Computational Study of Copper(II) Complexation and Hydrolysis in Aqueous Solutions Using Mixed Cluster/Continuum Models

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Supporting Information Available: Cartesian coordinates and total energies for all Cu(II) complexes optimized in the field of the continuum solvent (COSMO solvation model for water) at the B3LYP/6-311++G(d,p) level of theory, Table 1S summarizing gas-phase binding free energies and solvation free energies of Cu(II) complexes, and Table 2S showing aqueous reaction free energies calculated using complexes with one coordination shell (four equatorial ligands). This material is available free of charge via the Internet at http://pubs.acs.org.

Table 1S. Total electronic binding energies ($\Delta E_{0K,bind}$), gas-phase binding free energies ($\Delta G^{o}_{bind,\,g}$), and solvation energies (ΔG^{*}_{solv}) for Cu(II) complexes (kcal/mol)[a]

complex	$\Delta E_{0K,bind}$[b]	$\Delta G^{o}_{bind,\,g}$[c]	ΔG^{*}_{solv}[d]
$[Cu(H_2O)_4]^{2+}$	-310.95	-271.25	-210.52
$[Cu(H_2O)_5]^{2+}$	-342.62	-289.05	-197.78
$[Cu(H_2O)_6]^{2+}$	-372.07	-304.08	-187.52
$[Cu(H_2O)_8]^{2+}$	-424.52	-332.92	-168.32
$[Cu(H_2O)_{18}]^{2+}$	-579.71	-363.35	-149.40
$[Cu(MeNH_2)(H_2O)_3]^{2+}$	-335.81	-295.33	-200.11
$[Cu(MeNH_2)(H_2O)_4]^{2+}$	-365.34	-310.27	-188.99
$[Cu(MeNH_2)(H_2O)_5]^{2+}$	-392.50	-324.49	-178.41
$[Cu(MeNH_2)(H_2O)_7]^{2+}$	-438.94	-346.88	-162.92
$[Cu(MeNH_2)(H_2O)_{18}]^{2+}$	-587.78	-370.41	-147.08
$[Cu(OH)(H_2O)_3]^{+}$	-575.46	-533.88	-71.14
$[Cu(OH)(H_2O)_4]^{+}$	-595.46	-540.74	-68.18
$[Cu(OH)(H_2O)_5]^{+}$	-614.00	-546.97	-65.75
$[Cu(OH)(H_2O)_7]^{+}$	-647.53	-556.42	-62.95
$[Cu(OH)(H_2O)_{17}]^{+}$	-773.21	-557.38	-69.52
$[Cu(OH)_2(H_2O)_2]$	-738.37	-695.02	-22.53
$[Cu(OH)_2(H_2O)_4]$	-772.40	-704.98	-21.36
$[Cu(OH)_2(H_2O)_6]$	-800.31	-707.66	-22.05
$[Cu(OH)_2(H_2O)_{16}]$	-905.54	-690.12	-47.98
$[Cu(OH)_3(H_2O)]^{-}$	-800.16	-757.38	-66.59
$[Cu(OH)_3(H_2O)_3]^{-}$	-826.85	-760.80	-69.02
$[Cu(OH)_3(H_2O)_{15}]^{-}$	-985.43	-771.18	-76.69

[a]The lowest energy structures in the aqueous phase for each cluster size. [b]Electronic binding energies obtained at the B3LYP/LACV3P+/6-311G++(d,p) level of theory. [c]ZPE and thermal corrections calculated using the B3LYP/LACVP/6-31G(d,p) method. The calculated (experimental) Gibbs free energy for $H^+ + OH^- = H_2O$ is 382.14 (383.7±0.3) kcal/mol. [d]The electrostatic contribution to the solvation free energy (ΔG^{*}_{solv}) with full geometry optimization in the solvent reaction field at the COSMO-B3LYP/LACV3P+/6-311G++(d,p) level. The calculated ΔG^{*}_{solv} for H_2O and $MeNH_2$ are -5.12 and -8.34 kcal/mol, respectively.

Table 2S. Gibbs free energies of aqueous reactions calculated using complexes with only the inner coordination shell around the Cu^{2+} ion (four equatorial ligands) [a]

	COSMO		Jaguar		expt
	BS1	BS1(corr)[b]	BS1	BS1(corr)[b]	
$\Delta G^*_{compl, aq}$	-14.51	-14.51	-12.40	-12.40	-5.61
$\Delta G^*_{1,hydr, aq}$	-5.12	2.91	5.12	8.83	10.85
$\Delta G^*_{2,hydr, aq}$	5.61	13.64	11.04	14.75	11.25
$\Delta G^*_{3,hydr, aq}$	11.70	19.73	8.99	12.70	14.19
MUE[c]	8.25	6.19	4.49	3.45	

[a]BS1 is the LACV3P+/6-311G++(d,p) basis set. [b]Using a constant empirical correction term to minimize the systematic errors in the calculated hydrolysis constants. [c]MUE denotes mean unsigned error (also called mean absolute error) for the complexation and three hydrolysis reactions.

Cartesian coordinates and absolute energies (in Hartrees) for optimized structures at the COSMO-B3LYP/ LACV3P+/6-311G++(d,p) level of theory

$[Cu(H_2O)_4]^{2+}$, E = -501.7444587
Cu 0.0002513 0.0003065 -0.0000112
O 1.3323009 1.4317355 0.1357866
H 1.3656347 2.1075774 -0.5558864
H 2.2414648 1.2474320 0.4079586
O -1.3454869 1.4204806 -0.1349077
H -2.2345045 1.2244938 -0.4605643
H -1.4343385 2.0533482 0.5919074
O -1.3297807 -1.4354199 0.1339525
H -1.4281293 -2.0494127 -0.6075940
H -2.2124799 -1.2631312 0.4890876
O 1.3465114 -1.4173596 -0.1359123
H 2.2584777 -1.2303790 -0.3962406
H 1.3717694 -2.1003069 0.5491964

$[Cu(H_2O)_5]^{2+}$, E = -578.2331476
Cu 0.0107005 -0.0035178 0.4315695
O 0.0810335 1.3976162 -0.9299860
H -0.0001884 1.1032709 -1.8706772
H -0.4902925 2.1659547 -0.7962950
O -0.0678201 1.4306615 1.7818899
H -0.4419857 1.2314200 2.6510021
H 0.7173227 1.9776812 1.9264921
O -0.0239393 -1.4055601 -0.9334891
H -0.0063086 -1.0985857 -1.8738537
H 0.6133755 -2.1263764 -0.8386798
O -0.0091467 -1.3909358 1.8120874
H 0.4861455 -1.3793848 2.6402588
H -0.5311105 -2.2018843 1.7686571
O -0.0380746 0.0024371 -3.1960301
H 0.7224487 0.0012162 -3.7919684
H -0.8241501 0.0052853 -3.7578714

$[Cu(H_2O)_6]^{2+}$, E = -654.7222684
Cu 0.0000878 -0.0000852 0.0000144
O 0.0067839 1.4090870 -1.3695496
H -0.0289962 1.1020943 -2.3084286
H -0.6310606 2.1277390 -1.2641402
O -0.0073303 1.4093191 1.3693289
H 0.0290347 1.1028260 2.3083270
H 0.6293873 2.1288977 1.2634256
O -0.0141333 -1.4094469 -1.3691112
H 0.0196218 -1.1030652 -2.3081903
H 0.6223018 -2.1295725 -1.2653117
O 0.0135637 -1.4094326 1.3694430
H -0.0210108 -1.1026387 2.3084498
H -0.6231053 -2.1293532 1.2655168
O 0.0026214 0.0003291 -3.6375998
H 0.7807468 0.0205598 -4.2099102
O -0.0018027 0.0004372 3.6374732
H -0.7792629 0.0209417 4.2106628
H 0.7669671 -0.0192016 4.2223670

