Supplementary material

Metal-histidine-glutamate as a regulator of enzymatic cycles : a case study of carbonic anhydrase

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Table S1. Interatomic distances (in Å) between Zn and C of the carboxylic moiety of the Zn-His-Glu triad, and between Zn and C of the carboxylic moiety of model of Glu106 (in bracket).

X	X_{OH}•H_2O	X_{NH}•H_2O	X_{OH}•OH^-	X_{NH}•OH^-
1	7.626	7.159	7.638	7.262
2	7.669	7.205	7.657	7.280
3	-	-	7.575	7.317
4	7.668	7.208	-	-
5	7.655 (5.291)	7.297 (5.060)	-	-
6	7.435	6.371	7.604	7.281
7	7.174	6.399	7.607	7.355
8	7.326	6.390	-	-
9	7.292 (6.051)	6.367 (5.973)	-	-
10	6.831 (5.347)	6.522 (5.234)	-	-
11	7.027 (4.960)	6.955 (4.878)		
12	6.767 (5.005)	6.955 (5.166)		
Exp.[a]	6.993 (5.209)			

[a] Ref 4.

a) Absolute electronic energies, gas phase and solvation free energies for complexes **1-12**

	E^a	E^b	E^c	$H_{corr}{}^d$	$G^1{}_{coor}{}^e$	$\Delta G^4{}_{solv}{}^f$	$\Delta G^{78}{}_{solv}{}^f$
$\mathbf{1_{NH}\bullet H_2O}$	-2755.286611	-2763.125572	-2759.477441	0.341916	0.259358	-238.11	-336.52
$\mathbf{1_{OH}\bullet H_2O}$	-2755.317940	-2763.149038	-2759.502565	0.344405	0.257204	-183.64	-264.26
$\mathbf{2_{NH}\bullet H_2O}$	-2811.483396 (-2819.298952)	-2819.722847 (-2819.726659)	-2815.924722	0.386537 (0.361515)	0.290529 (0.268490)	-224.26	-320.49
$\mathbf{2_{OH}\bullet H_2O}$	-2811.508945 (-2819.320623)	-2819.742084 (-2819.746437)	-2815.945202	0.387649 (0.363184)	0.290423 (0.266916)	-171.71	-251.71
$\mathbf{4_{NH}\bullet H_2O}$	-2926.542220	-2935.515897	-2931.426883	0.447999	0.342024	-200.54	-293.05
$\mathbf{4_{OH}\bullet H_2O}$	-2926.565764	-2935.533138	-2931.445383	0.449967	0.337854	-151.59	-229.12
$\mathbf{5_{NH}\bullet H_2O}$	-3210.143128	-3220.894479		0.552635	0.421768	-57.49	-116.19
$\mathbf{5_{OH}\bullet H_2O}$	-3210.156740	-3220.902713		0.553265	0.421136	-31.38	-81.96
$\mathbf{6_{NH}\bullet H_2O}$	-3002.353170	-3011.799116	-3007.504814	0.463504	0.362143	-140.83	-215.64
$\mathbf{6_{OH}\bullet H_2O}$	-3002.368262	-3011.809091	-3007.515917	0.464364	0.360711	-118.83	-184.68
$\mathbf{7_{NH}\bullet H_2O}$	-3418.359208	-3430.441705		0.639532	0.497698	-87.03	-152.63
$\mathbf{7_{OH}\bullet H_2O}$	-3418.368641	-3430.448802		0.639787	0.493822	-78.49	-139.49
$\mathbf{7_{TS}\bullet H_2O}$	-3418.357063	-3430.445784		0.634590	0.492247	-77.95	-140.08
$\mathbf{8_{NH}\bullet H_2O}$	-3117.408892	-3127,586463		0.526612	0.414538	-115.94	-188.20
$\mathbf{8_{OH}\bullet H_2O}$	-3117.423214	-3127.596625		0.527178	0.412401	-92.34	-155.52
$\mathbf{9_{NH}\bullet H_2O}$	-3591.833956	-3604.992270		0.706979	0.563307	34.35	-5.94
$\mathbf{9_{OH}\bullet H_2O}$	-3591.841800	-3604.997597		0.707226	0.561670	45.56	10.67
$\mathbf{10_{NH}\bullet H_2O}$	-4007.834723	-4023.626264		0.883723	0.708484	92.22	56.94
$\mathbf{10_{OH}\bullet H_2O}$	-4007.831614	-4023.621313		0.882908	0.703742	96.52	62.26
$\mathbf{11_{NH}\bullet H_2O}$	-4161.595720 (-4177.555072)	-4178.462341 (-4178.473617)				-27.78	-99.24
$\mathbf{11_{OH}\bullet H_2O}$	-4161.607823 (-4177.563879)	-4178.468961 (-4178.481278)				4.60	-54.89
$\mathbf{12_{NH}\bullet H_2O}$	-4161.538730[g]	-4178.414929[g]	-25330.922880[h] (-25342.682776)				1845.02
$\mathbf{12_{OH}\bullet H_2O}$	-4161.553700[g]	-4178.430332[g]	-25330.985767[h] (-25342.752555)				1955.89
$\mathbf{1_{NH}\bullet OH^-}$	-2754.880681	-2762.739337	-2759.093539	0.32886	0.246297	-89.50	-139.49
$\mathbf{1_{OH}\bullet OH^-}$	-2754.895363	-2762.747898	-2759.103928	0.329980	0.246143	-57.70	-97.74
$\mathbf{2_{NH}\bullet OH^-}$	-2811.075957 (-2818.897568)	-2819.334133 (-2819.337603)	-2815.538301	0.372903 (0.348386)	0.278956 (0.257734)	-77.36	-126.82

$\mathbf{2_{OH}{\bullet}OH^-}$	-2811.085301 (-2818.904355)	-2819.339182 (-2819.342790)	-2815.544690	0.373065 (0.348885)	0.277202 (0.253995)	-52.09	-93.76
$\mathbf{3_{NH}{\bullet}OH^-}$	-2867.281942	-2875.937132	-2871.990687	0.417228	0.316467	-45.52	-88.28
$\mathbf{3_{OH}{\bullet}OH^-}$	-2867.283159	-2875.935306	-2871.993414	0.416336	0.312103	-27.91	-66.15
$\mathbf{6_{NH}{\bullet}OH^-}$	-3001.903416	-3011.366859	-3007.068680	0.449415	0.340788	-76.99	-129.70
$\mathbf{6_{OH}{\bullet}OH^-}$	-3001.910932	-3011.370832	-3007.073631	0.449431	0.340291	-55.23	-100.67
$\mathbf{7_{NH}{\bullet}OH^-}$	-3417.896389	-3429.996151		0.624849	0.472517	-58.91	-112.63
$\mathbf{7_{OH}{\bullet}OH^-}$	-3417.899492	-3429.997030		0.624505	0.471271	-41.84	-89.45
$\mathbf{7_{TS}{\bullet}OH^-}$	-3417.891423	-3429.997846		0.619307	0.467889	-47.32	-96.44

a. absolute energy at the HF/BS1 level in u.a. Values in bracket are at the B3LYP/BS1 level.
b. absolute energy at the B3LYP/BS2//HF/BS1 level in u.a. Values in bracket are at the B3LYP/BS2//B3LYP/BS1 level
c. absolute energy at the MP2/BS2//HF/BS1 level in u.a.
d. Thermal correction to Enthalpy computed at the HF/BS1 level in u.a. Values in bracket are at the B3LYP/BS1 level.
e. Thermal correction to Gibbs Free Energy computed at the HF/BS1 level in u.a. Values in bracket are at the B3LYP/BS1 level.
f. in kJ/mol
g. absolute energy computed only for the inner shell.
h. Single-point energy computed at the B3LYP level with BS2 and STO-3G used for atoms belonging to the inner and outer layers, respectively. Values in brackets are at the HF level with the BS2 and 3-21G composite basis set.

b) Cartesian coordinates of the stationary points.

$\mathbf{1_{NH}{\bullet}H_2O}$

C	-3.909136	1.480213	1.304480
N	-3.168182	1.206702	2.438801
C	-3.716757	1.895226	3.406489
N	-4.756539	2.586784	2.961539
C	-4.896935	2.335667	1.618107
Zn	-1.529049	0.046632	2.712921
N	-0.881599	0.136039	4.557187
C	-0.936485	-0.851705	5.528585
C	-0.377952	-0.375887	6.660850
N	0.020696	0.899963	6.391785
C	-0.290059	1.165232	5.152017
N	0.001125	-0.005840	1.384961
C	0.005502	-0.017495	0.002808
C	1.276160	-0.026098	-0.434534
N	2.056823	-0.019927	0.696000
C	1.256561	-0.007501	1.752790
O	-2.392147	-1.871168	2.323854

O	1.157730	2.451471	8.026168
C	1.246991	1.765286	9.084104
C	1.904933	2.459832	10.263665
O	0.846448	0.613496	9.204726
H	-3.274363	-2.138076	2.562824
H	-1.906657	-2.661344	2.108043
H	-3.679192	1.044102	0.356841
H	-3.386926	1.909520	4.424137
H	-1.367873	-1.810608	5.334521
H	-0.083804	2.108196	4.687361
H	1.608700	-0.001733	2.763021
H	-0.897302	-0.020238	-0.568176
H	3.053559	-0.020439	0.725396
H	1.692419	-0.035043	-1.417492
H	-0.213987	-0.790294	7.630754
H	-5.668525	2.781185	1.030126
H	-5.330537	3.187213	3.513227
H	0.498285	1.553294	7.076378
H	1.942655	1.808661	11.126320
H	2.909753	2.765811	9.990362
H	1.352575	3.361556	10.508150

1_{OH}•H_2O

C	-1.437243	-2.761611	-.535439
N	-2.240357	-1.774797	-.236238
C	-3.519529	-2.225764	-.495767
C	-3.458580	-3.489047	-.950758
N	-2.122827	-3.811939	-.968435
Zn	-1.509621	.000000	.437845
O	-2.436742	-.000014	2.378282
N	-2.240360	1.774799	-.236230
C	-1.437250	2.761622	-.535407
N	-2.122837	3.811952	-.968396
C	-3.458587	3.489049	-.950740
C	-3.519532	2.225760	-.495766
N	.416213	-.000001	.559229
C	1.307657	.000028	-.451260
N	2.548935	.000016	-.071934
C	2.500479	-.000024	1.294070
C	1.206620	-.000035	1.689725
O	5.190380	.000047	-1.225139
C	6.084923	-.000002	-.257315
O	5.802068	-.000053	.902195
C	7.493162	.000015	-.785815
H	-2.493991	.765775	2.940690
H	-2.494041	-.765825	2.940654
H	-4.380118	1.613607	-.335315

H -.371055 2.739946 -.447280
H .789270 -.000064 2.676147
H 1.006528 .000057 -1.482906
H -.371047 -2.739927 -.447325
H -4.380118 -1.613620 -.335297
H -1.729044 -4.680829 -1.257009
H -4.217130 -4.174674 -1.257366
H 3.397455 -.000042 1.875556
H -4.217139 4.174674 -1.257348
H -1.729057 4.680849 -1.256954
H 4.295839 .000032 -.854155
H 7.649388 -.874283 -1.407565
H 7.649398 .874371 -1.407480
H 8.193737 -.000029 .035745

2_{NH}•H_2O

C	1.033777	3.878967	0.426058
N	1.545110	2.764695	-0.213889
C	2.054879	3.192604	-1.338427
N	1.906443	4.505085	-1.454712
C	1.253747	4.963678	-0.335879
Zn	1.334769	0.861849	0.440029
O	1.329655	1.133920	2.571375
N	2.918235	-0.303266	-0.078246
C	2.793223	-1.533314	-0.505092
N	3.981296	-2.067322	-0.754983
C	4.943387	-1.127967	-0.472978
C	4.274747	-0.039243	-0.055451
N	-0.334903	-0.132619	0.369201
C	-1.441758	0.079787	-0.324331
N	-2.319993	-0.872467	-0.145467
C	-1.787899	-1.786074	0.717302
C	-0.559377	-1.330535	1.038691
O	-4.589473	-0.909023	-1.320432
C	-5.129444	-1.990791	-0.972205
O	-4.617325	-2.814251	-0.218010
C	-6.511010	-2.257673	-1.544716
N	-3.302918	-4.681275	1.776440
H	-3.810701	-4.758719	2.638900
H	-3.162607	-5.618773	1.446127
H	2.004620	1.294537	3.222504
H	0.561220	0.803667	3.029678
H	4.663032	0.905159	0.259672
H	1.867938	-2.054529	-0.637137
H	0.170099	-1.760259	1.694006
H	-1.616989	0.922432	-0.960418
H	0.551906	3.811083	1.376581

H	2.530885	2.586073	-2.079741
H	1.012689	5.994172	-0.196346
H	2.207771	5.057066	-2.228281
H	-2.320811	-2.663991	1.017214
H	5.986073	-1.322788	-0.593341
H	4.140058	-2.994155	-1.086613
H	-3.271731	-0.916223	-0.610097
H	-7.188763	-1.469015	-1.233841
H	-6.466823	-2.231567	-2.628610
H	-6.892206	-3.215272	-1.216433
H	-3.915318	-4.227066	1.117623

2_{NH}•H_2O optimized at the B3LYP/BS1 level

C	-3.072366	-2.493738	1.006805
N	-2.794066	-1.541351	0.036926
C	-3.401732	-1.944235	-1.077468
N	-4.053323	-3.101040	-0.852657
C	-3.858473	-3.469036	0.462962
Zn	-1.558286	-0.021551	0.294645
O	-1.648642	0.124568	2.445096
N	-2.295849	1.688599	-0.413707
C	-1.524780	2.649634	-0.920084
N	-2.286288	3.684432	-1.323372
C	-3.609485	3.384773	-1.070658
C	-3.602956	2.140381	-0.506108
N	0.350712	-0.059727	0.287339
C	1.232545	-0.916467	-0.260921
N	2.483634	-0.506180	-0.071017
C	2.452831	0.673223	0.631232
C	1.130070	0.951806	0.856081
O	4.478579	-1.756013	-0.969990
C	5.486286	-0.998518	-0.733044
O	5.419375	0.114623	-0.166539
C	6.842564	-1.537805	-1.187651
N	5.055571	2.414548	1.575831
H	5.507251	2.324571	2.485844
H	5.401042	3.290008	1.182770
H	-2.196023	0.664683	3.037821
H	-0.759571	0.091038	2.840016
H	-4.438098	1.547514	-0.163968
H	-0.446481	2.619788	-0.995253
H	0.686631	1.790139	1.376497
H	0.976362	-1.825130	-0.787553
H	-2.693312	-2.401214	2.012742
H	-3.388191	-1.437587	-2.031438
H	-4.283155	-4.369151	0.879135
H	-4.587694	-3.617195	-1.540522

H	3.355469	1.213580	0.910520
H	-4.411161	4.066107	-1.309391
H	-1.938944	4.538296	-1.742482
H	3.344867	-1.010629	-0.427961
H	7.076663	-2.457579	-0.638675
H	6.804509	-1.802730	-2.250087
H	7.633503	-0.803816	-1.017414
H	5.440621	1.665350	0.989246

