.345445000	0.223204000
H	1.116569000	3.843473000	0.233321000
H	-3.563463000	4.093711000	-0.429582000
H	-1.115766000	4.583783000	-0.142622000
H	-4.289301000	1.730644000	-0.352632000
H	2.743038000	2.041892000	0.585566000
H	2.707801000	-2.645458000	0.836912000
H	0.344267000	-3.323051000	0.457693000
N	-2.397023000	0.949410000	-0.086298000
O	-1.596595000	-1.858144000	0.007828000
H	-5.541952000	-1.758395000	0.942749000
H	-4.924049000	-0.878083000	2.066305000
H	-4.820457000	-1.450901000	-2.147347000
H	-3.756063000	-2.569471000	-2.028483000