H -0.7654427 -0.0185057 -4.2234298

$[Cu(H_2O)_8]^{2+}$, E = -807.6923175
Cu -0.0011771 0.0007596 0.0028671
O 1.4002358 1.3230740 -0.3479025
H 2.3157860 1.0747371 -0.0950821
H 1.2130370 2.2654566 -0.1458578
O -1.3053508 1.4175526 0.3657436
H -2.2335497 1.2413218 0.1000156
H -1.0443358 2.3435860 0.1693116
O 1.3012046 -1.4158504 -0.3637370
H 2.2332039 -1.2409153 -0.1092398
H 1.0425275 -2.3431833 -0.1688415
O -1.4023777 -1.3210473 0.3577978
H -2.3163559 -1.0748890 0.0957685
H -1.2135833 -2.2641836 0.1614467
O -0.1261731 -3.6768890 0.0063307
H -0.0466154 -4.2505303 0.7790704
O 3.6121182 -0.1357944 0.2191456
H 4.0115641 -0.1584910 1.0978297
O 0.1306881 3.6779637 -0.0002595
H 0.0622136 4.2515874 -0.7740796
O -3.6072589 0.1288018 -0.2453643
H -3.9934330 0.1463408 -1.1300878
H -0.2397558 -4.2658961 -0.7504741
H -4.3520893 0.1533802 0.3689086
H 0.2387676 4.2668187 0.7574763
H 4.3478355 -0.1582794 -0.4060158

$[Cu(H_2O)_{18}]^{2+}$-5c, E = -1572.4947612
Cu -0.4093641 -0.2444167 0.2485693
O 0.5197104 0.5292896 1.8539066
O 1.3535738 -0.6926163 -0.5529461
O -1.2522025 -0.2632607 -1.5716911
O -2.2055422 0.1799483 1.0201109
H 0.2013046 1.3889611 2.2144933
H 0.6651028 -0.1177367 2.5749020
H 1.7445444 -0.0338762 -1.1789193
H 2.0484858 -1.0003500 0.0741297
H -1.3845733 -1.1467382 -1.9852024
H -0.9363114 0.3958368 -2.2327277
H -2.5073783 1.1167149 0.9238532
H -2.8695168 -0.4256856 0.6312094
O -1.0908496 3.7999074 -1.3187208
O 2.2165755 1.2077000 -2.2644052
O -2.5879383 2.8283123 0.9218267
O -0.2787757 3.0713448 2.3856260
O 1.0322078 4.4687760 0.4271768
O -0.3312324 1.8484194 -2.9844479
O 3.2195910 3.2381506 -0.6004112
H 2.8009205 0.9034950 -2.9697215
H 1.3835093 1.4989406 -2.6997407
H -3.4259716 3.2258900 1.1868115
H -1.9298905 3.0689412 1.6080057
H -0.2115776 3.4173158 3.2835329
H 0.2819416 3.6480298 1.8178904

H 1.8712922 4.0833320 0.0767413
H 1.2015822 5.4078417 0.5672386
H -0.6011791 1.9983736 -3.8981164
H -0.6465079 2.6246755 -2.4521908
H 3.8708364 3.7873881 -1.0510462
H 2.9604779 2.5480609 -1.2425521
H -1.7571691 3.5147625 -0.6682120
H -0.3456415 4.1356380 -0.7833501
O -0.7449941 -2.3564766 1.0167345
O 3.0069180 -1.9382286 1.1897674
O -3.4028769 -2.1194915 0.1381307
O -1.8752510 -2.8086469 -2.1692614
O 0.0451097 -4.2575034 -0.7787006
O 0.9950147 -1.8305548 3.1095183
O 2.7447044 -4.0235892 -0.6954955
H 3.8861972 -1.6191934 1.4258531
H 2.4937253 -1.9854626 2.0218650
H -4.2682076 -2.4821071 0.3583587
H -3.1773513 -2.4450092 -0.7522102
H -2.1691496 -3.1041059 -3.0387086
H -1.1782836 -3.4322693 -1.8808463
H 1.0319344 -4.2400364 -0.8259175
H -0.1974857 -5.1649080 -0.5587926
H 0.9817772 -2.1411589 4.0220463
H 0.2633568 -2.2762621 2.6426960
H 3.2618699 -4.8122967 -0.4976155
H 2.9554015 -3.3815245 0.0089852
H -1.7135368 -2.4610259 1.0416435
H -0.4257423 -3.0786537 0.4279123

$[Cu(H_2O)_{18}]^{2+}$-6c, E = -1572.4926114
Cu 0.2306701 0.0103763 -0.0162487
O 0.5528895 0.1225916 1.9614183
O 2.1882591 -0.2082935 -0.3101594
O -0.0628610 0.1422778 -2.0007983
O -1.7559152 -0.1025851 0.2671621
H 0.0766998 0.7759207 2.5206736
H 0.6441564 -0.7309146 2.4346035
H 2.7304605 0.5062219 -0.7148280
H 2.7202357 -0.6527795 0.3866879
H -0.0165959 -0.6719445 -2.5549481
H 0.3907677 0.8827728 -2.4505806
H -2.2435464 0.7047095 0.5352568
H -2.2333898 -0.5980177 -0.4276814
O -0.0399077 -2.4408798 0.1236834
O 3.5236996 -1.8415401 1.4348892
O -2.4151235 -2.1813816 -1.4168875
O -0.2388300 -2.23283166 -3.2836254
O 1.3705047 -3.8571419 -1.7663094
O 1.0750270 -2.4761275 2.5850257
O 3.8631447 -3.3610803 -0.96995158
H 4.2575186 -1.5909785 2.0088009
H 2.8117284 -2.1830684 2.0155155
H -3.2630710 -2.6277901 -1.5269737
H -1.9290816 -2.2723643 -2.2572211
H -0.2453166 -2.3270569 -4.2439625

H 0.4187417 -2.8731618 -2.9303721
H 2.3336385 -3.7113969 -1.5698573
H 1.2525219 -4.8124325 -1.8368638
H 0.8576410 -3.0663425 3.3160604
H 0.5472676 -2.7474629 1.8013814
H 4.6532178 -3.8947857 -1.1044043
H 3.9284994 -2.9471407 -0.0918561
H -0.9732291 -2.5709788 -0.1242431
H 0.4721238 -3.0001557 -0.5037043
O -0.0012346 2.4917101 -0.1134224
O 3.5514370 1.8813605 -1.4155324
O -2.4979103 2.3524795 1.1963415
O-0.5658502 2.2477549 3.2610561
O 1.3114829 3.7644056 1.9372407
O 1.1526954 2.5771239 -2.5562292
O 3.7622659 2.9478776 1.2312424
H 4.3282464 1.7403792 -1.9707161
H 2.8567865 2.2761141 -1.9861620
H -3.3525049 2.7999967 1.2156831
H -2.0994234 2.4315245 2.0847403
H -0.6866865 2.2885679 4.2176974
H 0.1441755 2.8856503 3.0287851
H 2.2560535 3.4960601 1.7943053
H 1.3119257 4.7270717 2.0052907
H 0.9523735 3.2078049 -3.2579536
H 0.6465804 2.8405138 -1.7557795
H 4.5960002 3.3493838 1.4988729
H 3.8447349 2.7013340 0.2927079
H -0.9444782 2.6489158 0.0762905
H 0.4798646 3.0123842 0.5699144