2_{OH}•H_2O

C	2.780323	-1.488847	-0.465797
N	2.938912	-0.255799	-0.062589
C	4.301733	-0.040697	-0.004361
C	4.942743	-1.161817	-0.378119
N	3.955394	-2.072298	-0.668972
Zn	1.339480	0.938867	0.382088
N	-0.308658	-0.039968	0.269315
C	-1.426354	0.144739	-0.450225
N	-2.328067	-0.777711	-0.288380
C	-1.785725	-1.655039	0.607842
C	-0.554127	-1.217259	0.956855
N	1.726592	2.844737	-0.197143
C	2.300042	3.264340	-1.292321
N	2.268505	4.588939	-1.365010
C	1.628030	5.063027	-0.245261
C	1.295668	3.975265	0.470641
O	1.233969	1.203435	2.528628
O	-4.934821	-1.201299	-1.374400
C	-5.480374	-2.312127	-0.936092
C	-6.855437	-2.535185	-1.503598
O	-4.942185	-3.058431	-0.172898
N	-3.194393	-4.777776	1.928854
H	-3.662607	-4.820244	2.815339
H	-3.057491	-5.726397	1.631682
H	1.861958	1.253010	3.240955
H	0.428722	0.829599	2.877987
H	4.713929	0.895952	0.303345
H	1.838492	-1.976385	-0.610168
H	0.158422	-1.644292	1.635246
H	-1.556887	0.988328	-1.100845
H	0.785294	3.914094	1.406494
H	2.741749	2.643860	-2.043204
H	1.473185	6.105053	-0.073266
H	2.637218	5.138543	-2.110052
H	-2.305765	-2.529762	0.936488
H	5.980658	-1.396796	-0.462382
H	4.089060	-3.011715	-0.973749

H	-4.050012	-1.076760	-0.992914
H	-7.498410	-1.704498	-1.235612
H	-6.801688	-2.569971	-2.585774
H	-7.266336	-3.458494	-1.123355
H	-3.836743	-4.358043	1.280596

2_{OH}•H_2O optimized at the B3LYP/BS1 level

C	2.981639	-1.515243	-0.392321
N	3.022724	-0.217303	-0.100594
C	4.359292	0.146002	-0.099792
C	5.123732	-0.948683	-0.391989
N	4.231282	-1.986169	-0.573000
Zn	1.345950	0.824810	0.241911
N	-0.199226	-0.267984	0.251278
C	-1.389080	-0.203764	-0.403550
N	-2.228521	-1.173628	-0.071022
C	-1.566661	-1.936245	0.863919
C	-0.321953	-1.392098	1.072375
N	1.606932	2.718231	-0.270788
C	2.034200	3.221499	-1.426166
N	1.943154	4.565567	-1.404267
C	1.430016	4.952075	-0.182647
C	1.222060	3.795512	0.513450
O	1.215710	1.106108	2.392519
O	-4.718924	-1.269900	-1.246682
C	-5.554530	-2.254108	-0.916437
C	-6.872462	-2.149826	-1.653105
O	-5.298420	-3.139006	-0.116108
N	-3.392871	-4.464003	1.903792
H	-3.894262	-4.488683	2.791439
H	-3.300447	-5.437111	1.613182
H	1.869916	1.023382	3.104918
H	0.431180	0.599123	2.673362
H	4.675901	1.156689	0.110563
H	2.083879	-2.113895	-0.464977
H	0.484471	-1.720803	1.717072
H	-1.622116	0.573596	-1.121770
H	0.834236	3.654066	1.510385
H	2.403007	2.657591	-2.270458
H	1.261557	5.987061	0.070457
H	2.199798	5.184131	-2.163205
H	-2.026573	-2.814200	1.314772
H	6.190186	-1.082455	-0.484888
H	4.469468	-2.942881	-0.802274
H	-3.847423	-1.353481	-0.745753
H	-7.356629	-1.195434	-1.419770
H	-6.700243	-2.169249	-2.734507

H	-7.524317	-2.975524	-1.365901
H	-4.031632	-4.029587	1.232448

4_{NH}•H_2O

C	-2.507196	2.835671	-1.170160
N	-2.076801	2.126335	-0.065150
C	-2.194647	2.933880	0.954032
N	-2.675164	4.110540	0.572706
C	-2.880686	4.068084	-0.785213
Zn	-1.258004	0.261933	-0.115905
O	-1.991683	-0.524951	-1.885517
N	-1.901808	-0.853864	1.473287
C	-3.176558	-1.074712	1.957206
C	-3.109019	-1.888290	3.025351
N	-1.773889	-2.166602	3.194334
C	-1.094921	-1.530247	2.247938
N	0.671297	0.027050	-0.318328
C	1.301606	-1.198083	-0.493072
C	2.637604	-1.011275	-0.459403
N	2.830605	0.326165	-0.268781
C	1.656838	0.899549	-0.192736
O	5.023505	1.625052	0.020668
C	5.931340	0.754770	0.028591
O	5.742092	-0.453505	-0.087940
C	7.349370	1.276317	0.191977
O	-4.298946	-1.898532	-2.362620
C	-4.410385	-3.312028	-2.344362
N	5.147284	-3.366021	-0.690301
H	5.527083	-3.658276	-1.572345
H	5.490980	-4.014927	-0.005832
H	-2.815571	-1.003209	-2.062190
H	-1.366946	-0.758593	-2.564581
H	-4.037905	-0.636969	1.500916
H	-0.030895	-1.579658	2.145059
H	0.749697	-2.103726	-0.638087
H	1.531391	1.951896	-0.044124
H	-2.512647	2.403961	-2.146693
H	-1.944439	2.701644	1.967649
H	-3.261285	4.902050	-1.332077
H	-2.843098	4.890414	1.170157
H	3.453530	-1.697419	-0.547749
H	-3.862297	-2.287907	3.667576
H	-1.375546	-2.746285	3.900637
H	3.758473	0.828895	-0.169170
H	7.590622	1.928807	-0.641316
H	7.416936	1.873952	1.095092
H	8.062657	0.464133	0.234587

H	5.559052	-2.470939	-0.478776
H	-4.959588	-1.529993	-2.935267
H	-5.384694	-3.614120	-1.982386
H	-4.240995	-3.728972	-3.329278
H	-3.653280	-3.679612	-1.668178

4_{OH}•H_2O

C	-2.942433	2.645527	-1.283375
N	-2.396540	2.068290	-0.153879
C	-2.592259	2.914971	0.818928
N	-3.232356	3.995033	0.386232
C	-3.464422	3.841283	-0.959585
Zn	-1.340328	0.319848	-0.116345
O	-1.969513	-0.577535	-1.894718
N	-1.983975	-0.800316	1.485588
C	-1.142432	-1.434210	2.257635
N	-1.785558	-2.089590	3.217819
C	-3.132851	-1.867839	3.059008
C	-3.242872	-1.068230	1.983551
N	0.575583	0.161327	-0.257796
C	1.565342	1.056670	-0.126324
N	2.761654	0.547914	-0.173050
C	2.571042	-0.793369	-0.352137
C	1.241893	-1.041591	-0.406612
O	5.362924	1.683114	0.024075
C	6.313554	0.779129	-0.012994
O	6.110435	-0.394640	-0.113762
C	7.685151	1.389474	0.085640
N	5.139162	-3.450132	-0.510418
H	5.467021	-3.780225	-1.399461
H	5.521781	-4.066685	0.182703
H	-2.691527	-1.196699	-2.067902
H	-1.261177	-0.784368	-2.496333
H	-4.125170	-0.670013	1.531167
H	-0.078577	-1.439349	2.139998
H	0.722755	-1.968946	-0.549694
H	1.376634	2.105225	0.004829
H	-2.914375	2.154985	-2.231169
H	-2.287989	2.779699	1.835297
H	-3.964832	4.583069	-1.541542
H	-3.486449	4.781497	0.942537
H	3.387274	-1.480303	-0.426730
H	-3.863205	-2.291674	3.712082
H	-1.356919	-2.645544	3.924790
H	4.485695	1.268829	-0.046876
H	7.835718	2.079332	-0.737025
H	7.766625	1.956770	1.005842

H	8.436759	0.614593	0.060380
H	5.557778	-2.548909	-0.363518
O	-3.978556	-2.377200	-2.404073
C	-3.856470	-3.780747	-2.259037
H	-4.646001	-2.175052	-3.047015
H	-4.790026	-4.214973	-1.924102
H	-3.551380	-4.244664	-3.189017
H	-3.098161	-3.956030	-1.510729

5_{NH}•H_2O

C	2.311981	-1.358216	-1.428806
N	0.998066	-1.273633	-1.004381
C	0.329839	-2.174798	-1.669791
N	1.130865	-2.832148	-2.500650
C	2.404251	-2.321850	-2.361940
Zn	0.267400	0.035116	0.346074
N	-1.717301	-0.160882	0.488525
C	-2.446696	-0.624344	1.566473
C	-3.761205	-0.587183	1.256766
N	-3.839419	-0.101440	-0.017326
C	-2.616831	0.134531	-0.431463
N	0.635758	2.027612	0.030359
C	1.834500	2.642452	-0.285635
C	1.617067	3.963362	-0.418046
N	0.273712	4.154379	-0.178866
C	-0.264974	2.969434	0.083581
O	1.137817	-0.396324	2.120501
O	-5.809997	0.441659	-1.634182
C	-6.893509	0.213486	-1.042974
C	-8.155209	0.487186	-1.852084
O	-7.002995	-0.203297	0.106020
O	3.429717	-1.594483	2.213090
C	3.883217	-2.898104	1.985009
O	5.303291	0.142329	1.585100
C	5.264873	0.801188	0.541119
C	6.429976	1.747577	0.271772
O	4.373630	0.756367	-0.331105
N	-6.711035	-1.386298	2.891379
N	5.559178	-1.215639	-2.665526
H	-7.197278	-0.823363	3.565142
H	-7.124074	-2.300118	2.931450
H	1.964932	-0.936442	2.141102
H	1.231376	0.251032	2.809345
H	3.074815	-0.723858	-1.024434
H	-0.716957	-2.372074	-1.573337
H	-1.969659	-0.947678	2.466865
H	-2.398666	0.522072	-1.405497

H	-1.301175	2.827779	0.307157
H	2.748284	2.087537	-0.382143
H	-0.215843	5.020253	-0.199460
H	2.273489	4.771442	-0.652791
H	-4.631318	-0.857250	1.818264
H	3.243576	-2.663967	-2.924917
H	0.850912	-3.563977	-3.113399
H	-4.704974	0.081296	-0.604517
H	-8.158615	1.521170	-2.182904
H	-8.154681	-0.132560	-2.743652
H	-9.045581	0.286557	-1.270595
H	-6.925707	-1.007000	1.982665
H	4.117551	-0.945373	1.952858
H	4.047605	-3.084284	0.927978
H	4.807923	-3.083050	2.520608
H	3.130911	-3.588135	2.346658
H	6.061755	2.711251	-0.064028
H	7.048887	1.870673	1.150189
H	7.036929	1.339774	-0.532351
H	5.227324	-0.502310	-2.038201
H	6.311503	-1.685328	-2.195942
H	5.960589	-0.749525	-3.458208

5_{OH}•H_2O

C	-1.882403	2.533435	0.248563
N	-0.683643	1.942020	-0.104445
C	0.201114	2.896316	-0.167710
N	-0.348775	4.071515	0.121713
C	-1.683142	3.856326	0.391401
Zn	-0.241125	-0.034080	-0.483228
O	-1.226302	-0.434360	-2.219830
N	1.707166	-0.196203	-0.659757
C	2.442010	-0.635176	-1.735589
C	3.754692	-0.569204	-1.405633
N	3.864989	-0.093509	-0.127842
C	2.635542	0.105601	0.258526
N	-1.011680	-1.340075	0.860060
C	-0.337452	-2.269348	1.476427
N	-1.118234	-2.929331	2.326296
C	-2.384061	-2.387291	2.252673
C	-2.307666	-1.404303	1.337845
O	-3.671027	-1.318573	-2.246930
C	-4.180852	-2.608977	-2.069241
O	-5.495251	0.374135	-1.388365
C	-5.449256	0.868059	-0.256665
O	-4.527047	0.739705	0.572517
C	-6.646240	1.703799	0.186813

O	5.985428	0.472238	1.598200
C	7.217848	0.257525	1.211457
O	7.525860	-0.174402	0.140614
C	8.216938	0.619863	2.279387
N	-5.501534	-1.325099	2.864476
N	7.073126	-1.296757	-2.863310
H	7.652718	-0.721282	-3.445902
H	7.484937	-2.211556	-2.859969
H	-2.127775	-0.833291	-2.208359
H	-1.197904	0.140692	-2.974475
H	-3.075232	-0.742984	0.988305
H	0.700876	-2.481905	1.331234
H	1.975827	-0.963072	-2.642162
H	2.379037	0.479447	1.232720
H	1.233763	2.767403	-0.415170
H	-2.785092	1.965748	0.370195
H	0.127100	4.944517	0.139550
H	-2.346462	4.650581	0.652535
H	4.614092	-0.827287	-1.989714
H	-3.207313	-2.721112	2.844266
H	-0.830489	-3.680825	2.910361
H	5.332303	0.234993	0.908004
H	8.105198	1.665534	2.543582
H	8.023556	0.035774	3.172231
H	9.219963	0.432866	1.925218
H	7.152680	-0.938487	-1.928140
H	-4.313658	-0.660163	-1.906990
H	-4.296933	-2.851321	-1.017195
H	-5.142441	-2.714286	-2.559795
H	-3.487371	-3.312962	-2.513020
H	-6.308576	2.627873	0.644100
H	-7.307089	1.917727	-0.642431
H	-7.198476	1.155450	0.945630
H	-5.202062	-0.605979	2.226280
H	-6.304213	-1.762563	2.450238
H	-5.822836	-0.864751	3.696202

6_{NH}•H_2O

C	0.467560	-2.781898	-0.824956
N	0.232346	-1.478575	-0.421958
C	-1.081473	-1.331690	-0.468129
N	-1.679194	-2.429334	-0.863662
C	-0.714671	-3.368557	-1.097197
Zn	1.519478	-0.092621	0.147773
N	3.449807	-0.773576	0.328473
C	4.542474	-0.216676	-0.114838
N	5.608311	-0.944420	0.200179

