

Supporting Information for

# Computational Insights on the Chemical Reactivity of Functionalized and Crosslinked Polyketones to Cu<sup>2+</sup> Ion for Wastewater Treatment

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**Table S1.** Calculated complexation energies and adsorption Gibbs free energies at 298K (in eV)

Complex	$\Delta E_{\text{com}}$	$\Delta G_{\text{ads}}$
<b>[Cu(H<sub>2</sub>O)<sub>5</sub>]<sup>2+</sup></b>		
<b>A2P-Cu(II)</b>	-0.69	-0.67
<b>BA-Cu(II)</b>	-1.18	-2.39
<b>DAP-Cu(II)</b>	-1.70	-1.61
<b>HAMC-Cu(II)</b>	-0.97	-0.83
<b>PAMBA-Cu(II)</b>	-1.19	-1.09

## Cartesian coordinates of the optimized structures

### A2P

C	8.062926838881	3.486328781777	1.230438434728
C	9.285023691926	4.161992837444	1.111074422960
C	9.972396047149	4.005518602416	2.358938113840
C	9.172322457761	3.246104992982	3.212435649398
N	8.001902900150	2.935194745003	2.517435259652
H	10.957019762163	4.423580645538	2.620548180852
C	9.430340668478	2.834276306658	4.632895740022
H	9.510891713380	1.730319820453	4.771950635933
H	10.391854144208	3.274974412862	4.971537195540
H	8.641474481461	3.194746293450	5.335831787902
C	7.006497265783	1.953174879131	2.951803737287
H	7.057968422969	1.878534909217	4.060844092650
H	5.985053030905	2.330597661536	2.714422807009
C	7.192526216856	0.559350859459	2.308180533047
H	6.350192392631	-0.092019696051	2.645635917904
H	7.061950712610	0.667644837255	1.206939532110

C	8.542459147367	-0.111119523084	2.619281700771
H	9.367205702816	0.611522947019	2.409301574167
H	8.596716813792	-0.330391633913	3.712898285048
C	8.821374735565	-1.409530180516	1.835189318412
H	9.740411648368	-1.884070485269	2.255895429544
H	7.998268471458	-2.146297999092	2.011537273457
C	9.019655608450	-1.211045622286	0.320264992587
H	8.065869725738	-0.894317753490	-0.165332042951
H	9.736612180333	-0.373422857526	0.142036150273
C	9.538970500285	-2.484461039286	-0.376910509727
H	8.865715685874	-3.342781318685	-0.153077219281
H	10.533623366857	-2.779310610855	0.024784779471
C	6.904817374430	3.464694750970	0.269291665945
H	6.172477161098	2.670006364539	0.532869837911
H	7.261543533351	3.205744064343	-0.756141602314
C	6.157143166962	4.836449719019	0.192159311172
H	5.936143536910	5.194475017041	1.222576421828
H	6.851125770856	5.592631779020	-0.238715388834
C	1.287231173217	4.059141179118	-1.019655691728
H	0.895510460076	4.402515063502	-0.035770772555
H	0.674356396875	4.586932303244	-1.786457908385
C	1.008589709632	2.530300745754	-1.133838399304
H	1.721099969324	1.980506443510	-0.469768938179
H	1.206540942605	2.167160288078	-2.167504834186
C	-0.391046472296	2.150186325522	-0.672268694055
C	-1.230206105753	1.249214283291	-1.565854501253
H	-2.013659337320	0.755032160049	-0.952898804113
H	-0.601318740487	0.460117402989	-2.037785184749
C	-1.922720686593	2.085228384547	-2.702204923626
H	-2.403337900649	2.973718866795	-2.237179015903
H	-1.142786766916	2.483320872992	-3.390647040210
O	-0.840704211690	2.621170652372	0.381006540063
C	-6.087443495207	-0.657965574232	-3.701216372623
H	-5.910680623483	-1.759622797992	-3.752094880109
H	-6.421075585381	-0.472097237090	-2.658721087410
C	-7.259730109066	-0.333600290333	-4.675897305178
H	-6.931092728585	-0.560559388149	-5.714697389259
H	-7.464183603109	0.760597086962	-4.652422690430
C	-8.525024880863	-1.112780110636	-4.432267146887
C	-9.017570831851	-2.199878480028	-5.155978907045
N	-9.457557544910	-0.822071569836	-3.430632194473
C	-10.282417988284	-2.578602789374	-4.605317257198
H	-8.515301716611	-2.661096415461	-6.020812296594
C	-10.541028660129	-1.703672917682	-3.540501313574
C	-11.743369772299	-1.674544200120	-2.633685631877
H	-12.664962976081	-1.787332574543	-3.252408519059
H	-11.853248993039	-0.686401970927	-2.134932803751
C	-11.749974921072	-2.776113673091	-1.543268285173
H	-12.134372122296	-3.746174771212	-1.937386035442
H	-10.700143226297	-3.009781027930	-1.230921861799
C	-12.478339520103	-2.410724426292	-0.243165734505
C	-12.867348430778	-3.577832341652	0.658284626915
H	-13.177593872447	-3.210025337971	1.658290393716
H	-13.716407970456	-4.136079500818	0.198522574483
H	-12.031266408263	-4.306927221661	0.760019703752
O	-12.698100164398	-1.247897248608	0.077489046208