$[Cu(MeNH_2)H_2O)_3]^{2+}$, E = -521.2028367
Cu -0.0005160 -0.0875719 0.2319961
O 0.0069072 0.2788425 2.1723521
H 0.7930801 0.6808787 2.5649040
H -0.7722602 0.6871396 2.5724129
O 2.0021077 -0.0307116 0.3675619
H 2.5090171 -0.8528153 0.3184665
H 2.5134954 0.6476713 -0.0938026
O -2.0019140 -0.0270801 0.3792921
H -2.5071323 -0.8511643 0.3484492
H -2.5166042 0.6404527 -0.0941258
H -0.8215035 -1.1083754 -1.8865588
N -0.0063109 -0.5313426 -1.6914051
H 0.8011619 -1.1185788 -1.8883532
C 0.0002293 0.6568558 -2.5905536
H -0.8836509 1.2602362 -2.3973324
H 0.8931064 1.2478723 -2.4006333
H -0.0039319 0.3345874 -3.6309705

$[Cu(MeNH_2)H_2O)_4]^{2+}$, E = -597.6906921
Cu 0.2314310 0.1366007 -0.2185251
O -1.4491657 0.2608800 0.8459385
H -1.3525283 0.1363479 1.8205980
H -2.0378256 1.0136836 0.7056203
O 1.2543662 -0.0968228 1.4521640

H 0.7536335 -0.2269214 2.2915168
H 2.0301373 -0.6706653 1.4653491
O 1.9197229 -0.1364417 -1.2870503
H 2.3349787 -1.0080054 -1.3321920
H 2.6315168 0.5134369 -1.2066052
O -0.6275243 -0.2517016 3.3486976
H -0.8655755 -1.0939968 3.7573266
H -0.6750400 0.4125393 4.0484049
N -0.7620065 0.4421554 -1.9057928
H -0.0810860 0.7426507 -2.5995043
H -1.4094937 1.2190114 -1.7942079
C -1.4896668 -0.7610099 -2.3964114
H -2.2202537 -1.0661049 -1.6512602
H -1.9980614 -0.5343691 -3.3329415
H -0.7782117 -1.5675277 -2.5597876

$[Cu(MeNH_2)H_2O)_5]^{2+}$, E = -674.1756557
Cu 0.3262615 0.0077809 -0.1539756
O 0.2533110 2.0074671 -0.1187073
H -0.6426576 2.3958703 0.0357557
H 0.8802927 2.4992694 0.4260965
O 0.3072931 -1.9927861 -0.1669522
H 0.9681194 -2.4821013 0.3385335
H -0.5712318 -2.4100955 0.0109938
O -1.6206965 -0.0228280 0.0297034
H -2.1708504 0.7843795 0.0914846
H -2.1481521 -0.8443401 0.0981982
O -2.3514478 2.5678186 0.1889516
H -2.8139442 3.0276513 -0.5233925
H -2.6835077 2.9467175 1.0129179
N 2.2939282 0.0392533 -0.4220864
H 2.5395836 -0.7514628 -1.0142121
H 2.5189417 0.8654007 -0.9724836
C 3.1187949 0.0182432 0.8184714
H 2.8790548 0.8873752 1.4268260
H 2.9001256 -0.8851603 1.3832974
H 4.1778782 0.0369439 0.5649022
O -2.2674095 -2.6348826 0.2156987
H -2.5602348 -3.0128250 1.0547687
H -2.7392219 -3.1171485 -0.4754059

$[Cu(MeNH_2)H_2O)_7]^{2+}$, E = -827.1420392
Cu -0.0682651 -0.0057458 -0.1700022
O -0.0873045 1.9806284 -0.2307426
H 0.6483924 2.4359335 0.2471117
H -0.9405976 2.4019011 0.0089206
O -2.0372402 0.0266105 -0.2929572
H -2.5663886 -0.7758058 -0.1044271
H -2.5442389 0.8448594 -0.1082672
O -0.1481307 -1.9862506 -0.1661774
H -1.0128410 -2.3944885 0.0564030
H 0.5803951 -2.4666840 0.2945139
O 2.1071522 -2.8752951 0.9581615
H 2.1536931 -3.0399848 1.9078163
O 2.1143628 2.8138455 1.0265920
H 2.0704214 2.9742725 1.9769036

O -2.7085375 2.5812678 0.2618997
H -3.2002462 3.1257233 -0.3661203
O -2.7790772 -2.5236868 0.2563242
H -3.2583228 -3.0641322 -0.3840870
H 2.5928987 -3.5990697 0.5445491
H -3.1147475 -2.7790638 1.1248336
H -3.0286541 2.8293857 1.1382580
H 2.6361964 3.5402689 0.6647234
N 1.9298677 -0.0326606 -0.1551717
H 2.2450788 -0.8806584 0.3185788
H 2.2593342 0.7545828 0.4049674
C 2.5277069 0.0391465 -1.5161015
H 2.2223537 0.9641956 -1.9993948
H 3.6156220 0.0088213 -1.4550722
H 2.1775633 -0.8022246 -2.1104327

$[Cu(MeNH_2)H_2O)_{17}]^{2+}$-5c, E = -1591.9393107
Cu -0.5347309 -0.2715659 0.1058875
O -0.0155032 0.5373483 1.8974234
O 1.4083021 -0.6509247 -0.2324053
O -0.8664189 -0.2524061 -1.9109995
O -0.5601782 3.8943780 -1.6136236
H -0.2854060 1.4467372 2.1606630
H 0.0045207 -0.0690058 2.6609922
H 1.9285652 -0.0091141 -0.7717843
H 1.9355690 -0.8873626 0.5631243
H -0.7549839 -1.1340850 -2.3339756
H -0.3869466 0.4314488 -2.4341830
H -2.6612614 1.0787246 0.0405952
H -2.9373510 -0.4885693 -0.3884018
O -0.8322443 -2.4414189 0.7108041
O 2.6917883 -1.6962165 1.9349657
O -3.0358779 -2.6932418 -0.8965983
O -0.8431891 -2.8415567 -2.7020960
O 0.7254409 -4.1385919 -0.8010755
O 0.2375600 -1.8500095 3.2231493
O 3.2648541 -3.7446607 0.0912704
H 3.4104457 -1.2515692 2.3997524
H 1.9713208 -1.8166050 2.5867496
H -3.7699730 -3.3171327 -0.8734480
H -2.5215177 -2.9029111 -1.6964756
H -0.8020030 -3.1038618 -3.6290408
H -0.1700526 -3.3709556 -2.2289088
H 1.6765546 -4.0546576 -0.5509552
H 0.5050729 -5.0715483 -0.6936065
H 0.0165087 -2.2289554 4.0815871
H -0.3048756 -2.3135055 2.5583144
H 3.7341231 -4.5050741 0.4522359
H 3.1844043 -3.1066129 0.8255316
H -1.7167258 -2.6672347 0.3523535
H -0.2199858 -3.0518796 0.2422197
O 2.7267144 1.1701645 -1.7514444
O -2.5917777 3.0845421 0.1549651
O -0.6776565 3.1485955 2.1875461
O 1.1193337 4.4698972 0.5783389
O 0.4208796 1.8545949 -3.0400746