C	5.179869	-2.048977	0.894905
C	3.842269	-1.933635	0.968519
N	1.374440	1.532843	-1.087868
C	0.939898	1.523145	-2.319078
N	0.861150	2.756656	-2.802558
C	1.261795	3.627745	-1.816876
C	1.575066	2.859457	-0.759160
O	1.244325	0.798557	1.954898
O	-0.994008	2.076354	2.111349
C	-2.059441	1.473198	1.970699
N	-3.013813	1.910428	1.168914
C	-2.868486	3.126970	0.399138
C	-2.351047	0.211642	2.745201
O	-4.295960	-2.381777	-1.007148
C	-4.697636	-1.317668	-0.511163
C	-6.197321	-1.087342	-0.450634
O	-3.960709	-0.422806	-0.050895
H	1.683101	0.625051	2.778968
H	0.414676	1.304924	2.138350
H	3.137127	-2.592735	1.427369
H	4.596910	0.701587	-0.660225
H	1.454655	-3.186943	-0.892908
H	-1.641979	-0.454632	-0.227291
H	0.669837	0.651427	-2.877004
H	1.902895	3.153175	0.213676
H	0.543630	3.002673	-3.714458
H	1.276175	4.685399	-1.960108
H	-0.950287	-4.354846	-1.431613
H	5.853443	-2.792460	1.259676
H	6.552089	-0.723511	-0.030949
H	-2.731288	-2.496584	-0.950018
H	-6.737104	-1.879271	-0.949982
H	-6.509860	-1.038772	0.588162
H	-6.439833	-0.132101	-0.904345
H	-3.706693	1.242728	0.874077
H	-2.590394	3.947365	1.044979
H	-2.113010	3.027020	-0.373990
H	-3.817443	3.348806	-0.067055
H	-3.096057	-0.399232	2.257767
H	-1.438091	-0.355066	2.880681
H	-2.710497	0.499561	3.728174

6_{OH}•H_2O

C	3.549188	2.568734	0.203781
N	2.470958	1.885878	-0.320805
C	1.910314	2.693898	-1.177952
N	2.561970	3.850895	-1.234918

C	3.615608	3.790107	-0.355084
Zn	1.724011	0.005304	0.093675
O	1.293318	-0.111265	2.089439
N	0.128515	-0.316793	-0.968248
C	-0.085754	-1.330658	-1.873739
C	-1.373519	-1.255674	-2.283001
N	-1.986159	-0.210473	-1.650793
C	-1.060326	0.304150	-0.894079
N	3.302641	-1.309765	0.016874
C	4.229544	-1.429959	-0.892064
N	5.020898	-2.464607	-0.630122
C	4.574368	-3.058382	0.526210
C	3.510141	-2.335820	0.917471
O	-1.222881	0.014370	2.713925
C	-2.251952	-0.438611	2.217747
C	-2.309547	-1.840526	1.666895
N	-3.370489	0.265455	2.181678
C	-3.455136	1.611096	2.709453
O	-4.790222	0.022481	-2.082079
C	-5.609362	-0.253672	-1.101522
O	-5.256112	-0.483038	0.022377
C	-7.047589	-0.252455	-1.537649
H	1.737027	0.332517	2.802535
H	0.342356	-0.170189	2.345093
H	2.879094	-2.467899	1.768592
H	4.356510	-0.793365	-1.742000
H	0.685178	-2.020060	-2.151596
H	-1.227345	1.145449	-0.249218
H	1.043874	2.469269	-1.763706
H	4.191828	2.132518	0.937633
H	2.319654	4.624934	-1.813388
H	4.292610	4.603680	-0.216077
H	-1.896715	-1.874975	-2.981638
H	5.046731	-3.918555	0.946133
H	5.795835	-2.758452	-1.182723
H	-3.856215	-0.006543	-1.811849
H	-7.297125	0.711234	-1.966299
H	-7.191042	-0.999024	-2.310358
H	-7.689798	-0.463465	-0.695918
H	-4.129130	-0.075934	1.627749
H	-3.107591	1.637127	3.732464
H	-2.861821	2.307000	2.126368
H	-4.489181	1.922407	2.678730
H	-3.162468	-1.994833	1.022327
H	-1.401878	-2.052122	1.118039
H	-2.367759	-2.527741	2.505096

7_{NH}•H_2O

C	3.377807	-1.814344	-1.460906
N	2.751516	-0.964551	-0.572562
C	3.709648	-0.293330	0.016087
N	4.899025	-0.658596	-0.431435
C	4.708944	-1.630551	-1.377988
Zn	0.757598	-0.724989	-0.270237
N	-0.322392	-2.358088	-0.589794
C	-1.637393	-2.393350	-0.700217
N	-2.085601	-3.624275	-0.783818
C	-1.009102	-4.463931	-0.725890
C	0.080850	-3.681216	-0.603590
N	0.058792	0.979501	-1.102130
C	0.158284	1.311336	-2.439206
C	-0.456882	2.489426	-2.645658
N	-0.934853	2.883704	-1.423159
C	-0.607320	1.958330	-0.537601
O	0.687609	-0.262963	1.759347
O	7.107169	0.643248	0.735087
C	8.296496	0.851077	0.855936
N	8.765732	1.731578	1.745022
C	9.313128	0.125811	0.009363
O	-2.568326	4.826937	-0.226842
C	-3.371731	5.730219	-0.129175
N	-3.912276	6.061975	1.047881
C	-3.807256	6.529428	-1.332320
O	-4.703553	-3.989203	-0.798718
C	-5.229265	-2.984548	-0.299000
C	-6.744111	-2.959526	-0.184465
O	-4.609979	-1.983115	0.117097
N	-3.109042	-1.048969	2.282749
C	-2.800697	0.206357	2.000800
C	-3.883927	1.013536	1.329507
C	-2.230266	-1.933839	3.013116
O	-1.718263	0.717691	2.295067
H	1.045568	-0.825319	2.436307
H	-0.165089	0.082256	2.092109
H	3.570535	0.457690	0.764333
H	2.827774	-2.483862	-2.086457
H	1.108864	-3.962848	-0.520645
H	-2.298229	-1.554598	-0.703152
H	-0.874756	2.013316	0.496514
H	0.659503	0.682972	-3.143641
H	-1.482118	3.700900	-1.203648
H	-0.597351	3.070264	-3.530107
H	-1.112919	-5.525481	-0.774588
H	5.776925	-0.274075	-0.112369

H	5.521257	-2.091823	-1.894535
H	-3.110173	-3.852112	-0.819818
H	-7.183205	-3.872108	-0.562181
H	-7.027761	-2.819987	0.854038
H	-7.131950	-2.110747	-0.738725
H	9.735705	1.912580	1.858471
H	8.120669	2.225476	2.321102
H	10.333697	0.418265	0.217144
H	9.209184	-0.939005	0.180861
H	9.095414	0.319146	-1.034179
H	-4.511382	7.315766	-1.094899
H	-2.929621	6.966281	-1.793137
H	-4.259196	5.854603	-2.049499
H	-4.572702	6.797246	1.145432
H	-3.645515	5.552049	1.860815
H	-3.864049	-1.461805	1.756673
H	-1.406602	-2.291235	2.403069
H	-1.834233	-1.428382	3.883618
H	-2.802888	-2.789616	3.339964
H	-4.508123	1.444104	2.106962
H	-3.448352	1.825485	0.763631
H	-4.503629	0.392246	0.697324

7_{OH}•H_2O

C	2.505389	-2.858644	-0.701083
N	2.285462	-1.576526	-0.242857
C	3.467355	-1.085980	0.030370
N	4.424155	-1.965888	-0.215821
C	3.828483	-3.107494	-0.685712
Zn	0.455243	-0.687631	-0.109561
N	-1.059016	-1.816588	-0.567963
C	-2.165994	-1.495505	-1.250913
N	-3.089392	-2.414928	-1.247724
C	-2.557351	-3.435102	-0.511749
C	-1.321014	-3.080048	-0.090143
N	0.541062	1.204979	-0.872630
C	0.638036	1.568339	-2.199411
C	0.611517	2.911370	-2.289656
N	0.496225	3.374454	-1.005036
C	0.457559	2.325129	-0.199415
O	0.310254	-0.143202	1.902862
O	7.097221	-1.200752	0.325046
C	8.287251	-1.430052	0.279008
N	9.183941	-0.580857	0.791389
C	8.823895	-2.689612	-0.355318
O	0.340734	5.933092	0.195886
C	-0.040944	7.084102	0.203155

N	0.094566	7.859404	1.284053
C	-0.682756	7.710090	-1.010570
O	-5.824615	-2.239946	-1.905679
C	-6.589443	-1.721503	-0.984292
C	-8.040219	-1.715656	-1.379527
O	-6.189272	-1.293457	0.064297
N	-4.128855	-1.195554	2.249357
C	-3.229345	-0.239013	2.107738
C	-3.570721	0.879311	1.152891
C	-3.922801	-2.321582	3.136610
O	-2.183207	-0.217475	2.749428
H	0.827981	-0.543338	2.591638
H	-0.610302	-0.105456	2.238650
H	3.660751	-0.102095	0.401744
H	1.700294	-3.490752	-1.007651
H	-0.618700	-3.621051	0.511177
H	-2.276087	-0.554378	-1.754070
H	0.368831	2.399956	0.862978
H	0.718159	0.842737	-2.980100
H	0.440033	4.335815	-0.703048
H	0.662452	3.566623	-3.130796
H	-3.093908	-4.345243	-0.340010
H	5.410559	-1.804162	-0.074965
H	4.390176	-3.972317	-0.961315
H	-4.882794	-2.262692	-1.648512
H	-8.161847	-1.173920	-2.310373
H	-8.371216	-2.733629	-1.550785
H	-8.634467	-1.259189	-0.602206
H	10.161339	-0.755360	0.767242
H	8.861719	0.255070	1.226352
H	9.904554	-2.738679	-0.367723
H	8.439080	-3.542407	0.191701
H	8.454726	-2.750205	-1.371842
H	-1.037789	8.717419	-0.838224
H	0.043651	7.725894	-1.814845
H	-1.513321	7.089371	-1.323261
H	-0.210311	8.804309	1.307003
H	0.523362	7.479073	2.098548
H	-4.892055	-1.230170	1.604055
H	-3.132743	-2.967240	2.773518
H	-3.665455	-1.975498	4.127726
H	-4.843513	-2.885081	3.187251
H	-3.824373	1.756197	1.739550
H	-2.697526	1.118967	0.559261
H	-4.397883	0.635932	0.502169

7_{TS}•H_2O 1 imaginary frequency

C	-0.484218	2.087871	-0.271284
N	0.165970	1.128756	-0.886239
C	0.477994	1.623278	-2.136867
C	0.002321	2.876889	-2.243450
N	-0.605914	3.152953	-1.046466
Zn	0.658199	-0.714619	-0.209373
O	0.621775	-0.404099	1.856562
N	2.633041	-1.070777	-0.554226
C	3.181787	-1.972383	-1.442509
C	4.523786	-1.876711	-1.389918
N	4.798687	-0.907017	-0.461589
C	3.645635	-0.457512	0.004975
N	-0.510192	-2.254202	-0.597100
C	-1.818724	-2.238667	-0.809025
N	-2.337556	-3.438830	-0.871889
C	-1.308306	-4.318123	-0.691654
C	-0.182497	-3.593776	-0.520235
O	-1.833625	0.527741	2.255910
C	-2.927994	0.052143	1.948627
C	-3.964884	0.906224	1.262973
N	-3.279675	-1.191679	2.224124
C	-2.424011	-2.114837	2.935781
O	-4.767118	-3.863602	-1.043704
C	-5.479450	-3.004324	-0.456496
O	-5.041995	-2.025264	0.145312
C	-6.972498	-3.240931	-0.533772
O	-1.962563	5.430898	-0.047421
C	-2.769589	6.331355	-0.132858
C	-3.440066	6.668970	-1.441907
N	-3.099166	7.078252	0.926452
O	7.129975	0.252086	0.626103
C	8.334456	0.350510	0.731773
C	9.269861	-0.508374	-0.082969
N	8.893681	1.224142	1.574790
H	0.949392	-1.034130	2.487425
H	-0.246939	-0.096239	2.175700
H	3.572535	0.310522	0.745328
H	2.573574	-2.612437	-2.044561
H	0.820082	-3.925363	-0.348785
H	-2.409877	-1.352956	-0.905356
H	-0.880739	2.027799	0.720603
H	1.017035	1.045077	-2.856165
H	-1.077347	4.006466	-0.786227
H	0.038741	3.583906	-3.042296
H	-1.460601	-5.375670	-0.700346
H	5.707113	-0.578963	-0.166937
H	5.292446	-2.397955	-1.916145

H	-3.501092	-3.651169	-0.962605
H	-7.278321	-3.274512	-1.573633
H	-7.207149	-4.207047	-0.100355
H	-7.516483	-2.463592	-0.015310
H	9.877442	1.316982	1.674848
H	8.303698	1.805462	2.127850
H	10.315483	-0.311252	0.112297
H	9.060223	-1.549153	0.133274
H	9.068404	-0.338249	-1.133842
H	-4.209986	7.423357	-1.348530
H	-2.684535	7.022012	-2.134480
H	-3.873907	5.766361	-1.853587
H	-3.753455	7.823493	0.873686
H	-2.661716	6.891046	1.801444
H	-4.066959	-1.567729	1.724705
H	-1.609077	-2.474225	2.316404
H	-2.019783	-1.639999	3.819715
H	-3.018270	-2.963986	3.240205
H	-4.396793	1.566302	2.008494
H	-3.486919	1.525556	0.514621
H	-4.747518	0.315978	0.809566

8_{NH}•H_2O

C	-1.800131	1.685963	2.121030
N	-1.215526	0.481515	1.780393
C	-0.506536	0.114319	2.812766
N	-0.606012	1.001516	3.795842
C	-1.428772	2.017379	3.370357
Zn	-1.304330	-0.481744	-0.037401
O	-1.411682	0.953701	-1.435429
N	0.210385	-1.755316	-0.116809
C	1.486886	-1.473014	0.079970
N	2.246756	-2.531785	-0.070179
C	1.436368	-3.584116	-0.391261
C	0.177442	-3.104032	-0.421872
N	-3.146349	-1.363015	-0.311277
C	-3.763640	-1.487597	-1.540598
C	-4.923697	-2.150079	-1.387413
N	-5.014518	-2.432600	-0.045517
C	-3.932163	-1.944225	0.550997
O	4.835832	-2.196845	0.252865
C	5.059492	-0.976569	0.251171
O	4.184685	-0.092045	0.159295
C	6.505379	-0.522924	0.350848
O	0.837435	2.331313	-1.679525
C	1.968893	1.857053	-1.588892
C	2.480013	0.863475	-2.601787

N	2.805892	2.210299	-0.626838
C	2.444671	3.182985	0.380116
O	-2.973475	3.206339	-0.978855
H	-3.873672	3.374420	-1.225622
H	-2.070499	1.652570	-1.363958
H	-0.582797	1.406169	-1.684663
H	-3.325435	-1.089443	-2.429720
H	-3.752726	-2.027337	1.601916
H	-0.736337	-3.613761	-0.640877
H	1.906791	-0.520619	0.322552
H	0.087557	-0.772763	2.876213
H	-2.423413	2.221549	1.437694
H	-0.142959	0.945229	4.676220
H	-1.660180	2.859242	3.984485
H	1.820760	-4.564237	-0.569232
H	-5.676288	-2.443258	-2.085333
H	-5.756763	-2.920670	0.405315
H	3.294848	-2.491038	0.039858
H	7.158014	-1.346392	0.604299
H	6.812873	-0.109814	-0.605677
H	6.596738	0.267125	1.087963
H	3.591330	1.607944	-0.443680
H	2.172571	4.123162	-0.080008
H	1.609087	2.845935	0.986060
H	3.300098	3.339712	1.021027
H	3.291612	0.267141	-2.211948
H	1.668834	0.224301	-2.926760
H	2.829127	1.418339	-3.466897
C	-2.180315	4.353787	-1.253777
H	-2.475789	5.180769	-0.619850
H	-1.155545	4.086270	-1.049743
H	-2.268041	4.643325	-2.293656