O 3.4456803 3.1480112 0.1000587
H 3.4411960 0.8152012 -2.2943272
H 2.0284266 1.4740333 -2.3733518
H -3.4131086 3.5860282 0.2154620
H -2.1131851 3.2382341 0.9931384
H -0.8057866 3.5237674 3.0668932
H 0.0235940 3.6845854 1.7527766
H 2.0039049 4.0529002 0.4447631
H 1.2831373 5.4018055 0.7657087
H 4.1892904 3.6760464 -0.2115563
H 3.2941434 2.4675973 -0.5858548
N -2.5045705 0.1055275 0.3168968
C -3.1457290 -0.1360532 1.6305722
H -2.7201015 0.5336995 2.3728401
H -4.2206727 0.0380983 1.5682736
H -2.9729313 -1.1630920 1.9435496
H 0.0400602 2.6587626 -2.5988718
H 0.3606732 1.9956811 -3.9923329
H -1.3678166 3.6496332 -1.1217618
H 0.0676108 4.1852742 -0.9237096

$[Cu(MeNH_2)H_2O)_{17}]^{2+}$-6c, E = -1591.9350804
Cu -0.5967258 -0.0204848 -0.0942999
O -0.4017958 0.8195661 1.7523539
O 1.3968409 -0.3342258 -0.1078445
O -0.6953786 -0.6572967 -2.0553805
H -0.6896187 1.7334413 1.9665659
H -0.3660621 0.2626744 2.5524982
H 1.9973420 0.1667632 -0.7028369
H 1.8370241 -0.4515522 0.7611131
H -0.5308305 -1.6134212 -2.2163163
H -0.1370969 -0.1345467 -2.6662493
H -2.8670852 0.9908395 -0.5563139
H -2.9191824 -0.6396140 -0.7397123
O -0.8015587 -2.2247724 0.8821389
O 2.5237213 -1.0685925 2.2865839
O -2.8896582 -2.9539410 -0.7609398
O -0.5441268 -3.3586501 -2.3013676
O 0.9879963 -4.1069470 -0.1237407
O -0.0187366 -1.3524596 3.3673416
O 3.4092741 -3.2704023 0.7806646
H 3.1600176 -0.5325338 2.7744686
H 1.7529031 -1.1930197 2.8776812
H -3.5745871 -3.6200227 -0.6356388
H -2.2947437 -3.2989779 -1.4503640
H -0.4123762 -3.7684810 -3.1640549
H 0.1263251 -3.7423274 -1.6997415
H 1.9079679 -3.8733749 0.1478441
H 0.8343862 -5.0021362 0.2008606
H -0.3210595 -1.6781357 4.2224765
H -0.4583545 -1.8891451 2.6775603
H 3.9441238 -3.9049584 1.2706077
H 3.2107549 -2.5472963 1.4064740
H -1.6423553 -2.5616838 0.5108070
H -0.1265641 -2.8659716 0.5746761
O -0.3905790 2.2544936 -1.1218666

O 3.0191964 1.0459936 -1.8242180
O -2.8369750 3.1650655 -0.2542644
O -1.0584147 3.4550322 1.9505621
O 1.0773241 4.1318317 0.3077648
O 0.7632125 1.2999776 -3.3633861
O 3.5813843 3.1069830 0.0143168
H 3.7671239 0.5496956 -2.1781881
H 2.3998260 1.1835770 -2.5719020
H -3.3734713 3.8940783 -0.5847564
H -2.4573385 3.4623884 0.5922023
H -1.2083332 3.8830508 2.8015216
H -0.2503303 3.8568380 1.5736953
H 2.0214691 3.8478678 0.2818366
H 1.0542412 5.0102373 -0.0896923
H 0.6120620 1.6304431 -4.2561889
H 0.2744108 1.8877620 -2.7469043
H 4.2886492 3.6984489 -0.2667677
H 3.4999356 2.4364054 -0.6909316
H -1.2871601 2.6391278 -1.0480028
H 0.1841519 2.8930454 -0.6506203
N -2.6256378 0.1069229 -0.1124936
C -3.3750802 -0.0035968 1.1622044
H -3.1237553 0.8346146 1.8054033
H -4.4497089 -0.0013962 0.9750032
H -3.1051592 -0.9269699 1.6683890

$[Cu(OH)(H_2O)_3]^+$, E = -501.3127813
Cu 0.0068586 -0.0527844 0.0026992
O 1.9348328 0.5616549 0.0188616
H 2.2640584 1.1138663 -0.7028967
H 2.4859026 -0.2340846 0.0323184
O -0.5861135 1.8559651 0.0536501
H -1.2981098 2.1406970 -0.5336860
H 0.0480869 2.5819309 0.1069682
O -1.9573265 -0.5018779 -0.0576983
H -2.1885828 -1.3894821 -0.3611094
H -2.4851012 -0.3354280 0.7352967
O 0.6542519 -1.7979291 -0.0028833
H 0.0168847 -2.4201296 0.3635946

$[Cu(OH)(H_2O)_4]^+$-4c-A, E = -577.7984618
Cu 0.0114883 0.0610262 0.4616863
O 0.0670623 1.4081776 -1.0245866
H -0.0370129 1.0594767 -1.9388058
H -0.5110446 2.1753111 -0.9318396
O -0.0415509 1.3236524 1.8350780
H 0.2586009 2.1885217 1.5366040
O 0.0138048 -1.4233171 -0.8748129
H 0.0377287 -1.1705744 -1.8246424
H 0.6266561 -2.1578835 -0.7469801
O 0.0005083 -1.3589562 1.9112649
H -0.0512663 -0.9049356 2.7640667
H -0.7026482 -2.0220049 1.9044347
O -0.0524838 -0.1211141 -3.2464911
H 0.6988384 -0.1167284 -3.8531398
H -0.8431092 -0.1750163 -3.7984158

$[Cu(OH)(H_2O)_4]^+$-4c-B, E = -577.7969052
Cu 0.0256884 -0.3786594 -0.0077920
O 1.3913186 0.9013900 -0.1498837
H 2.1861743 0.6380172 0.3259072
O -1.4026765 1.0300554 0.0190163
H -2.0612284 0.9610211 0.7218937
H -1.0089204 1.9484999 0.0632927
O 1.2686455 -1.9726902 0.0835486
H 2.1252980 -1.8636112 -0.3501518
H 1.4484060 -2.3545890 0.9538041
O -1.4521280 -1.7303638 -0.0326556
H -2.2861054 -1.4928904 -0.4587777
H -1.2178270 -2.6128447 -0.3495427
O 0.0858331 3.1819201 0.0969991
H 0.1260894 3.7576105 -0.6747313
H 0.7990427 2.5028344 -0.0107376

$[Cu(OH)(H_2O)_4]^+$-5c, E = -577.7932255
Cu -0.0199826 -0.1365248 0.1540670
O 1.8975907 -0.8370392 0.2723588
H 2.6097256 -0.1865729 0.2250227
H 2.1310789 -1.5613439 -0.3215947
O 0.7384314 1.6414175 0.8116925
H 0.6062294 2.3690696 0.1903553
H 0.5561365 1.9833225 1.6958088
O -1.9623269 0.4666575 0.4850032
H -2.4593384 -0.3642434 0.4856432
H -2.1974506 0.9335148 1.2971797
O -0.7243418 -1.8323543 -0.2685697
H -0.3626007 -2.4982830 0.3264946
O 0.0809719 0.9553839 -1.8539972
H 0.6643663 0.5966171 -2.5332772
H -0.7698422 1.0791542 -2.2918024

$[Cu(OH)(H_2O)_5]^+$-4c, E = -654.2826563
Cu -0.0435379 0.0192997 -0.0507539
O 1.4067911 0.0929814 1.3253535
H 1.1327124 -0.0030763 2.2657424
H 2.1754937 -0.4739041 1.1856098
O -1.4100335 0.1183040 1.4192697
H -2.1886453 -0.4382608 1.2945067
H -1.0845362 -0.0181056 2.3374339
O -1.3659091 -0.1001390 -1.3876532
H -2.1645157 0.3800945 -1.1454145
O 1.4249161 -0.0749936 -1.4187853
H 2.1316288 0.5772480 -1.3343046
H 1.0676888 -0.0149275 -2.3493079
O 0.0769070 -0.0891227 3.6680306
H 0.1055140 -0.8971893 4.1958945
H 0.0909395 0.6439604 4.2966595
O 0.0085543 -0.0553173 -3.6319763
H -0.0403266 0.7403628 -4.1731252
H -0.7230898 0.0060211 -2.9653874

$[Cu(OH)(H_2O)_5]^+$-5c, E = -654.2774283
Cu 0.0360029 -0.3957606 0.1943360

O 1.5069227 0.7187134 0.6601214
H 1.6770540 0.6665104 1.6076939
O -1.4029823 0.9035954 0.9315160
H -1.5127638 0.9091240 1.8909695
H -1.0910645 1.8014267 0.6794240
O 1.3268524 -1.9419725 -0.1965150
H 2.2181465 -1.6132254 -0.0144940
H 1.2306904 -2.7618352 0.3059584
O -1.4860584 -1.7021851 -0.0777027
H -2.3579425 -1.2860444 -0.0859296
H -1.4594957 -2.2997530 -0.8360201
O 0.1399595 2.8133882 -0.2071126
H 0.3876468 3.7360866 -0.0879528
H 0.8578408 2.2465374 0.1790190
O -0.2423307 0.5755661 -1.8451832
H 0.3774704 0.3252154 -2.5398533
H -0.0949699 1.5238339 -1.6846768

$[Cu(OH)(H_2O)_7]^+$-4c, E = -807.2487004
Cu -0.0728861 0.0056986 -0.3243778
H -2.2981220 0.2016163 -1.2386175
O 0.1603152 1.9899912 -0.3809390
H -0.6097732 2.4613122 0.0262564
O -0.1967422 -1.9887351 -0.3685959
H -1.0391202 -2.3083763 0.0423025
O 1.9089130 -0.1692845 -0.2651101
H 2.4094523 0.5906352 0.1015957
H 2.2705533 -1.0087782 0.0899746
O -1.9866178 0.1799114 -0.3254105
H -2.6448274 -1.2937521 0.3600009
H -2.3726063 1.7491048 0.3480318
O -2.1820460 2.6574505 0.6910179
O -2.6245069 -2.2214314 0.7017215
H -2.7972933 3.2538944 0.2506883
H -3.3325581 -2.6970403 0.2536586
H 0.5614261 -2.4701721 0.0207603
H 0.9944000 2.3353958 -0.0030349
O 2.2958431 -2.7492734 0.5118672
H 2.8299584 -3.3354147 -0.0386472
H 2.4878494 -2.9949542 1.4253647
O 2.7391640 2.2934958 0.5289595
H 2.9306309 2.5082864 1.4503850
H 3.3899676 2.7740273 0.0020990

$[Cu(OH)(H_2O)_7]^+$-5c, E = -807.2447638
Cu 0.1644842 -0.3747341 0.5417265
H 1.7699607 0.1757212 -1.1957789
O 0.9627595 1.3497686 1.3001486
H 1.9036746 1.3171681 1.5120286
H 0.8108418 2.1687982 0.7490609
O -0.2565055 -2.3599506 0.2229764
H -0.0392576 -2.6251415 -0.7096696
H 0.1992706 -2.9780046 0.8074797
O -0.3398052 -0.7517100 2.4740073
H -0.3860033 0.0491948 3.0125802
H -1.1449634 -1.2544315 2.6517021

O 0.8540960 -0.1222013 -1.2364570
H 0.6963405 -1.5850460 -2.1416914
H -0.0563662 3.0603197 -1.0103874
O 0.4556120 3.4259097 -0.2586771
O 0.3772106 -2.5002488 -2.3457701
H -0.0724090 4.1428968 0.1102354
H 1.1458006 -3.0023317 -2.6381454
O -1.8846973 0.4561599 0.0640482
H -1.8089852 0.9738750 -0.7616695
H -2.5948615 -0.1790893 -0.0815842
H -0.1042673 1.0673880 -1.9643450
O -0.7807547 1.7886061 -2.0770083
H -0.9719091 1.8731813 -3.0172366

$[Cu(OH)(H_2O)_7]^+$-6c, E = -807.2368402
Cu -0.0061762 -0.4449916 0.0018358
H 2.2249121 0.5824219 -0.0123225
O -0.1813935 -0.5067923 2.1146755
H 0.4926766 -1.0652188 2.5205452
H -0.0217316 0.4070431 2.4369130
O -0.1951068 -0.5259386 -2.1090538
H -0.0324132 0.3846780 -2.4393585
H 0.4760471 -1.0899679 -2.5121580
O -1.4896224 -1.8313611 0.0144947
H -2.0590742 -1.7893624 0.7936098
H -2.0692811 -1.7961400 -0.7574527
O 1.3338683 0.9468021 -0.0097824
H 0.8622926 1.8881919 -1.3866860
H 0.8674322 1.9117042 1.3711540
O 0.2381776 2.1539359 2.0954342
O 0.2343010 2.1325526 -2.1132397
H 0.6515559 2.8365242 2.6341256
H 0.6586334 2.7994603 -2.6629429
O -1.5572409 1.3542056 -0.0011039
H -1.2847575 1.8772669 -0.7717368
H -1.2788648 1.8843237 0.7627705
O 1.4476844 -2.1796213 0.0013320
H 2.4111189 -2.1790861 0.0083248
H 1.1785796 -3.1049390 0.0144648

$[Cu(OH)(H_2O)_{17}]^+$-5c, E = -1572.0447568
Cu -0.2575155 -0.2661004 0.1912706
O 0.7733020 0.5808817 1.7336418
O 1.4087113 -0.6342160 -0.6848597
O -1.3121783 -0.3821746 -1.5415776
O -2.0092048 0.1458704 1.1270073
H 0.4314320 1.4169904 2.1191950
H 0.9287168 -0.0773422 2.4428706
H 1.9506130 0.7582089 -1.5551658
H 2.4895145 -1.4985394 0.3060310
H -1.4988802 -1.2584483 -1.9418115
H -1.0602377 0.2797927 -2.2239801
H -2.3496404 1.0693347 1.0792674
H -2.6997726 -0.4663985 0.8038136
O -1.3341719 3.7693323 -1.2489010
O 2.1455982 1.5422523 -2.1274632

O -2.5721909 2.7875894 1.1161216
O -0.1582834 3.1075301 2.3698766
O 0.8220747 4.6706644 0.3398399
O -0.5757626 1.8099591 -2.9663987
O 3.0814899 3.6681724 -0.7380696
H 1.2926694 1.7305780 -2.5576364
H -3.3997992 3.1331206 1.4723141
H -1.8622184 3.0442903 1.7431917
H -0.0255947 3.4401704 3.2658032
H 0.2926310 3.7396942 1.7660263
H 1.6915334 4.3926608 -0.0455784
H 0.8792348 5.6219321 0.4860305
H -0.8658042 1.9776393 -3.8693899
H -0.9083485 2.5609871 -2.4167978
H 3.6106639 4.2248751 -1.3201197
H 2.7833970 2.9005452 -1.2861025
H -1.9181601 3.4540988 -0.5352809
H -0.5679442 4.1561350 -0.7816357
O -0.6473508 -2.4130657 1.0930624
O 3.0713196 -2.0972211 0.8451308
O -3.3497396 -2.1396483 0.3684385
O -2.0278505 -2.9631028 -2.0132150
O -0.0373599 -4.4189093 -0.7056511
O 1.1846777 -1.7579598 3.0633028
O 2.6690487 -4.2903598 -0.7429882
H 2.6471602 -2.1278243 1.7172180
H -4.1972974 -2.4926476 0.6626051
H -3.1823125 -2.5034243 -0.5209916
H -2.3931827 -3.2971433 -2.8402304
H -1.3230612 -3.5866470 -1.7449107
H 0.9481761 -4.4445902 -0.7840404
H -0.3048844 -5.3041628 -0.4304727
H 1.1399539 -2.0181344 3.9902658
H 0.4380919 -2.1950332 2.6104770
H 3.1721952 -5.0723702 -0.4899268
H 2.9078731 -3.5806468 -0.1004232
H -1.6182120 -2.4731019 1.1501957
H -0.3797451 -3.1622024 0.5172841
H 1.2142245 -1.2123097 -1.4326834