8_{OH}•H_2O

C	-1.497135	0.071742	2.959437
N	-1.982865	0.455900	1.812074
C	-2.777802	1.552473	2.075329
C	-2.758146	1.804692	3.396408
N	-1.937570	0.847703	3.945101
Zn	-1.498471	-0.437617	0.008458
O	-1.456911	1.007715	-1.394840
N	-3.121217	-1.518386	-0.678329
C	-3.575477	-1.489558	-1.981385
C	-4.588153	-2.364079	-2.116391
N	-4.752563	-2.934744	-0.876908
C	-3.853403	-2.398525	-0.057332
N	0.161741	-1.428490	0.252694

C	0.468809	-2.693508	-0.191881
C	1.785029	-2.907468	0.041304
N	2.324197	-1.795742	0.625293
C	1.328327	-0.962567	0.725342
O	0.975655	2.031521	-1.530018
C	2.082031	1.501864	-1.587140
C	2.338177	0.314937	-2.480815
N	3.112446	1.965314	-0.897323
C	3.005601	3.117563	-0.029207
O	-2.875014	3.388072	-1.097815
H	-3.668359	3.655216	-1.543471
O	5.132457	-1.682894	0.991947
C	5.812705	-0.788841	0.326056
O	5.313889	0.061170	-0.359635
C	7.296567	-0.940035	0.512302
H	-2.037361	1.774251	-1.373492
H	-0.563400	1.345180	-1.599344
H	-3.135859	-0.844742	-2.710127
H	-3.763013	-2.670833	0.972786
H	-0.264642	-3.335222	-0.635578
H	1.425635	0.022057	1.140684
H	-0.825937	-0.748649	3.103768
H	-3.280101	2.082956	1.295736
H	-1.697755	0.756046	4.907329
H	-3.232931	2.556244	3.987337
H	2.375365	-3.775360	-0.167825
H	-5.193204	-2.632793	-2.953676
H	-5.419798	-3.632341	-0.632196
H	4.171056	-1.607346	0.852578
H	7.539070	-0.880975	1.566995
H	7.606098	-1.918032	0.161893
H	7.819085	-0.169319	-0.034087
H	3.947365	1.416897	-0.858117
H	2.642661	3.975512	-0.578617
H	2.332172	2.931289	0.800439
H	3.988162	3.339356	0.361323
H	3.272248	-0.178498	-2.255567
H	1.526587	-0.393632	-2.382162
H	2.357532	0.665841	-3.507581
C	-1.941205	4.456740	-1.099328
H	-2.291713	5.271987	-0.478258
H	-1.016410	4.069430	-0.700410
H	-1.763810	4.815841	-2.105636

9_{NH}•H_2O

C	-3.311579	-1.136958	-0.296939
N	-2.265169	-1.820781	0.121090

C	-2.749688	-3.070772	0.450023
C	-4.076011	-3.098317	0.209090
N	-4.409231	-1.860500	-0.265055
Zn	-0.412023	-1.091083	0.261312
N	1.098612	-2.449106	0.387809
C	1.175088	-3.713416	-0.159143
C	2.455029	-4.129471	-0.127523
N	3.167550	-3.112632	0.452020
C	2.321814	-2.135438	0.737464
N	-0.001584	0.032791	-1.426270
C	-0.604949	0.099462	-2.578620
N	0.061836	0.887954	-3.418686
C	1.175230	1.363552	-2.763842
C	1.122897	0.829204	-1.531980
O	-0.100964	0.200327	1.747111
O	-2.199516	1.652555	2.704435
C	-3.265079	1.662454	2.105007
N	-3.436621	2.313643	0.958591
C	-2.371382	3.086355	0.358166
C	-4.472522	0.950250	2.663914
O	2.477751	0.913228	2.102014
C	2.819769	1.301193	3.410420
O	3.402300	2.867468	0.593276
C	3.689791	3.169007	-0.580051
C	3.806933	4.660444	-0.870207
O	3.886190	2.377598	-1.512532
O	-6.662115	-0.650809	-1.030515
C	-6.415888	0.564602	-1.063022
C	-7.549123	1.504706	-1.447575
O	-5.314336	1.084473	-0.804292
O	5.705520	-1.890279	0.302785
C	5.551006	-0.697844	0.079203
C	5.986506	0.342897	1.082959
N	5.029536	-0.234734	-1.054261
C	4.702056	-1.096255	-2.166070
H	0.777854	0.567710	1.929974
H	-0.782200	0.766648	2.139229
H	0.311819	-4.221232	-0.532251
H	2.619843	-1.210411	1.187899
H	-2.116785	-3.839205	0.839635
H	-3.326949	-0.117442	-0.614551
H	-1.513180	-0.402016	-2.837951
H	1.812033	0.975244	-0.731636
H	-0.211284	1.100751	-4.351191
H	1.893458	2.016324	-3.206260
H	-4.799410	-3.873417	0.334949
H	2.915776	-5.034985	-0.454882

H	4.169327	-3.001548	0.502965
H	-5.338759	-1.478161	-0.546796
H	-8.446182	0.958060	-1.704152
H	-7.757913	2.174052	-0.618324
H	-7.240464	2.121550	-2.285363
H	-4.256930	2.122890	0.410134
H	-1.989409	3.815946	1.059370
H	-1.543630	2.461621	0.039553
H	-2.771394	3.600334	-0.504537
H	-5.237845	0.788109	1.918383
H	-4.159479	0.005661	3.089250
H	-4.880060	1.556090	3.466884
H	2.824457	1.581674	1.479852
H	2.407948	0.571457	4.095673
H	3.895703	1.332364	3.536617
H	2.412199	2.277403	3.647582
H	2.880501	5.157361	-0.600587
H	4.587637	5.086150	-0.247939
H	4.034157	4.845208	-1.911936
H	4.765043	0.735374	-1.134835
H	5.941572	-0.084267	2.075504
H	7.019793	0.604010	0.874844
H	5.386636	1.241194	1.032115
H	4.665512	-0.492558	-3.062504
H	5.459413	-1.859094	-2.282199
H	3.739353	-1.583228	-2.044463

9_{OH}•H_2O

C	0.081556	-0.046678	2.772696
N	-0.367021	0.029855	1.554013
C	-1.499479	0.817334	1.606010
C	-1.715545	1.202902	2.875485
N	-0.692631	0.644710	3.608612
Zn	0.291741	-0.977121	-0.137318
O	0.022208	0.358956	-1.608310
N	-1.166753	-2.371841	-0.473058
C	-1.218859	-3.684541	-0.055109
C	-2.477002	-4.142735	-0.199513
N	-3.199737	-3.100917	-0.719912
C	-2.379729	-2.070510	-0.861700
N	2.139912	-1.594458	0.098524
C	2.726386	-2.738445	-0.383557
C	4.049835	-2.678989	-0.100299
N	4.315434	-1.509004	0.552752
C	3.156432	-0.914404	0.640737
O	2.170107	2.014793	-1.728082
C	3.346649	1.692801	-1.685572

C	3.894963	0.592911	-2.561432
N	4.215915	2.315251	-0.893850
C	3.809313	3.392058	-0.018921
O	-2.558033	1.073367	-2.077104
C	-2.824668	1.522929	-3.381663
O	6.948102	-0.778261	1.125632
C	7.443642	0.273812	0.535061
O	6.820435	1.011297	-0.176970
C	8.903101	0.468940	0.846714
H	-0.845288	0.736079	-1.812197
H	0.717163	1.010624	-1.776267
H	-0.354073	-4.192711	0.314130
H	-2.690201	-1.119229	-1.242965
H	2.164910	-3.495458	-0.891988
H	3.023274	0.047022	1.097539
H	0.950134	-0.589047	3.081721
H	-2.078349	1.060720	0.744397
H	-0.550328	0.736459	4.588421
H	-2.491876	1.801688	3.295708
H	4.820623	-3.388760	-0.320081
H	-2.916113	-5.092354	0.012294
H	-4.199335	-3.023438	-0.827079
H	6.005075	-0.934238	0.908966
H	9.038444	0.550568	1.919147
H	9.462714	-0.397666	0.513279
H	9.271026	1.357929	0.356384
H	5.130362	1.930046	-0.780852
H	3.321818	4.175808	-0.582317
H	3.121499	3.049226	0.746752
H	4.692834	3.794119	0.457121
H	4.891453	0.288865	-2.273908
H	3.233020	-0.261548	-2.517946
H	3.911152	0.954054	-3.584597
H	-2.983579	1.683100	-1.446151
H	-2.330662	0.853986	-4.074854
H	-3.889143	1.514576	-3.586377
H	-2.449096	2.528865	-3.533996
O	-3.703038	2.882986	-0.526222
C	-4.094533	3.119306	0.631962
O	-4.350939	2.279739	1.505246
C	-4.268097	4.592421	0.983360
H	-3.330664	5.116258	0.825647
H	-4.996776	5.037427	0.313266
H	-4.593007	4.720258	2.007665
N	-5.291663	-0.362993	0.816021
C	-5.706579	-0.785579	-0.375593
O	-5.795391	-1.969572	-0.668267

H	-5.078564	0.611767	0.966900
C	-6.107234	0.289164	-1.358023
H	-5.963652	-0.082008	-2.363722
H	-7.164778	0.495678	-1.222887
H	-5.554615	1.207206	-1.212838
C	-5.008416	-1.271635	1.901907
H	-5.040417	-0.712455	2.826946
H	-5.751174	-2.056871	1.935638
H	-4.028277	-1.729940	1.814275

10_{NH}•H_2O

C	2.489863	-1.840932	-0.641852
N	1.246774	-2.205460	-0.851615
C	1.309083	-3.461537	-1.419983
C	2.598470	-3.820372	-1.551445
N	3.332303	-2.778005	-1.050105
Zn	-0.433051	-1.193077	-0.347826
N	-2.096499	-1.788415	-1.359572
C	-2.229839	-2.577915	-2.482430
C	-3.537703	-2.677393	-2.795961
N	-4.211827	-1.939705	-1.864015
C	-3.319606	-1.430720	-1.039103
N	-0.391274	0.833131	-0.480597
C	0.634129	1.679255	-0.101265
C	0.214991	2.952566	-0.220035
N	-1.077507	2.883600	-0.678800
C	-1.392817	1.607548	-0.816311
O	-0.645682	-1.660267	1.606141
O	1.725014	-1.523391	2.922370
C	2.514699	-2.573182	3.404928
O	3.178078	0.309990	1.551239
C	3.404210	1.446652	2.040273
C	3.631621	1.497026	3.546253
O	3.456689	2.498936	1.406570
O	-6.798290	-1.291967	-1.386692
C	-6.872529	-0.238324	-0.748140
C	-8.229917	0.449049	-0.686360
O	-5.920348	0.326185	-0.162393
O	-3.039936	-1.929099	3.010835
C	-4.080496	-1.584142	2.479113
N	-4.368670	-0.304047	2.234963
C	-3.471724	0.763309	2.625579
C	-5.131043	-2.596087	2.086546
O	6.137687	-2.415610	-1.210002
C	6.718788	-1.377667	-0.947912
N	7.364374	-0.671628	-1.879240
C	6.745510	-0.836619	0.460480

O	-3.724394	3.683635	-0.995210
C	-4.826582	4.079471	-0.674377
N	-5.811801	3.263014	-0.303610
C	-5.132580	5.560961	-0.680495
N	5.192731	2.567723	-0.919407
C	6.488797	2.653960	-0.608751
O	7.379364	2.278724	-1.348601
C	4.741911	2.025453	-2.178526
C	6.804559	3.295075	0.723824
H	0.141395	-1.659313	2.171418
H	-1.431497	-1.753281	2.156499
H	2.804356	-0.930034	-0.170184
H	0.429830	-4.012344	-1.673991
H	-1.385389	-2.999393	-2.982932
H	-3.601585	-0.795530	-0.229211
H	-2.355707	1.293958	-1.154096
H	1.579599	1.321168	0.241338
H	-1.742942	3.615485	-0.829494
H	0.711339	3.874250	-0.013424
H	-4.037890	-3.193677	-3.585236
H	4.340328	-2.712706	-1.019934
H	3.056095	-4.701737	-1.942665
H	-5.223144	-1.761107	-1.768383
H	-9.023651	-0.234114	-0.955312
H	-8.406014	0.856400	0.303208
H	-8.234780	1.276357	-1.391914
H	-5.124776	-0.083080	1.614345
H	-3.327120	0.767612	3.698091
H	-2.499242	0.667554	2.156812
H	-3.912820	1.702577	2.323260
H	-5.745856	-2.262493	1.260784
H	-4.644732	-3.528209	1.833867
H	-5.772226	-2.772946	2.944564
H	2.282865	-0.856739	2.496540
H	1.861093	-3.294319	3.877455
H	3.057490	-3.069582	2.605067
H	3.228826	-2.220425	4.142429
H	2.808471	1.015867	4.064197
H	4.533294	0.942781	3.791792
H	3.733516	2.516774	3.891196
H	4.514410	2.674839	-0.185606
H	7.167771	4.300284	0.534858
H	5.943226	3.348259	1.374691
H	7.604635	2.744349	1.202210
H	3.710087	2.315915	-2.326913
H	5.339578	2.420017	-2.988312
H	4.801641	0.941712	-2.208550

H	6.998090	-1.648615	1.130962
H	7.456300	-0.031259	0.581876
H	5.754623	-0.482326	0.725858
H	7.620309	0.285104	-1.725347
H	7.273309	-0.979365	-2.822301
H	-6.138446	5.797192	-0.356870
H	-4.424349	6.064429	-0.033367
H	-4.985087	5.938149	-1.685523
H	-6.706885	3.622821	-0.068836
H	-5.703246	2.259890	-0.304523