$[Cu(OH)(H_2O)_{17}]^+$-4c, E = -1572.0420672
Cu -0.1494144 -0.0369076 -0.0114670
O 0.5226233 0.5655048 1.7788377
O 1.6457839 -0.3074994 -0.5899233
O -0.8987402 -0.2881990 -1.8403841
O -2.0040795 -0.0850524 0.7324902
H 0.0383981 1.3285201 2.1699936
H 0.4874174 -0.2034416 2.3935056
H 2.2802397 1.2106418 -1.2308131
H 2.4978834 -1.3233145 0.5309087
H -0.9491565 -1.1950967 -2.2184875
H -0.5797140 0.3784689 -2.4921770
H -2.4883876 0.7755478 0.7419950
H -2.5707129 -0.7786481 0.3249591
O -1.3674212 3.6029073 -1.2516914
O 2.4896739 2.0442341 -1.7140111

O -2.9112616 2.4325587 0.8694829
O -0.7260017 2.8955182 2.4820303
O 0.3304782 4.7119907 0.7228472
O -0.0739442 1.9883873 -3.0241178
O 2.8580649 4.1425743 -0.0289737
H 1.7263552 2.1598612 -2.3062739
H -3.8213023 2.6631173 1.0903655
H -2.3515583 2.7250365 1.6181075
H -0.2765805 3.6210379 1.9914255
H 1.2814143 4.5990860 0.4747207
H 0.2056152 5.6489802 0.9139294
H -0.5925988 2.6265469 -2.4788654
H 3.3820401 4.8216454 -0.4677557
H 2.7742689 3.3991648 -0.6734815
H -2.0480940 3.2168151 -0.6737500
H -0.7606971 4.0663799 -0.6423618
O -1.0787181 -3.4888021 1.4922131
O 2.9007719 -1.9868115 1.1432598
O -3.1105759 -2.3579936 -0.2077004
O -1.3668471 -2.9054831 -2.3101411
O 0.1482468 -4.6342928 -0.7974517
O 0.6199665 -1.8847008 2.9116548
O 2.7854958 -4.2967404 -0.2986767
H 2.2735775 -2.0397508 1.8844876
H -4.0510361 -2.5691973 -0.2283806
H -2.7370908 -2.6275217 -1.0701985
H -0.7596925 -3.5705468 -1.9151989
H 1.1256358 -4.5651377 -0.6596399
H -0.0369063 -5.5690154 -0.9471050
H -0.0398309 -2.4865598 2.4946413
H 3.2408976 -5.0109676 0.1603893
H 2.8940551 -3.4919393 0.2634221
H -1.8911937 -3.1366312 1.0904668
H -0.6372949 -3.9756002 0.7696336
H 1.6207439 -0.7993343 -1.4191866
H -0.2304367 2.2187588 -3.9470927
H -1.5871006 -3.2206710 -3.1944738
H -0.7340572 3.1538792 3.4113330
H 0.6144243 -2.0743291 3.8567597

$[Cu(OH)(H_2O)_{17}]^+$-6c, E = -1572.0412073
Cu -0.3704782 -0.0020040 -0.0086210
O 0.1408990 0.8725029 1.7632325
O 1.4995465 -0.2750276 -0.4077346
O -0.9090294 -0.7034932 -1.8572598
O -2.3373333 0.0430067 0.5193206
H -0.3961123 1.6359583 2.0614396
H 0.2284029 0.2294498 2.4978566
H 2.2800006 0.9815904 -1.2042610
H 2.3953944 -0.9794759 0.8518735
H -0.9481892 -1.6670773 -2.0465306
H -0.4553649 -0.2312730 -2.5850887
H -2.8187443 0.8913912 0.4146233
H -2.8556333 -0.6836512 0.1230971
O -0.7094110 -2.3281812 1.1239236
O 2.8920675 -1.4951350 1.5416900

O -3.2394332 -2.4645944 -0.1984515
O -1.2976375 -3.3829288 -2.0511043
O 0.4734043 -4.4646621 -0.2181537
O 0.5828480 -1.3353368 3.2919636
O 3.0837660 -3.8564878 0.1716536
H 2.2954136 -1.5058093 2.3075158
H -4.0983111 -2.8796599 -0.0638505
H -2.8216060 -2.9156854 -0.9548772
H -1.4141234 -3.8150358 -2.9051429
H -0.6213759 -3.8977688 -1.5642074
H 1.4489113 -4.3413563 -0.1208684
H 0.2751852 -5.3452232 0.1211715
H 0.3609218 -1.5599739 4.2021297
H 0.0080867 -1.8761234 2.7098375
H 3.6646134 -4.4957438 0.5988755
H 3.0864624 -3.0521798 0.7439897
H -1.6613544 -2.4689630 0.9930534
H -0.2777173 -3.1029622 0.7102527
O -0.7478418 2.2575789 -1.0329244
O 2.7144284 1.6742445 -1.7723359
O -3.1738942 2.6131091 0.3837322
O -1.1709755 3.2733479 2.1941444
O 0.4512308 4.4139552 0.2750021
O 0.2574152 1.2853727 -3.3855777
O 3.0325844 3.9647277 -0.3452841
H 2.1214374 1.7389498 -2.5357700
H -4.0591532 2.9923009 0.3542864
H -2.7081168 3.0124205 1.1446832
H -1.2464199 3.6591461 3.0745025
H -0.5478092 3.8383477 1.6923457
H 1.4278109 4.3282995 0.1450351
H 0.2082147 5.2813952 -0.0682694
H -0.0667895 1.5857096 -4.2418790
H -0.1904031 1.8360113 -2.7102492
H 3.6955055 3.8150591 0.3368029
H 2.9758014 3.1280267 -0.8681273
H -1.6830567 2.4642831 -0.8684459
H -0.2621201 3.0096237 -0.6354195
H 1.5282199 -0.9439586 -1.1008501

$[Cu(OH)_2(H_2O)_2]$-cis, E = -500.8638308
Cu 0.0903788 -0.0000015 0.0006751
O 1.2813955 1.4769930 -0.0050788
H 2.1839048 1.1936552 0.1688758
O -1.3998884 1.4211215 0.0393430
H -2.1002285 1.3958517 -0.6246637
H -0.9546671 2.2737671 -0.0587363
O -1.4044805 -1.4148053 -0.0401755
H -0.9573917 -2.2680468 0.0438683
H -2.0975172 -1.3979009 0.6317878
O 1.2741469 -1.4829485 0.0036450
H 2.1782356 -1.2029560 -0.1677166

$[Cu(OH)_2(H_2O)_2]$-trans, E = -500.8636915
Cu -0.0002728 0.0004222 -0.0006357
O 2.0188380 -0.4743167 0.0557036

H 2.4733212 0.3589195 -0.1317293
H 2.3491956 -1.1189609 -0.5825321
O 0.6069128 1.7838704 0.0015456
H -0.1029582 2.4150416 -0.1464037
O -2.0197221 0.4715451 -0.0473655
H -2.4694598 -0.3580900 0.1659055
H -2.3473477 1.1317685 0.5761773
O -0.6050915 -1.7839140 -0.0109817
H 0.0995674 -2.4106045 0.1760849

$[Cu(OH)_2(H_2O)_4]$-cis, E = -653.8332547
Cu -0.0784576 0.0000877 0.0002517
O -1.3421909 -1.4282668 -0.1599735
O 1.4402696 -1.3680797 -0.1015560
O 1.4402831 1.3678738 0.1023096
H 2.1672922 1.2491466 -0.5203013
O -1.3422836 1.4284656 0.1607328
H -2.2034188 1.1728818 -0.1824732
H -0.6828417 2.9302143 -0.0259656
O 0.0349757 3.6157433 -0.1328266
H 1.1094273 2.2980439 0.0026028
H 2.1673266 -1.2508325 0.5212251
H 1.1089205 -2.2983391 -0.0033797
H -2.2035049 -1.1724493 0.1826003
O 0.0347574 -3.6159769 0.1305617
H -0.0268112 -4.2044489 -0.6295880
H -0.6832354 -2.9307086 0.0244409
H -0.0265703 4.2047835 0.6269069

$[Cu(OH)_2(H_2O)_4]$-trans, E = -653.8329916
Cu 0.0007496 -0.0618618 -0.0006210
O 1.3274383 -0.0395691 1.3601874
O -1.4426568 -0.0825527 1.4641481
O -1.3300036 -0.0115419 -1.3580232
H -2.1579470 -0.4185511 -1.0875807
O 1.4475678 -0.0574130 -1.4623138
H 2.1541370 0.5861705 -1.3338214
H 1.0668599 0.0859787 -2.3664468
O -0.0875429 0.1200088 -3.6374831
H -0.2102186 0.9605589 -4.0914521
H -0.7624438 0.0873218 -2.9030099
H 2.1704126 -0.4007115 1.0723368
H -1.0639605 0.0747214 2.3668714
H -2.1641455 0.5432684 1.3307178
O 0.0853046 0.2463148 3.6265751
H 0.1542713 -0.4871812 4.2469383
H 0.7640750 0.0863648 2.9142628

$[Cu(OH)_2(H_2O)_6]$-trans, E = -806.7959026
Cu -0.0000226 0.0000248 -0.4069825
O 1.8987322 0.4031113 -0.3633708
O -0.4177631 1.9863318 -0.3503129
O -1.8987414 -0.4030029 -0.3631890
O 0.4177506 -1.9862619 -0.3504483
H -0.2920603 -2.4929658 0.1060532
O -1.8921605 -2.7845788 0.8248016

H -2.4701275 -3.4355479 0.4125653
H -2.1105030 -1.9089742 0.4083117
H 0.2921790 2.4929674 0.1060787
O 1.8923488 2.7841068 0.8248707
H 2.4704842 3.4350103 0.4127672
H 2.1104433 1.9085376 0.4081991
H 2.2187443 0.5129770 -1.2666197
H -2.2187450 -0.5130167 -1.2664185
H 1.2825825 -2.1675657 0.0836479
H -1.2825141 2.1675955 0.0839416
O 2.9488803 -1.8384776 0.5962268
O -2.9489572 1.8387070 0.5961836
H 2.7251231 -0.9105865 0.3159270
H 3.1413332 -1.8029205 1.5393702
H -2.7252774 0.9108353 0.3157389
H -3.1416643 1.8031158 1.5392736

$[Cu(OH)_2(H_2O)_6]$-cis, E = -806.7929588
Cu 0.0825533 0.0210109 0.3621303
O -0.0013850 1.9657828 0.4200804
O 1.9924952 -0.0793195 0.3846688
O 0.0203349 -2.0127879 0.3184593
O -1.9455729 -0.0743148 0.2946732
H -2.3388466 -0.8362155 -0.1725172
H 2.3507596 0.7612196 0.0746971
O 2.1441920 2.7094565 -1.0355050
H 2.4258633 3.5925723 -0.7758834
H 1.3145908 2.5327042 -0.5238124
H 0.2256836 2.2511695 1.3126808
H -2.3596635 0.7608157 -0.0249974
O -2.4847004 2.4931501 -0.2943352
H -1.5158440 2.4885116 -0.0591670
H -2.5479661 2.8174531 -1.1990714
H -0.7377115 -2.4179158 -0.1446051
H 0.8593776 -2.4064219 -0.0198997
H 2.5464059 -1.5174015 -0.1865348
O 2.5458638 -2.4711590 -0.4884595
H 3.1440939 -2.9474355 0.0971365
O -2.4557642 -2.5636816 -0.8027601
H -3.0631952 -3.1687840 -0.3596989
H -2.5783761 -2.7129502 -1.7482312

$[Cu(OH)_2(H_2O)_{16}]$-cis-4c, E = -1571.5902416
Cu -0.1039797 -0.0298645 0.1391406
O 0.4588890 0.5462591 1.8865152
O 1.7210545 -0.2719626 -0.4605604
O -0.8368512 -0.2654652 -1.7285964
O -2.0171407 -0.1315621 0.8155551
H -0.3100082 2.0522986 2.2553084
H 0.4460036 -1.0875009 2.6537639
H 2.2943291 1.2467974 -1.1193175
H 2.4873222 -1.4227167 0.5982481
H -0.8942755 -1.1548344 -2.1407074
H -0.5367800 0.4155249 -2.3701285
H -2.4916628 0.7294583 0.7518339
H -2.5448939 -0.8133255 0.3475182

O -1.4323117 3.7266173 -1.2907972
O 2.4840585 2.0773753 -1.6206835
O -2.9020867 2.4255803 0.7817874
O -0.8095602 2.8985923 2.3908486
O 0.3087799 4.8387956 0.6301369
O -0.0631323 2.0508539 -2.9345711
O 2.8694044 4.2324591 -0.0213515
H 1.6991292 2.1863570 -2.1863813
H -3.7833763 2.6829788 1.0759865
H -2.2641021 2.6963328 1.4911700
H -0.3238111 3.5845326 1.8969397
H 1.2639543 4.7175838 0.4120262
H 0.1982669 5.7663630 0.8682546
H -0.6065762 2.6999158 -2.4247050
H 3.4070506 4.8819489 -0.4874338
H 2.7843177 3.4573887 -0.6282224
H -2.0718184 3.2852214 -0.7023785
H -0.8162073 4.1843886 -0.6849884
O -1.1720257 -3.6327659 1.3912203
O 2.8299512 -2.1461764 1.1807231
O -3.1214285 -2.3642541 -0.3141970
O -1.3143445 -2.8539238 -2.3898513
O 0.1382288 -4.6655810 -0.9137547
O 0.5874984 -2.0249270 2.9192862
O 2.7830726 -4.3018012 -0.4668293
H 2.1499480 -2.2232708 1.8791919
H -4.0651632 -2.5502580 -0.3770712
H -2.7285134 -2.5915473 -1.1794349
H -0.7342756 -3.5481646 -2.0037654
H 1.1175679 -4.5975600 -0.7925679
H -0.0467797 -5.5928343 -1.1037186
H -0.0779314 -2.5463229 2.4299155
H 3.2733544 -5.0385523 -0.0859441
H 2.8573938 -3.5559184 0.1788132
H -1.9596344 -3.2435684 0.9755862
H -0.6953286 -4.0571561 0.6530385
H 1.6788856 -0.7424408 -1.3011330
H 1.4031295 0.7296936 1.8214819
H -0.1897209 2.2550759 -3.8683323
H -1.4929732 -3.1155660 -3.3004720