10_{OH}•H_2O

C	-1.244992	1.641494	-0.901527
N	-0.282634	0.844865	-0.516623
C	0.723357	1.661416	-0.039111
C	0.333093	2.945188	-0.149319
N	-0.924075	2.910926	-0.703332
Zn	-0.431647	-1.198551	-0.479084
O	-0.579870	-1.661001	1.496244
N	1.271567	-2.169026	-1.013271
C	2.507102	-1.847614	-0.713823
N	3.358564	-2.738262	-1.202796
C	2.636159	-3.700181	-1.858794
C	1.345399	-3.342931	-1.733011
N	-2.114302	-1.666801	-1.424749
C	-2.338343	-2.355783	-2.589517
C	-3.674230	-2.375865	-2.816363
N	-4.304357	-1.701504	-1.809772
C	-3.335252	-1.308318	-1.024356
O	-6.938541	-1.103820	-1.455066
C	-7.190172	-0.209714	-0.554490
O	-6.350087	0.345659	0.112434
C	-8.661999	0.077808	-0.418947
O	1.767281	-1.675768	2.878631
C	2.532880	-2.785922	3.251132
O	3.249976	0.212434	1.623346
C	3.466784	1.320855	2.175280
O	3.515086	2.408450	1.602994
C	3.689945	1.288331	3.682853
O	-3.600125	3.776559	-1.042197
C	-4.694503	4.176853	-0.716451
C	-5.013747	5.654406	-0.735357
N	-5.675499	3.356126	-0.323024
O	-2.990763	-2.060668	2.885397
C	-4.080014	-1.666669	2.521483
C	-5.168743	-2.633749	2.122146
N	-4.377697	-0.363731	2.434998

C	-3.396961	0.659455	2.733706
O	6.186391	-2.418073	-1.243432
C	6.750094	-1.376111	-0.962097
C	6.793633	-0.876113	0.460943
N	7.360354	-0.627246	-1.884791
N	5.175809	2.554465	-0.769980
C	4.694734	2.045684	-2.032087
C	6.478953	2.647136	-0.494822
C	6.826589	3.246084	0.849560
O	7.352208	2.309782	-1.272996
H	0.203344	-1.710242	2.062758
H	-1.365237	-1.815497	2.028194
H	2.812028	-0.998627	-0.132641
H	0.470831	-3.839901	-2.092773
H	-1.540283	-2.766222	-3.172842
H	-3.507669	-0.735350	-0.136190
H	-2.180609	1.341303	-1.319030
H	1.637827	1.276833	0.355439
H	-1.562725	3.660587	-0.870027
H	0.826334	3.852525	0.119386
H	-4.216981	-2.819858	-3.625178
H	4.364298	-2.690727	-1.130055
H	3.102085	-4.530916	-2.340516
H	-5.970701	-1.295079	-1.562029
H	-9.195544	-0.842983	-0.214804
H	-8.834369	0.790015	0.374924
H	-9.039040	0.468994	-1.357333
H	-5.206666	-0.096651	1.949721
H	-3.033139	0.546299	3.745752
H	-2.547225	0.617428	2.062339
H	-3.871869	1.625746	2.635705
H	-6.158969	-2.209379	2.230624
H	-5.023205	-2.911819	1.083682
H	-5.081905	-3.524051	2.729250
H	2.337430	-0.993937	2.495373
H	1.866667	-3.525319	3.675652
H	3.043331	-3.228490	2.399995
H	3.273274	-2.519541	3.999228
H	2.869189	0.772751	4.170598
H	4.594945	0.727386	3.899248
H	3.784013	2.287846	4.084821
H	4.518239	2.627332	-0.012860
H	7.171112	4.262231	0.685359
H	5.984711	3.264357	1.527224
H	7.647858	2.690069	1.283973
H	3.652064	2.315872	-2.134787
H	5.255164	2.482227	-2.847127

H	4.777971	0.965524	-2.102160
H	7.060456	-1.705274	1.104180
H	7.500706	-0.069359	0.595403
H	5.804106	-0.536191	0.749462
H	7.599758	0.329657	-1.707051
H	7.253279	-0.907150	-2.834792
H	-6.025383	5.883241	-0.424706
H	-4.317724	6.167065	-0.082296
H	-4.857141	6.026661	-1.740518
H	-6.570781	3.699276	-0.066846
H	-5.539615	2.366298	-0.300852

11_{NH}•H_2O

C	-0.623472	0.570523	-1.438631
C	0.340013	1.430427	-1.805982
N	0.376542	2.380439	-0.815870
C	-0.517554	2.055095	0.103658
N	-1.165210	0.972353	-0.231526
C	1.277988	1.416016	-2.958265
Zn	-2.374539	-0.316739	0.707991
N	-4.263057	0.202794	0.020663
C	-4.439102	0.655142	-1.275554
C	-5.750979	0.855840	-1.517305
N	-6.383464	0.525033	-0.339989
C	-5.458631	0.146112	0.535227
C	-6.486067	1.322841	-2.738587
N	-1.787882	-2.182489	0.261409
C	-2.409716	-3.288377	-0.294865
C	-1.461811	-4.206149	-0.566773
N	-0.260384	-3.673067	-0.183691
C	-0.494177	-2.474813	0.296776
C	-3.881000	-3.360237	-0.542230
O	-2.184212	-0.326695	2.758406
O	2.158903	-4.403907	-0.772446
C	2.570874	-4.417066	-1.956986
O	3.734896	-4.322567	-2.322458
C	1.493537	-4.559953	-3.042244
O	-9.178863	0.590636	0.356496
C	-10.349449	0.691735	0.641811
N	-10.956591	1.883389	0.736008
C	-11.194978	-0.526079	0.924499
O	1.892618	4.713600	-1.500745
C	2.909430	5.381840	-1.545481
C	2.858119	6.803480	-2.054943
N	4.101234	4.930621	-1.166098
C	4.318167	3.619402	-0.604886
C	5.484833	3.690099	0.369170

O 6.356615 4.513993 0.210862
N 5.460669 2.772597 1.332476
C 6.524737 2.669792 2.306362
N 5.868804 -4.042950 -0.262087
C 6.491529 -5.234680 0.254353
C 6.148337 -2.839568 0.253067
O 6.968257 -2.662087 1.126027
C 5.338050 -1.687398 -0.311860
C 4.242706 -1.260953 0.669361
C 3.330357 -0.197494 0.046798
C 2.427928 0.445957 1.089056
O 2.783681 1.513133 1.596244
O 1.378097 -0.174193 1.384675
O 0.184596 0.450827 3.631576
C 1.027382 -0.008252 4.661876
H -12.249660 -0.303495 1.022143
H -11.050134 -1.241223 0.125299
H -10.844212 -0.981111 1.843789
H -11.914048 1.977674 0.981435
H -10.423098 2.709865 0.581877
H -7.040108 2.233809 -2.537988
H -5.781972 1.522395 -3.535595
H -7.187495 0.570551 -3.083425
H -7.370445 0.565278 -0.154484
H -5.692381 -0.161517 1.532448
H -3.609183 0.812899 -1.929713
H -4.450686 -3.220980 0.373171
H -4.206814 -2.604690 -1.250620
H -4.142951 -4.330175 -0.947119
H -1.535665 -5.179218 -1.001213
H 0.278109 -1.814166 0.649099
H -1.347999 0.021201 3.154189
H 1.954890 0.550281 4.661523
H 0.523067 0.144500 5.607946
H 1.254032 -1.064025 4.547838
H 0.678524 0.358759 2.791188
H 0.893725 -5.446585 -2.855084
H 0.824420 -3.703191 -3.014409
H 1.939656 -4.628270 -4.025260
H 5.116720 -4.141623 -0.922322
H 6.154256 -6.077088 -0.335189
H 7.571116 -5.167777 0.188727
H 6.230921 -5.408021 1.293871
H 6.019526 -0.860383 -0.482076
H 4.892913 -1.970295 -1.259006
H 3.644316 -2.122075 0.946658
H 4.706622 -0.877417 1.572700

H 3.940380 0.571949 -0.414523
H 2.725739 -0.663507 -0.724164
H 4.615921 2.244112 1.471888
H 6.424400 1.727116 2.825931
H 7.485916 2.698222 1.812827
H 6.486797 3.478386 3.029268
H 2.448131 6.796113 -3.057628
H 2.181194 7.369749 -1.426347
H 3.824949 7.289990 -2.067197
H 4.899501 5.526947 -1.172040
H 3.427268 3.270645 -0.109538
H 4.574955 2.904980 -1.381958
H 1.256565 2.356790 -3.497335
H 2.294851 1.245587 -2.624485
H 1.011830 0.619140 -3.640957
H 0.981692 3.185901 -0.814661
H -0.661163 2.613585 1.003272
H -0.938363 -0.324559 -1.930918
H 0.703592 -4.057367 -0.382585
H -2.277585 -1.198139 3.128339

11_{NH}•H_2O optimized at the B3LYP/BS1 level
C -0.642323 0.567954 -1.418182
C 0.351690 1.412354 -1.823541
N 0.428649 2.383263 -0.845113
C -0.472755 2.098943 0.110645
N -1.155013 1.001693 -0.205981
C 1.275178 1.349305 -2.985339
Zn -2.396944 -0.221229 0.716803
N -4.221112 0.298051 -0.031298
C -4.398373 0.750505 -1.333301
C -5.736941 0.925867 -1.593513
N -6.373074 0.577180 -0.414239
C -5.441421 0.207317 0.485644
C -6.490686 1.373349 -2.817197
N -1.890497 -2.090180 0.280181
C -2.497833 -3.202205 -0.299870
C -1.512818 -4.111240 -0.589581
N -0.314371 -3.566818 -0.193429
C -0.569464 -2.361534 0.319435
C -3.969884 -3.319798 -0.545302
O -2.082601 -0.293645 2.711882
O 2.101381 -4.185781 -0.731570
C 2.498438 -4.370159 -1.932280
O 3.686427 -4.371392 -2.315792
C 1.402660 -4.629775 -2.993726
O -9.087330 0.280470 0.049471

C -10.086257 0.596213 0.699767
N -10.200862 1.792141 1.326263
C -11.250563 -0.360012 0.836510
O 1.877411 4.652929 -1.563954
C 2.926424 5.319128 -1.603951
C 2.901838 6.748890 -2.114153
N 4.124346 4.846600 -1.222014
C 4.332089 3.536885 -0.638899
C 5.499095 3.632277 0.351974
O 6.388146 4.470533 0.168926
N 5.447283 2.729561 1.347371
C 6.499501 2.615412 2.342618
N 5.737092 -4.164564 -0.287084
C 6.312490 -5.393119 0.218294
C 6.038618 -2.976253 0.288618
O 6.847901 -2.850471 1.212686
C 5.271231 -1.780295 -0.273163
C 4.155601 -1.342396 0.684621
C 3.322865 -0.193625 0.084265
C 2.452899 0.477152 1.142829
O 2.849377 1.536126 1.689244
O 1.359949 -0.124424 1.444317
O 0.162975 0.541654 3.573173
C 0.953199 0.024266 4.650006
H -12.088611 0.045237 1.410125
H -11.599354 -0.633156 -0.163765
H -10.897386 -1.276310 1.319531
H -11.026469 2.053438 1.843630
H -9.452584 2.467546 1.247687
H -7.046811 2.299725 -2.631106
H -5.793162 1.557798 -3.638101
H -7.207721 0.611251 -3.142902
H -7.389032 0.568125 -0.249585
H -5.678352 -0.119636 1.487788
H -3.554410 0.929181 -1.983323
H -4.551200 -3.247223 0.383784
H -4.338278 -2.537884 -1.221690
H -4.197299 -4.288122 -1.000385
H -1.570607 -5.087885 -1.046182
H 0.202235 -1.684922 0.687316
H -1.185104 0.070973 3.131942
H 1.942610 0.492961 4.629922
H 0.457341 0.271764 5.593876
H 1.078438 -1.066010 4.584924
H 0.709919 0.390788 2.704683
H 0.870947 -5.561294 -2.759310
H 0.660727 -3.821221 -2.989137

H 1.840427 -4.713297 -3.991068
H 4.974819 -4.224223 -0.977874
H 6.100441 -6.197693 -0.491307
H 7.395938 -5.285634 0.334226
H 5.901689 -5.670824 1.199714
H 5.985427 -0.958835 -0.408163
H 4.839754 -2.030344 -1.249631
H 3.495125 -2.192341 0.888675
H 4.605736 -1.029017 1.634741
H 3.997878 0.553871 -0.349712
H 2.694895 -0.599138 -0.717920
H 4.572425 2.197739 1.479951
H 6.769201 1.563930 2.484832
H 7.370490 3.171309 1.991901
H 6.181152 3.029627 3.307909
H 2.484056 6.757142 -3.125683
H 2.233478 7.340014 -1.479813
H 3.888538 7.220291 -2.130738
H 4.947945 5.440265 -1.187347
H 3.423851 3.190878 -0.141100
H 4.590712 2.802295 -1.414998
H 1.378783 2.325912 -3.471064
H 2.275783 1.026032 -2.674340
H 0.909349 0.630127 -3.723226
H 1.056081 3.201542 -0.897048
H -0.588519 2.676143 1.015379
H -0.985162 -0.340348 -1.891311
H 0.657968 -3.924119 -0.401722
H -2.088943 -1.228493 2.973902

11_{OH}•H_2O
C -0.636852 0.549461 -1.422995
C 0.312511 1.422365 -1.794319
N 0.325236 2.386064 -0.816623
C -0.573476 2.054938 0.098945
N -1.196632 0.957669 -0.228566
C 1.252632 1.408288 -2.943293
Zn -2.394132 -0.384325 0.669839
N -4.283521 0.200418 -0.018908
C -4.461106 0.658559 -1.312367
C -5.773770 0.857518 -1.554628
N -6.405553 0.519492 -0.378710
C -5.478211 0.137318 0.494294
C -6.512819 1.325159 -2.774966
N -1.815653 -2.216911 0.237017
C -2.456170 -3.309861 -0.299988
C -1.515013 -4.248644 -0.550644

N -0.283979 -3.771061 -0.188843
C -0.518136 -2.573013 0.271310
C -3.928008 -3.349854 -0.537875
O -2.209147 -0.404109 2.735852
O 2.363978 -4.336602 -0.777142
C 2.638903 -4.464139 -2.050314
O 3.771496 -4.502941 -2.433772
C 1.461652 -4.568271 -2.995935
O -9.210447 0.595659 0.335047
C -10.361089 0.708104 0.686566
N -10.909778 1.903773 0.949122
C -11.248237 -0.499958 0.865817
O 1.872081 4.700129 -1.535208
C 2.894049 5.358107 -1.597136
C 2.858975 6.760047 -2.160310
N 4.078852 4.912254 -1.189985
C 4.279664 3.619933 -0.580730
C 5.493245 3.697293 0.334196
O 6.368672 4.503696 0.114532
N 5.502614 2.805087 1.320678
C 6.605342 2.721699 2.252041
N 6.010159 -4.003071 -0.237732
C 6.710414 -5.153152 0.279557
C 6.151413 -2.792057 0.328312
O 6.909066 -2.582496 1.244881
C 5.291277 -1.686503 -0.254361
C 4.270620 -1.171940 0.761815
C 3.336570 -0.139419 0.123577
C 2.454329 0.532898 1.168637
O 2.857568 1.581100 1.682943
O 1.386172 -0.050827 1.448388
O 0.116053 0.521060 3.664809
C 0.949539 0.022507 4.682036
H -12.287216 -0.248499 1.035868
H -11.167462 -1.122468 -0.015664
H -10.881309 -1.072513 1.710064
H -11.850355 2.006102 1.249971
H -10.346532 2.720635 0.866211
H -7.074429 2.230749 -2.570597
H -5.809916 1.533862 -3.570827
H -7.208034 0.568732 -3.123524
H -7.391748 0.556633 -0.192441
H -5.710561 -0.178658 1.489246
H -3.631190 0.818513 -1.966026
H -4.493535 -3.177824 0.376233
H -4.247323 -2.603702 -1.261200
H -4.219566 -4.321756 -0.919840

H -1.643111 -5.229683 -0.962850
H 0.247336 -1.913613 0.635402
H -1.411799 0.002521 3.144028
H 1.878531 0.578635 4.712824
H 0.437883 0.138245 5.629717
H 1.177289 -1.028589 4.530190
H 0.621948 0.455997 2.829943
H 0.816846 -3.704370 -2.889416
H 1.824487 -4.643788 -4.010024
H 0.870130 -5.443934 -2.751041
H 5.294846 -4.148425 -0.918577
H 6.524172 -5.992482 -0.377773
H 7.775526 -4.964586 0.317404
H 6.379035 -5.410850 1.280361
H 5.958401 -0.878499 -0.538531
H 4.785270 -2.029741 -1.150290
H 3.679106 -1.997584 1.144554
H 4.798369 -0.735022 1.602167
H 3.932387 0.614340 -0.380570
H 2.711847 -0.632847 -0.613516
H 4.657927 2.289938 1.509233
H 6.500787 1.811557 2.826017
H 7.545609 2.694896 1.718964
H 6.621718 3.567923 2.931183
H 2.448417 6.719790 -3.161944
H 2.188876 7.357433 -1.553500
H 3.831316 7.234782 -2.190471
H 4.885747 5.495965 -1.222564
H 3.403541 3.319742 -0.029809
H 4.477880 2.864892 -1.336166
H 1.218376 2.340704 -3.496249
H 2.272663 1.259278 -2.607688
H 0.998807 0.598762 -3.616186
H 0.919373 3.198588 -0.819357
H -0.738364 2.622506 0.989186
H -0.929742 -0.360807 -1.900497
H 1.414736 -4.236275 -0.572236
H -2.178672 -1.313099 3.017189

11_{OH}•H_2O optimized at the B3LYP/BS1 level
C -0.651975 0.571629 -1.409631
C 0.338203 1.420387 -1.812825
N 0.405941 2.395262 -0.837566
C -0.500718 2.108030 0.114106
N -1.173914 1.006986 -0.203405
C 1.262007 1.357758 -2.973080
Zn -2.415512 -0.261897 0.667835

N -4.236296 0.327885 -0.067630
C -4.411928 0.813708 -1.357228
C -5.750673 0.988552 -1.618866
N -6.389433 0.604301 -0.451876
C -5.457472 0.215397 0.440973
C -6.503769 1.461917 -2.834043
N -1.920599 -2.101618 0.237405
C -2.565143 -3.195490 -0.323159
C -1.601250 -4.136428 -0.599794
N -0.364954 -3.656898 -0.231695
C -0.601222 -2.445319 0.264163
C -4.040112 -3.258215 -0.555375
O -2.112334 -0.347419 2.682863
O 2.175130 -4.237412 -0.736433
C 2.484190 -4.437645 -2.007423
O 3.650956 -4.493454 -2.375440
C 1.327774 -4.622314 -2.984380
O -9.126692 0.355921 -0.020764
C -10.036708 0.615592 0.769524
N -9.968566 1.645432 1.648506
C -11.294978 -0.224123 0.800806
O 1.899796 4.634802 -1.589098
C 2.959138 5.282030 -1.647893
C 2.960907 6.693011 -2.209298
N 4.147547 4.804558 -1.242373
C 4.332514 3.512409 -0.613954
C 5.529108 3.613915 0.340763
O 6.428319 4.429612 0.109303
N 5.487997 2.742074 1.363483
C 6.560375 2.644255 2.338273
N 5.775807 -4.184524 -0.232007
C 6.391379 -5.398820 0.262087
C 6.014839 -2.973582 0.342761
O 6.799758 -2.799669 1.276278
C 5.215319 -1.814379 -0.247714
C 4.192202 -1.268820 0.755545
C 3.354021 -0.135553 0.140760
C 2.483806 0.545500 1.198076
O 2.900140 1.594092 1.753502
O 1.383507 -0.041837 1.475049
O 0.116859 0.573491 3.591692
C 0.897695 0.032080 4.660252
H -12.029600 0.110213 1.538485
H -11.752305 -0.207785 -0.193049
H -11.019146 -1.261103 1.015013
H -10.724517 1.868128 2.278126
H -9.157487 2.249093 1.644352

H -7.079260 2.370848 -2.622583
H -5.803207 1.685923 -3.642524
H -7.203657 0.697540 -3.190470
H -7.405881 0.589440 -0.291110
H -5.695014 -0.143501 1.432034
H -3.566211 1.011429 -1.999417
H -4.616615 -3.139235 0.373568
H -4.389334 -2.482638 -1.251089
H -4.312272 -4.228660 -0.982678
H -1.724040 -5.119866 -1.035765
H 0.173087 -1.779645 0.637272
H -1.250149 0.053193 3.107870
H 1.885007 0.506982 4.670883
H 0.387775 0.246265 5.605108
H 1.033034 -1.055317 4.566252
H 0.677469 0.450825 2.734341
H 0.595220 -3.816173 -2.879636
H 1.715610 -4.655617 -4.003373
H 0.806225 -5.561609 -2.765128
H 5.050530 -4.265706 -0.944601
H 6.885730 -5.946629 -0.549937
H 7.132877 -5.114447 1.010973
H 5.652101 -6.064845 0.727508
H 5.929558 -1.022404 -0.505848
H 4.707877 -2.122730 -1.169634
H 3.522115 -2.073552 1.079433
H 4.724925 -0.908114 1.643247
H 4.026604 0.602742 -0.312074
H 2.716779 -0.552223 -0.648444
H 4.606335 2.228180 1.530241
H 6.829839 1.595011 2.498256
H 7.426012 3.189052 1.957975
H 6.263448 3.079684 3.301007
H 2.549353 6.671863 -3.223216
H 2.298212 7.316898 -1.600940
H 3.955082 7.148069 -2.235991
H 4.983377 5.381921 -1.233298
H 3.429545 3.210174 -0.079184
H 4.549231 2.741750 -1.367742
H 1.355523 2.330652 -3.468464
H 2.267564 1.049630 -2.661560
H 0.902608 0.628645 -3.704622
H 1.034307 3.211065 -0.887440
H -0.627210 2.687957 1.015647
H -0.985224 -0.343739 -1.875896
H 1.169355 -4.115098 -0.561020
H -2.029216 -1.297777 2.868045

12_{NH}•H_2O (only the inner shell and link atoms)

Zn	-0.302152	-0.048399	-0.026641
O	0.139649	2.018417	-0.097076
H	-0.190406	2.426198	-0.914638
H	-0.106660	2.573003	0.661645
C	4.777035	0.318434	7.718228
C	3.804994	0.469256	6.549649
O	2.831792	-0.228573	6.355554
N	4.105659	1.499070	5.743411
H	4.594817	1.186429	8.363217
H	5.801092	0.452761	7.334381
H	3.450911	1.753479	5.036215
H	4.886056	2.114893	5.904217
C	-0.818648	-1.713718	5.211387
C	-0.272678	-0.990606	4.012574
N	0.991574	-0.451264	3.948276
C	-0.803558	-0.800649	2.789099
C	1.176569	0.013570	2.719862
N	0.118274	-0.178287	1.975917
H	-1.902917	-1.560161	5.253934
H	-0.405576	-1.286846	6.131740
H	1.653201	-0.411739	4.709111
H	-1.771654	-1.082200	2.430862
H	2.084278	0.485292	2.401920
C	-5.167406	-2.365514	-1.121037
C	-4.133543	-1.327925	-0.778956
N	-4.424685	-0.025495	-0.458325
C	-2.802860	-1.440465	-0.628210
C	-3.294421	0.592581	-0.164492
N	-2.279332	-0.228682	-0.224995
H	-4.744796	-3.066155	-1.847656
H	-6.035375	-1.899376	-1.596892
H	-5.334751	0.404956	-0.496684
H	-2.193044	-2.308180	-0.764949
H	-3.251502	1.626676	0.110953
C	2.034227	-2.743305	0.204861
C	1.269595	-2.525321	-1.075668
N	0.480108	-1.398412	-1.275855
C	1.221702	-3.268657	-2.197854
C	-0.012759	-1.505932	-2.499067
N	0.408727	-2.608036	-3.074845
H	1.452100	-2.359804	1.048191
H	2.967356	-2.150773	0.159432
H	1.671780	-4.206831	-2.453389
H	-0.708173	-0.826444	-2.950847
H	0.125377	-2.997274	-3.970096

C -1.595547 -5.934487 -4.077029
C -1.414493 -4.741583 -5.037259
O -2.405198 -4.363342 -5.663912
O -0.263685 -4.262022 -5.126552
H -0.701397 -6.043344 -3.455541
H -1.672123 -6.840264 -4.697473
C -0.871403 3.142511 -3.843905
O -0.925872 2.500070 -2.576169
H -1.905347 3.220382 -4.216531
H -1.585989 1.790853 -2.714698
C -9.289141 1.217661 0.099301
C -8.180468 1.138459 -0.991212
O -7.002386 1.115734 -0.701108
H -9.725397 2.238426 0.020426
N -8.609468 1.148574 -2.257719
C -7.729252 1.030926 -3.408323
C -7.996218 2.207773 -4.357639
O -9.065363 2.749231 -4.394174
H -9.576559 1.283157 -2.463215
H -6.712477 1.105887 -3.036577
N -6.934714 2.556594 -5.129533
C -6.956826 3.811829 -5.889783
H -6.023125 2.227817 -4.856576
H -7.994372 4.173832 -5.859314
C -4.604808 -1.757218 -6.694741
C -3.966311 -1.958912 -8.084477
O -4.388550 -1.373463 -9.049329
C -3.706387 -0.783824 -5.888054
C -4.279189 -0.439499 -4.510637
C -3.590097 0.778116 -3.925206
O -2.508628 0.583946 -3.335996
O -4.122566 1.887212 -4.113280
H -5.581333 -1.275780 -6.879183
H -2.709200 -1.194136 -5.775796
H -3.617854 0.125767 -6.475926
H -5.341602 -0.235406 -4.612023
H -4.151404 -1.287168 -3.844785
N -2.879200 -2.754853 -8.105320
C -2.284227 -3.191233 -9.355705
H -2.648732 -3.295449 -7.289768
H -2.332662 -2.341929 -10.053845
N -4.793452 -3.017036 -5.969736 Medium H
C -3.061293 -4.376756 -9.926578 Medium H
C -0.829374 -3.612425 -9.134224 Medium H
N -10.348840 0.229951 -0.148106 Medium H
C -8.694387 1.057069 1.493596 Medium H
C -7.906307 -0.307537 -4.119382 Medium H

C -6.571486 3.571928 -7.350070 Medium H
C -6.044660 4.829457 -5.204522 Medium H
C -0.306455 4.563418 -3.694634 Medium H
C -0.051293 2.338554 -4.842640 Medium H
C -2.845777 -5.787638 -3.239809 Medium H
C 2.397682 -4.207120 0.458113 Medium H
C -5.597385 -3.094604 0.145034 Medium H
C -0.512052 -3.208565 5.174295 Medium H
C 4.644486 -0.943040 8.536709 Medium H

12_{OH}•H_2O (only the inner shell and link atoms)
Zn -0.280161 -0.050958 -0.016161
O 0.201749 2.027857 -0.039098
H -0.122235 2.437536 -0.857464
H -0.036338 2.589304 0.716806
C 4.571792 0.239676 7.917770
C 3.750927 0.378481 6.638772
O 2.739422 -0.249741 6.403064
N 4.207434 1.321917 5.803126
H 4.205577 1.037197 8.575528
H 5.621120 0.488701 7.706233
H 3.653921 1.558132 5.008305
H 5.026471 1.878781 5.984913
C -0.932595 -1.682607 5.242590
C -0.360067 -0.965446 4.051330
N 0.908613 -0.434354 4.009457
C -0.869395 -0.766367 2.819312
C 1.114299 0.033138 2.784385
N 0.067707 -0.146482 2.023763
H -2.013583 -1.505030 5.277385
H -0.517425 -1.268847 6.167746
H 1.560732 -0.400653 4.778124
H -1.834422 -1.036230 2.444730
H 2.028593 0.502394 2.482770
C -5.220281 -2.182480 -1.124107
C -4.156759 -1.187905 -0.747331
N -4.417135 0.107981 -0.376131
C -2.827049 -1.333688 -0.616267
C -3.269769 0.689441 -0.070684
N -2.275201 -0.150339 -0.175318
H -4.811162 -2.881566 -1.860176
H -6.065755 -1.675831 -1.598407
H -5.320022 0.550069 -0.403383
H -2.229725 -2.199431 -0.805057
H -3.197711 1.710776 0.244659
C 1.891001 -2.776160 0.387412
C 1.248991 -2.531812 -0.949102

N 0.480734 -1.418353 -1.207894
C 1.257290 -3.288029 -2.070635
C 0.063122 -1.584115 -2.473725
N 0.490069 -2.688281 -3.027047
H 1.211989 -2.470721 1.191717
H 2.797219 -2.158000 0.493696
H 1.749306 -4.228502 -2.249588
H -0.601244 -0.898229 -2.958068
H -0.143253 -3.405175 -4.356046
C -1.668596 -5.406257 -3.778208
C -1.698697 -4.441518 -4.966094
O -2.609750 -4.426422 -5.745984
O -0.654238 -3.680414 -5.167196
H -0.981611 -5.045411 -3.009583
H -1.248475 -6.342932 -4.166805
C -0.770275 3.115379 -3.785193
O -0.846067 2.492510 -2.509946
H -1.798355 3.195540 -4.175250
H -1.470103 1.754341 -2.654135
C -9.285249 1.467572 0.024643
C -8.150674 1.368252 -1.032555
O -7.015158 1.084193 -0.725841
H -9.708866 2.494481 -0.050054
N -8.500099 1.638470 -2.300591
C -7.585118 1.418415 -3.409668
C -7.649191 2.590885 -4.399781
O -8.648713 3.230976 -4.577414
H -9.434081 1.905010 -2.530749
H -6.589018 1.393684 -2.981468
N -6.472955 2.792464 -5.033521
C -6.232783 3.875259 -5.988937
H -5.648351 2.336310 -4.679313
H -7.141746 4.496205 -6.008255
C -4.720190 -1.564079 -6.670264
C -4.143444 -1.715429 -8.090870
O -4.556007 -1.062356 -9.011530
C -3.776091 -0.630276 -5.867318
C -4.210823 -0.419498 -4.414579
C -3.454643 0.746854 -3.803128
O -2.345085 0.502052 -3.302014
O -3.969239 1.874985 -3.896573
H -5.700109 -1.071725 -6.789161
H -2.760583 -1.010904 -5.883403
H -3.768209 0.326383 -6.382614
H -5.279899 -0.217164 -4.385535
H -4.013426 -1.319034 -3.840993
N -3.087772 -2.556201 -8.182793