$[Cu(OH)_2(H_2O)_{16}]$-cis-5c, E = -1571.5886805
Cu -0.2067678 -0.2241065 0.3097822
O 0.6777328 0.5503425 1.8686508
O 1.5011746 -0.5627420 -0.5648915
O -1.2080128 -0.3466920 -1.4894878
O -2.0501070 0.0969426 1.1591105
H 0.0673210 2.1233334 2.2186153
H 0.9322427 -0.9419743 2.8125088
H 2.0116211 0.8079739 -1.4649987
H 2.4917516 -1.5274518 0.4236458
H -1.3863301 -1.2072269 -1.9219618
H -0.9622112 0.3301078 -2.1565621
H -2.3954515 1.0143473 1.0693113
H -2.7019831 -0.5100459 0.7602674
O -1.3402855 3.8413436 -1.2266969

O 2.2117142 1.5745975 -2.0629827
O -2.6424439 2.7361014 1.0453160
O -0.3240492 3.0286747 2.3429002
O 0.8285015 4.7145012 0.3518204
O -0.5018824 1.8867399 -2.9182014
O 3.1276634 3.7458726 -0.7270271
H 1.3575071 1.7716447 -2.4867578
H -3.4405641 3.0892322 1.4548405
H -1.8825497 2.9527543 1.6461392
H 0.1847329 3.6218570 1.7622123
H 1.6940721 4.4343770 -0.0305374
H 0.9005016 5.6596185 0.5282865
H -0.7812432 2.0424160 -3.8274377
H -0.8599043 2.6337579 -2.3783963
H 3.6208960 4.3100783 -1.3324661
H 2.8489035 2.9552653 -1.2512637
H -1.9342243 3.4866448 -0.5395674
H -0.5729085 4.1931081 -0.7330306
O -0.7478575 -2.5274342 0.9952602
O 2.9934843 -2.1854512 0.9756581
O -3.3902754 -2.1353051 0.1284173
O -1.9294195 -2.8893077 -2.1897568
O -0.0260948 -4.4760500 -0.8732048
O 1.0517853 -1.8752249 3.1114605
O 2.6790626 -4.3016051 -0.7223929
H 2.4822934 -2.2274765 1.8041835
H -4.2421366 -2.5205654 0.3611362
H -3.1657340 -2.4564231 -0.7635366
H -2.2273368 -3.1498928 -3.0686242
H -1.2550161 -3.5427887 -1.9181796
H 0.9608334 -4.4980814 -0.8927446
H -0.3111635 -5.3722426 -0.6604273
H 0.3789851 -2.3397377 2.5871868
H 3.1818443 -5.0810300 -0.4626478
H 2.8656593 -3.6094511 -0.0430926
H -1.7195458 -2.5473664 0.9479043
H -0.4502766 -3.2389405 0.3943552
H 1.5850037 0.7108716 1.5854762
H 1.3032568 -1.1331638 -1.3161725

$[Cu(OH)_3(H_2O)]^-$, E = -500.4014314
Cu 0.1925988 0.4928235 0.0399448
O -0.2662656 2.2612550 -0.3388569
O 1.5043248 -0.8579499 0.1466046
O -0.4123392 -2.7912338 -0.4061688
H 0.4276497 -2.3021894 -0.2770301
O -1.4666558 -0.3905878 0.4484300
H -2.1922756 0.2129859 0.2570380
H -1.0492004 -2.0862889 -0.1718716
H 1.8137383 -0.9865623 1.0491714
H -0.9673697 2.3258491 -0.9945358

$[Cu(OH)_3(H_2O)_3]^-$, E = -653.3649027
Cu 0.0291300 0.0029994 -0.1267468
O -1.3679045 -1.3393921 -0.2877825
O 1.3933791 -1.5854474 -0.2360173

O 1.6012430 1.0896594 0.0541727
O -1.1847698 1.5237987 -0.0129964
H -2.0311198 1.3178942 -0.4207947
H -0.6026539 3.0318013 0.1630792
O -0.1366969 3.9086940 0.2771338
H 1.3173532 2.0091015 0.0983739
H 2.1828871 -1.3475679 0.2633247
H 1.0213616 -2.4142160 0.1412431
H -2.2047919 -0.9818538 0.0211149
O -0.3030741 -3.5273277 0.5980904
H -0.4661241 -4.2697342 0.0069851
H -0.8774473 -2.7665878 0.2721112
H -0.2102985 4.1212261 1.2126643

$[Cu(OH)_3(H_2O)_{15}]^-$, E = -1571.132226
Cu -0.1201440 -0.0075075 -0.0685591
O 0.4006214 0.4928801 1.7330459
O 1.7427549 -0.3183037 -0.5918555
O -0.7068480 -0.2120569 -1.9188480
O -2.0721536 -0.0920897 0.5919848
H -0.3928662 1.9228549 2.1647329
H 0.3447334 -1.0860728 2.4972290
H 2.3719645 1.2269174 -1.0575440
H 2.4110762 -1.4574299 0.4796426
H -0.9066926 -1.9372211 -2.2073030
H -0.1353065 1.3433601 -2.5779557
H -2.5766954 0.7497193 0.5531318
H -2.6136102 -0.8218908 0.2231160
O -1.4002737 3.9652502 -1.2010553
O 2.5926316 2.1080818 -1.4555666
O -2.9706903 2.4733166 0.6816082
O -0.9032568 2.7559893 2.3639741
O 0.3348536 4.8401660 0.8669213
O 0.1491248 2.2539254 -2.8324642
O 2.8953492 4.1462154 0.2905575
H 1.8073810 2.2922717 -2.0115338
H -3.8419862 2.7381211 0.9978080
H -2.3265406 2.6550633 1.4147166
H -0.3974246 3.4847086 1.9605627
H 1.2893573 4.6797479 0.6728183
H 0.2700810 5.7446314 1.1936481
H -0.4183421 2.8522826 -2.3069710
H 3.4775356 4.7968057 -0.1167364
H 2.8290590 3.3951174 -0.3518514
H -2.0632126 3.4781019 -0.6797126
H -0.7966532 4.3437486 -0.5335464
O -1.2991901 -3.7296216 1.4449464
O 2.7432580 -2.1437526 1.1194231
O -3.1354578 -2.4342477 -0.3428197
O -1.2782870 -2.8514642 -2.2825837
O 0.1690667 -4.7663925 -0.7496622
O 0.4752763 -2.0089944 2.8278213
O 2.8258433 -4.4584887 -0.2654037
H 2.0373052 -2.2005742 1.7938000
H -4.0560806 -2.6483496 -0.5306138
H -2.6113962 -2.6597210 -1.1497082

H -0.6553768 -3.4596950 -1.8448457
H 1.1446472 -4.7328495 -0.6019350
H -0.0303557 -5.6691957 -1.0229791
H -0.1924309 -2.5595039 2.3743683
H 3.2684965 -5.1391309 0.2531583
H 2.8565867 -3.6310075 0.2793799
H -2.0489430 -3.3186792 0.9806454
H -0.7796519 -4.1548007 0.7358708
H 1.6854500 -0.7318519 -1.4609661
H -1.6520316 -0.0257093 -1.9420355
H 1.3450634 0.6794749 1.6986260