C -2.496999 -2.920115 -9.457799
H -2.884737 -3.166079 -7.416146
H -2.694941 -2.084803 -10.144725
N -4.891390 -2.851052 -5.992781 Medium H
C -3.148617 -4.194812 -9.989231 Medium H
C -0.987213 -3.122024 -9.293846 Medium H
N -10.339965 0.495011 -0.283078 Medium H
C -8.746951 1.268892 1.436106 Medium H
C -7.842891 0.086693 -4.110673 Medium H
C -5.983292 3.263626 -7.368432 Medium H
C -5.045702 4.718692 -5.513372 Medium H
C -0.201173 4.535771 -3.646369 Medium H
C 0.064593 2.286830 -4.749648 Medium H
C -3.051975 -5.643111 -3.214788 Medium H
C 2.269403 -4.244022 0.571594 Medium H
C -5.692874 -2.926168 0.117216 Medium H
C -0.659043 -3.184215 5.207142 Medium H
C 4.456668 -1.080636 8.637328 Medium H

1_{NH}•OH^-

C	0.737900	-1.179058	-1.586118
N	0.348105	0.003407	-0.989331
C	1.470607	0.581607	-0.612979
N	2.525114	-0.144809	-0.908322
C	2.084404	-1.274105	-1.530243
Zn	-1.523515	0.602396	-0.585580
N	-1.291072	1.620772	1.278579
C	-2.163734	2.649292	1.555580
C	-1.873037	3.162135	2.766064
N	-0.803951	2.430961	3.232661
C	-0.498082	1.525316	2.301400
N	-2.483927	-1.228313	-0.080174
C	-3.847726	-1.314400	-0.245421
C	-4.262616	-2.538181	0.132426
N	-3.127943	-3.207617	0.533221
C	-2.094479	-2.376269	0.382098
O	-2.932107	1.554267	-1.301783
O	4.991734	0.313750	-0.263207
C	5.616172	-0.726542	-0.600688
O	5.125634	-1.716720	-1.129977
C	7.112646	-0.707975	-0.310387
H	-2.914549	1.913928	-2.174450
H	-3.077819	-4.144582	0.862124
H	3.546096	0.067804	-0.664761
H	1.532601	1.529638	-0.121609
H	2.781058	-2.015028	-1.852793
H	-5.228489	-2.992160	0.154132

H	-1.084464	-2.644480	0.610243
H	-0.328580	2.560536	4.096391
H	-2.307683	3.957376	3.330089
H	0.303830	0.825129	2.406021
H	-2.918045	2.915945	0.847661
H	-4.395001	-0.480028	-0.626917
H	0.025580	-1.854139	-2.010693
H	7.279085	-0.510526	0.744202
H	7.576022	-1.646477	-0.585929
H	7.577102	0.103096	-0.863408

1_{OH}•OH^-

C	-3.933659	-1.261935	-0.247983
N	-2.568761	-1.190744	-0.096754
C	-2.186638	-2.340653	0.362758
N	-3.227979	-3.162219	0.527228
C	-4.359320	-2.480476	0.136292
Zn	-1.545190	0.624587	-0.617550
O	-2.970229	1.570834	-1.325402
N	-1.404444	1.638707	1.275360
C	-2.325466	2.614092	1.578856
C	-2.057627	3.111577	2.801394
N	-0.950858	2.423810	3.247725
C	-0.603558	1.557838	2.290940
N	0.303357	0.002857	-0.931711
C	1.447289	0.586988	-0.564498
N	2.521598	-0.114954	-0.811190
C	2.058883	-1.254498	-1.401426
C	0.706729	-1.188870	-1.482911
O	5.260117	0.209179	-0.354029
C	5.946708	-0.861512	-0.674922
C	7.423356	-0.675761	-0.434521
O	5.469195	-1.867167	-1.106461
H	-2.950104	1.935925	-2.195845
H	-3.184359	-4.099482	0.855044
H	4.303696	0.084434	-0.524017
H	1.473102	1.557324	-0.107079
H	2.730228	-2.024375	-1.719550
H	-5.329963	-2.923770	0.168323
H	-1.175908	-2.616750	0.577867
H	-0.480350	2.555229	4.113295
H	-2.529681	3.869959	3.385936
H	0.233957	0.897240	2.369760
H	-3.091628	2.861630	0.876876
H	-4.473936	-0.421982	-0.626930
H	0.007550	-1.884973	-1.899941
H	7.596705	-0.428038	0.606880

H	7.955831	-1.579043	-0.694151
H	7.787318	0.153338	-1.031305

2_{NH}•OH^-

C	-2.414679	-2.122100	0.549698
N	-2.775295	-0.963646	0.089926
C	-4.147262	-0.994000	-0.016972
C	-4.596414	-2.194994	0.393285
N	-3.474595	-2.907215	0.754638
Zn	-1.760216	0.815370	-0.485178
O	-3.151405	1.815556	-1.168677
N	0.069246	0.125381	-0.940398
C	0.385522	-1.091955	-1.510841
C	1.725645	-1.260033	-1.481083
N	2.235138	-0.134921	-0.900943
C	1.225929	0.654768	-0.604263
N	-1.411257	1.860171	1.345645
C	-2.225773	2.932674	1.632836
C	-1.862804	3.459007	2.817725
N	-0.808317	2.691308	3.258161
C	-0.581212	1.752388	2.337488
O	4.678056	0.521667	-0.151453
C	5.399575	-0.489433	-0.311107
C	6.862489	-0.326433	0.087920
O	5.027324	-1.571572	-0.759606
N	3.915026	-3.858172	-2.421356
H	-3.155491	2.148440	-2.052063
H	-3.449181	-3.842523	1.090989
H	3.239493	0.070283	-0.665389
H	1.352474	1.610096	-0.140694
H	2.349321	-2.064373	-1.808640
H	-5.578553	-2.607668	0.460935
H	-1.407914	-2.430671	0.737595
H	-0.290876	2.819695	4.097546
H	-2.238262	4.285451	3.379391
H	0.193476	1.020121	2.426389
H	-2.996119	3.217283	0.949608
H	-4.675079	-0.141874	-0.386433
H	-0.368310	-1.741225	-1.902246
H	6.927822	0.051325	1.103337
H	7.398912	-1.263221	0.007818
H	7.328948	0.412138	-0.557675
H	4.378685	-3.152799	-1.870234
H	4.341106	-3.840717	-3.329985
H	4.148492	-4.745757	-2.014839

2_{NH}•OH^- optimized at the B3LYP/BS1 level

C	-0.908795	2.354210	1.007239
N	-1.709356	1.800385	0.112656
C	-2.731258	2.701619	-0.119810
C	-2.538371	3.813340	0.653801
N	-1.375482	3.575091	1.364741
Zn	-1.769319	0.004086	-0.973787
N	0.118734	-0.507910	-1.022951
C	0.651114	-1.784206	-0.906124
C	2.013378	-1.694108	-0.763411
N	2.313924	-0.353636	-0.805200
C	1.170596	0.320259	-0.963457
N	-2.534577	-1.344025	0.436371
C	-2.040703	-2.063278	1.428632
N	-3.027181	-2.769728	2.033264
C	-4.216299	-2.484746	1.384864
C	-3.891877	-1.598601	0.394376
O	-3.319536	0.324148	-1.920465
O	4.344004	1.158508	-0.396581
C	5.245466	0.756878	0.415005
O	5.377016	-0.395230	0.883069
C	6.280407	1.820947	0.816802
N	4.764272	-3.129181	-0.040997
H	-3.326418	0.180346	-2.874965
H	-2.908877	-3.401756	2.812302
H	3.243398	0.133736	-0.656383
H	1.121892	1.397088	-1.029674
H	2.796456	-2.437875	-0.616785
H	-5.151524	-2.931474	1.684117
H	-1.001896	-2.106353	1.723081
H	-0.935057	4.206142	2.019270
H	-3.098167	4.728835	0.764315
H	-0.003048	1.919837	1.405417
H	-3.504023	2.444718	-0.831201
H	-4.493766	-1.110565	-0.359686
H	0.020584	-2.661125	-0.936562
H	5.799292	2.792200	0.974600
H	6.824249	1.517012	1.715367
H	7.003160	1.947310	0.000296
H	4.949777	-2.161185	0.266385
H	5.464768	-3.330972	-0.754784
H	5.006478	-3.722870	0.752646

2_{OH}•OH^-

C	0.277853	-1.214825	-1.381236
N	0.007644	0.029730	-0.866231
C	1.211567	0.506905	-0.541782
N	2.205111	-0.308327	-0.782847

C	1.617662	-1.416489	-1.323189
Zn	-1.764297	0.831313	-0.520808
N	-1.473649	1.872036	1.340741
C	-2.287915	2.938034	1.644513
C	-1.937434	3.435168	2.846126
N	-0.888445	2.654538	3.279171
C	-0.654102	1.737679	2.335487
N	-2.935749	-0.868251	0.073869
C	-4.305785	-0.812892	-0.029602
C	-4.829807	-1.979933	0.391189
N	-3.754056	-2.759144	0.756064
C	-2.646824	-2.042126	0.541081
O	-3.113603	1.894697	-1.210971
O	4.827670	0.332224	-0.156946
C	5.769478	-0.534397	-0.423820
O	5.587372	-1.605505	-0.923051
C	7.132764	-0.028121	-0.027263
H	-3.096758	2.217183	-2.098147
H	-3.786310	-3.692059	1.097330
H	3.936739	0.013620	-0.423593
H	1.345526	1.484529	-0.119876
H	2.187299	-2.270003	-1.628271
H	-5.835930	-2.329349	0.464075
H	-1.659369	-2.409362	0.725844
H	-0.381718	2.759824	4.127670
H	-2.317306	4.248494	3.423946
H	0.118650	1.001711	2.407815
H	-3.047455	3.242130	0.957717
H	-4.778299	0.068107	-0.405857
H	-0.495681	-1.851011	-1.760708
H	7.142377	0.204483	1.031790
H	7.882913	-0.772798	-0.249679
H	7.349905	0.888714	-0.564036
N	4.063988	-4.072148	-2.359323
H	4.471316	-3.302401	-1.858387
H	4.226368	-3.897033	-3.333772
H	4.596463	-4.888565	-2.120978

2_{OH}•OH^- optimized at the B3LYP/BS1 level

C	-2.124001	-2.182204	1.290384
N	-2.582704	-1.403940	0.327889
C	-3.943119	-1.622614	0.250966
C	-4.308125	-2.549129	1.189571
N	-3.137830	-2.894918	1.843560
Zn	-1.742581	0.011015	-1.015194
O	-3.243352	0.314941	-2.049785
N	0.138287	-0.415362	-0.877974

C	0.704966	-1.668786	-0.721156
C	2.050635	-1.509643	-0.481147
N	2.340054	-0.164369	-0.492131
C	1.178121	0.440417	-0.736251
N	-1.934222	1.768849	0.132355
C	-3.010816	2.600789	-0.105597
C	-2.942894	3.679740	0.733335
N	-1.799060	3.491296	1.490102
C	-1.222436	2.329744	1.092391
O	4.464837	1.358158	-0.060376
C	5.614783	0.811038	0.294767
C	6.697024	1.854272	0.513693
O	5.819337	-0.386698	0.437607
N	4.915143	-3.316182	0.136823
H	-3.335949	-0.181990	-2.872496
H	-3.048243	-3.569444	2.589911
H	3.716559	0.655491	-0.217004
H	1.068448	1.514572	-0.823636
H	2.816398	-2.256515	-0.301615
H	-5.258948	-2.987319	1.450260
H	-1.090229	-2.262849	1.595126
H	-1.443966	4.114770	2.200660
H	-3.576915	4.543064	0.862062
H	-0.303890	1.940059	1.507101
H	-3.725458	2.332926	-0.871009
H	-4.516689	-1.080846	-0.488197
H	0.114825	-2.571355	-0.807679
H	6.375446	2.576858	1.271582
H	7.622823	1.371091	0.829754
H	6.868130	2.413077	-0.412992
H	5.130743	-2.320287	0.233804
H	5.423110	-3.627256	-0.690999
H	5.369218	-3.776044	0.925966

3_{NH}•OH^-

C	-3.529588	-1.053822	0.916028
N	-2.240376	-0.896201	0.898006
C	-1.714891	-1.878607	1.702881
C	-2.715059	-2.624937	2.207054
N	-3.872451	-2.083148	1.694855
Zn	-1.485765	0.660573	-0.330667
O	-3.123936	1.256500	-1.001773
N	-1.059680	2.263261	0.979802
C	-0.078293	2.656668	1.864946
C	-0.426003	3.837223	2.409926
N	-1.639187	4.166704	1.846766
C	-1.969797	3.192709	0.998068

N	0.209982	-0.039477	-1.118619
C	0.407213	-0.740924	-2.292363
C	1.704747	-1.100784	-2.380522
N	2.304643	-0.614617	-1.251872
C	1.388136	0.004508	-0.537225
O	4.583961	-0.491533	0.136724
C	5.616382	-1.098742	-0.242843
C	6.821969	-0.982879	0.686263
O	5.730603	-1.755522	-1.268892
N	4.327120	-2.618172	-3.855440
N	3.143585	1.032873	2.312530
H	-3.270501	1.388090	-1.925544
H	-2.718896	-3.469185	2.860366
H	3.282202	-0.690179	-0.928312
H	1.612435	0.470516	0.399120
H	2.259577	-1.645889	-3.116249
H	-4.798720	-2.403558	1.859951
H	-0.661511	-1.977867	1.852436
H	0.060478	4.463696	3.124393
H	-2.173195	4.985352	2.026516
H	0.804123	2.075494	2.039130
H	-2.861883	3.165110	0.407817
H	-4.213836	-0.437663	0.371326
H	-0.393047	-0.931768	-2.975507
H	6.559743	-1.351993	1.673693
H	7.667260	-1.539468	0.303682
H	7.095726	0.062425	0.797492
H	4.750178	-2.314646	-2.990426
H	4.867351	-2.207179	-4.595086
H	4.478693	-3.608897	-3.913108
H	3.708994	0.523534	1.645821
H	3.193318	0.523766	3.176777
H	3.616826	1.903907	2.474089

3_{OH}•OH^-

C	-0.077817	2.257386	2.157769
N	-1.014118	2.157797	1.152431
C	-1.774790	3.206285	1.243151
N	-1.390492	3.987001	2.255901
C	-0.300146	3.389809	2.851957
Zn	-1.458089	0.767879	-0.389112
N	0.258565	-0.048708	-0.901342
C	0.538791	-1.373632	-1.128533
C	1.879888	-1.501620	-1.285275
N	2.455844	-0.266491	-1.163147
C	1.452796	0.543875	-0.943549
N	-2.604548	-0.764591	0.566549

C	-2.357778	-1.859132	1.359629
C	-3.523207	-2.455216	1.674212
N	-4.498296	-1.703825	1.057146
C	-3.891752	-0.705817	0.407279
O	-2.923872	1.676281	-1.126119
O	4.999048	0.651231	-0.618576
C	6.053420	-0.076028	-0.891081
O	6.019833	-1.152745	-1.408146
C	7.332422	0.604418	-0.475868
N	4.495080	-3.857127	-2.364667
N	2.595893	-0.146641	2.293213
H	-2.948765	1.897331	-2.044361
H	-3.751224	-3.318713	2.259133
H	4.159905	0.225162	-0.905600
H	1.574819	1.598685	-0.789753
H	2.460484	-2.380234	-1.479448
H	-5.477483	-1.871605	1.080301
H	-1.363564	-2.133994	1.638180
H	0.199115	3.822845	3.690386
H	-1.813138	4.846538	2.519907
H	0.682338	1.515892	2.300086
H	-2.597264	3.405308	0.588670
H	-4.385236	0.049779	-0.167392
H	-0.231358	-2.116606	-1.169155
H	7.301419	0.827551	0.584795
H	8.177272	-0.031384	-0.696221
H	7.429831	1.546484	-1.003972
H	4.899168	-3.004422	-2.019744
H	4.315193	-3.713296	-3.341153
H	5.206944	-4.561673	-2.303364
H	3.311702	0.345639	1.790492
H	2.216658	-0.802336	1.634351
H	3.056684	-0.681279	3.006697

6_{NH}•OH^-

C	4.453759	2.444250	0.390432
N	3.291761	1.719361	0.541729
C	2.700726	2.191002	1.596521
N	3.414896	3.172295	2.150068
C	4.544629	3.348085	1.383591
Zn	2.806286	0.312770	-0.976011
O	4.059886	0.815834	-2.225760
N	0.828320	0.024017	-0.731266
C	0.287644	-0.405915	0.388684
N	-1.021545	-0.492333	0.302690
C	-1.378311	-0.094816	-0.950835
C	-0.230603	0.224775	-1.589197

N	3.607637	-1.568538	-0.308746
C	4.950690	-1.772981	-0.531769
C	5.286759	-3.011721	-0.126363
N	4.123693	-3.573452	0.347333
C	3.152708	-2.667889	0.209450
O	-2.585954	-1.317288	2.278982
C	-3.740323	-1.215571	1.820418
O	-4.017159	-0.812545	0.682412
C	-4.887225	-1.655070	2.719834
H	4.132190	0.394713	-3.067627
H	1.760852	1.862830	1.986807
H	3.159442	3.692501	2.958106
H	5.279029	4.087856	1.613287
H	5.099485	2.259606	-0.440084
H	5.544671	-1.010498	-0.985528
H	6.213941	-3.540659	-0.132473
H	4.014656	-4.491702	0.713347
H	2.137549	-2.855088	0.488375
H	-0.086877	0.582110	-2.586382
H	-2.402837	-0.082770	-1.247005
H	0.830851	-0.658856	1.275490
H	-1.667262	-0.811529	1.063335
H	-5.180850	-2.663804	2.440584
H	-4.587744	-1.661308	3.759730
H	-5.749159	-1.013344	2.579988
H	-5.670117	-0.380529	-0.209176
N	-6.487082	-0.109024	-0.725190
C	-6.819613	1.185513	-0.825130
O	-7.778712	1.575438	-1.447643
C	-7.274214	-1.127793	-1.373627
H	-6.828770	-2.090669	-1.159132
H	-8.296896	-1.125521	-1.013808
H	-7.300499	-0.984514	-2.448272
C	-5.911927	2.153759	-0.093312
H	-5.572423	2.906149	-0.796106
H	-6.493744	2.660960	0.668829
H	-5.060504	1.669396	0.365607

6_{OH}•OH^-

C	-0.567557	4.109222	0.341055
N	-1.787869	3.680895	0.255551
C	-2.596047	4.790305	0.336456
C	-1.832383	5.889662	0.482403
N	-0.532135	5.437781	0.484692
Zn	-2.712033	1.755151	-0.116500
N	-1.127650	0.606149	-0.424652
C	-0.087514	0.508350	0.408077

N	0.848481	-0.316022	0.016768
C	0.394252	-0.807354	-1.172228
C	-0.811565	-0.248679	-1.446751
N	-3.442849	1.107167	1.788810
C	-4.719148	1.449872	2.172439
C	-5.010857	0.841760	3.337655
N	-3.890360	0.111023	3.665009
C	-2.988444	0.303262	2.698598
O	-4.332117	2.328811	-0.794573
O	3.256504	-1.064512	1.138001
C	3.911206	-1.940042	0.427556
C	5.219380	-2.334016	1.061541
O	3.519566	-2.385042	-0.616081
H	-4.405631	2.677851	-1.668926
H	-2.026948	-0.164562	2.690658
H	-3.775152	-0.473455	4.460618
H	-5.885304	0.847864	3.949931
H	-5.315752	2.082215	1.552173
H	-3.656356	4.690535	0.260247
H	-2.075965	6.924766	0.576916
H	0.288527	5.993443	0.561089
H	0.309544	3.499331	0.294707
H	-1.462063	-0.396571	-2.284407
H	0.963648	-1.518323	-1.733103
H	-0.032177	1.065751	1.324793
H	2.402577	-0.815475	0.715084
H	5.840510	-1.454205	1.186421
H	5.034846	-2.744986	2.047633
H	5.729440	-3.061806	0.447683
H	4.397456	-3.736389	-1.920819
N	4.907484	-4.383096	-2.483659
C	5.814025	-3.873088	-3.484485
C	4.674947	-5.702105	-2.367304
H	6.805005	-4.292145	-3.360365
H	5.473508	-4.110391	-4.486030
H	5.870224	-2.797449	-3.379249
O	5.229621	-6.525844	-3.050392
C	3.666652	-6.105216	-1.310948
H	3.252510	-5.263759	-0.770651
H	2.864022	-6.651382	-1.792771
H	4.148520	-6.781579	-0.614292

7_{NH}•OH^-

C	2.111055	2.765248	0.027970
N	1.238605	1.886561	0.437069
C	0.567874	2.470675	1.484647
C	1.058776	3.708953	1.687719

N	2.044267	3.881815	0.747401
Zn	1.176989	0.060657	-0.581617
O	2.488958	0.338760	-1.878714
N	-0.771652	-0.461051	-0.615122
C	-1.857803	0.384499	-0.708000
C	-2.989252	-0.350584	-0.688941
N	-2.595880	-1.653298	-0.588402
C	-1.279540	-1.671455	-0.549986
N	2.108305	-1.434871	0.559674
C	1.818496	-2.169482	1.684538
C	2.839832	-3.011014	1.938467
N	3.767146	-2.784821	0.951884
C	3.282512	-1.834927	0.156862
O	-4.240472	-3.775678	-0.438398
C	-5.376377	-3.273215	-0.411420
O	-5.622362	-2.058209	-0.451640
C	-6.566361	-4.221194	-0.326423
N	-7.305134	0.280695	-0.217977
C	-7.263901	0.969527	0.930822
O	-7.801577	2.042122	1.078122
C	-8.027593	0.783555	-1.359411
C	-6.498925	0.310783	2.060943
O	6.229367	-4.284591	0.530835
C	6.633994	-5.238630	-0.089932
C	8.088547	-5.638830	-0.039913
N	5.831114	-5.984040	-0.867150
O	3.520291	6.350293	0.278819
C	3.421258	7.376404	-0.350898
C	4.507549	8.423512	-0.306887
N	2.361579	7.640877	-1.132866
H	2.288618	0.290775	-2.800629
H	-0.213917	1.961076	2.005499
H	0.808558	4.467691	2.395973
H	2.602771	4.706067	0.613109
H	2.788561	2.597806	-0.782597
H	3.782191	-1.439270	-0.702200
H	4.645587	-3.258786	0.837289
H	2.994164	-3.732398	2.710271
H	0.903899	-2.038686	2.222016
H	-1.738735	1.444662	-0.774850
H	-4.023584	-0.095244	-0.731411
H	-0.708132	-2.571729	-0.468867
H	-3.231295	-2.475616	-0.537823
H	-7.202156	-4.078809	-1.195062
H	-6.247917	-5.253955	-0.275825
H	-7.161775	-3.978463	0.548321
H	-6.829881	-0.600385	-0.293054

H	-7.902041	0.084970	-2.176310
H	-9.085715	0.887839	-1.145287
H	-7.654639	1.754335	-1.666065
H	-5.802320	1.031516	2.473366
H	-7.202147	0.052630	2.845987
H	-5.968787	-0.578301	1.747673
H	2.280883	8.480869	-1.655759
H	1.633156	6.966309	-1.209125
H	5.375249	8.037656	-0.830026
H	4.215171	9.364255	-0.756020
H	4.788559	8.586250	0.725007
H	6.163189	-6.763570	-1.384436
H	4.869204	-5.739848	-0.948083
H	8.280906	-6.611688	-0.474387
H	8.666436	-4.893506	-0.574774
H	8.413358	-5.631771	0.991891

7_{OH}•OH^-

Zn	1.391457	0.029316	-0.498374
O	2.783048	0.137887	-1.752252
H	2.600934	0.122252	-2.679198
N	2.167907	-1.573506	0.650950
C	3.322310	-2.058203	0.292857
N	3.692682	-3.062190	1.086557
C	2.703012	-3.232003	2.023590
C	1.766246	-2.304594	1.741479
H	3.889624	-1.687669	-0.534783
H	4.534750	-3.601745	0.997002
H	2.761307	-3.979733	2.783587
H	0.837787	-2.110664	2.234086
O	6.017860	-4.768678	0.574521
C	6.217481	-5.614531	-0.263816
N	5.281864	-5.976684	-1.158550
H	4.396224	-5.521474	-1.148217
H	5.450782	-6.659185	-1.859346
C	7.555243	-6.305891	-0.371706
H	7.520004	-7.213139	-0.961904
H	8.259839	-5.618748	-0.827566
H	7.909065	-6.533121	0.624478
N	1.820442	1.799606	0.579385
C	2.864474	2.485297	0.211401
N	3.014955	3.576739	0.960452
C	1.992059	3.590220	1.877129
C	1.260784	2.485327	1.628997
H	3.509683	2.197971	-0.591830
H	3.735894	4.267697	0.855283
H	1.887405	4.367952	2.601212

H	0.377164	2.135412	2.117846
O	4.952970	5.704155	0.413385
C	4.964920	6.572874	-0.425289
N	3.965235	6.734165	-1.309395
H	3.192160	6.106733	-1.290059
H	3.981244	7.438090	-2.009173
C	6.130244	7.525094	-0.545768
H	5.903514	8.404123	-1.136157
H	6.438248	7.822898	0.447049
H	6.957451	6.996920	-1.007464
N	-0.575496	-0.173356	-0.487406
C	-1.291102	-1.298763	-0.458827
N	-2.586607	-1.119199	-0.460656
C	-2.745118	0.236433	-0.498161
C	-1.522142	0.819986	-0.516879
H	-0.832959	-2.268595	-0.432198
H	-3.951889	-2.213961	-0.422845
H	-3.717975	0.681549	-0.508782
H	-1.253734	1.856363	-0.546393
O	-4.701285	-2.859224	-0.398430
C	-5.859390	-2.267213	-0.386428
O	-6.009801	-1.075434	-0.403132
C	-7.005745	-3.244574	-0.350286
H	-7.672755	0.127567	-0.424994
N	-8.519989	0.654869	-0.438893
C	-9.026982	1.139227	0.707165
O	-10.022858	1.818250	0.746582
C	-9.128614	0.962718	-1.710588
C	-8.272906	0.774201	1.969384
H	-6.960560	-3.886746	-1.222725
H	-7.948304	-2.717069	-0.328914
H	-6.915062	-3.877714	0.525028
H	-8.571398	0.456547	-2.488043
H	-9.117091	2.028734	-1.907921
H	-10.158718	0.628744	-1.740251
H	-7.388094	0.179690	1.782734
H	-7.990822	1.688668	2.477992
H	-8.942501	0.229787	2.625670

7_{TS}•OH^- 1 imaginary frequency

C	1.674680	-2.272887	1.712551
N	2.069793	-1.565812	0.603025
C	3.190663	-2.102301	0.209993
N	3.543539	-3.115458	0.997946
C	2.580368	-3.237472	1.968880
Zn	1.336722	0.055412	-0.528973
O	2.692038	0.143546	-1.815806

N	-0.650648	-0.144564	-0.526101
C	-1.594564	0.855765	-0.574822
C	-2.822156	0.289392	-0.556955
N	-2.650166	-1.063310	-0.500875
C	-1.353363	-1.265127	-0.487349
N	1.745391	1.830180	0.523350
C	2.773204	2.528703	0.130866
N	2.922275	3.625505	0.869951
C	1.917728	3.631167	1.806190
C	1.196724	2.515187	1.580018
O	-4.455003	-2.739020	-0.419289
C	-5.616381	-2.227229	-0.405528
O	-5.850793	-1.030076	-0.434414
C	-6.747385	-3.235038	-0.353022
O	5.794822	-4.917843	0.531650
C	6.018447	-5.868214	-0.179325
N	5.094404	-6.377723	-1.011284
C	7.374202	-6.531975	-0.188718
O	4.869081	5.748534	0.379420
C	4.984476	6.689244	-0.369105
N	4.043372	7.008674	-1.273512
C	6.219165	7.557384	-0.344482
N	-8.324655	0.618545	-0.384743
C	-8.742173	1.142179	0.777436
O	-9.707445	1.862264	0.866127
C	-9.007624	0.913362	-1.619963
C	-7.926916	0.766092	1.998009
H	2.491281	0.128750	-2.738828
H	3.746494	-1.760980	-0.637756
H	4.358445	-3.692070	0.887072
H	2.632866	-3.982161	2.732212
H	0.773950	-2.036843	2.237300
H	4.195544	-5.951967	-1.059298
H	5.280076	-7.151519	-1.604800
H	7.374912	-7.496523	-0.680722
H	8.071932	-5.876946	-0.698706
H	7.711102	-6.644844	0.832777
H	3.407751	2.245565	-0.682304
H	3.633011	4.324879	0.749959
H	1.816768	4.411836	2.527548
H	0.328538	2.157104	2.090169
H	3.225794	6.444709	-1.344183
H	4.141412	7.774686	-1.897289
H	6.100665	8.485462	-0.889492
H	6.471563	7.770515	0.685372
H	7.039680	6.997055	-0.778914
H	-0.913108	-2.240418	-0.443935

H	-3.563549	-1.899688	-0.462549
H	-3.800389	0.716973	-0.577670
H	-1.318299	1.888612	-0.614906
H	-7.500022	0.051343	-0.410606
H	-7.708301	-2.740627	-0.308875
H	-6.622308	-3.875367	0.513374
H	-6.702854	-3.870054	-1.231654
H	-8.509892	0.381525	-2.420409
H	-8.989741	1.975183	-1.839709
H	-10.044245	0.599615	-1.579808
H	-7.058883	0.165786	1.760270
H	-7.615005	1.675998	2.497541
H	-8.566158	0.221158	2.684141