N	9.652960803903	-2.355785048157	-1.831095138545
C	10.760893677803	-1.835024988133	-2.507021557068
C	8.632702155745	-2.620764444401	-2.744677796780
C	10.444203224240	-1.781048587178	-3.873547093442
C	9.110288181182	-2.278425483684	-4.012123322665
H	8.550847346273	-2.376509810213	-4.955555421180
C	12.051553898093	-1.424903440246	-1.841598224013
H	12.340551363770	-0.414317612397	-2.216817052289
H	11.924737577121	-1.307917702698	-0.743013165193
C	13.238385359585	-2.379269381294	-2.108184442960
H	13.368546570949	-2.560390916328	-3.200575522745
H	14.196628814370	-1.897839901788	-1.781647792104
C	13.186017033281	-3.720423069569	-1.368210109615
C	14.009278760721	-4.850037801455	-1.976662643262
H	14.100032014742	-5.694655391477	-1.263105195043
H	13.497223617640	-5.211072092980	-2.899818180383
H	15.018593227209	-4.500747725331	-2.291963222362
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C	7.280492985718	-3.164282224709	-2.361829779701
H	7.170975145919	-3.201990719550	-1.255137405765
H	7.167594609761	-4.223879163420	-2.698560534093
C	6.092406922804	-2.339315920291	-2.943985034828
H	6.257701268506	-1.264254144275	-2.709547921176
H	6.118424972411	-2.401080904587	-4.055661237473
C	4.749288420213	-2.819192674140	-2.466740742118
C	3.947123638265	-3.842847787310	-2.994786616286
N	4.180479167493	-2.410640584707	-1.255371375747
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C	3.028048380705	-3.164931499709	-1.006057339149
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H	5.741840187260	-1.210621785362	-0.496495056503
C	2.178332611653	-2.987561531904	0.219938359221
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C	0.735805329158	-1.214823817364	1.401978463325
C	-0.494334843155	-1.627091467763	2.193602211990
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H	-0.697486958035	0.274770951619	3.229725902259
H	0.050394300412	-0.994265722845	4.199123533221
C	-2.095544226312	-1.137197728234	4.121959751876
C	-2.423850028476	-2.243679426268	4.915581086515
N	-3.253167265709	-0.361207896118	3.968537124913
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H	-2.477018640319	1.529417163567	3.433485906086
H	-4.251470713204	1.435599267024	3.513568327327
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H	-0.385706735794	-2.716779570788	2.427941688514
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C	-5.696224800882	-0.366413199499	4.714051978057
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H	-6.422087323867	-1.472026922186	6.445325209066
H	-6.696903476392	-2.295853918009	4.902063102203
C	-8.145633430348	-0.762555067945	5.405942646586
C	-8.751569615006	0.079040635033	6.349580913829
N	-9.105087076191	-1.065240505073	4.428994327627
C	-10.105344221210	0.279213432036	5.924473416780
C	-10.308161300601	-0.433116949917	4.743000903234
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H	-7.642477383965	-0.427353895985	2.133123509225
C	-8.428762224513	-1.887278312885	0.704834453689
H	-9.354077826186	-2.505591635858	0.589948787937
H	-7.601222411132	-2.621912026833	0.858971310349
C	-8.178004408226	-1.124267127494	-0.613225779877
H	-8.077212708468	-1.875310547209	-1.431943448690
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H	-10.271082427366	-0.509297833810	-0.659504176899
H	-9.155554015848	0.831868747873	-0.405026613080
C	-9.360747318737	0.290743051968	-2.477013382245
H	-10.240395410715	0.964731476985	-2.613663438307
H	-8.475802689659	0.901304745271	-2.759642878316
C	-3.406730086743	0.682785876238	1.650466771909
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C	4.695810110324	0.904354908117	-1.780854822457
H	4.202700097472	1.890305091032	-1.929212611713
H	4.707678633000	0.373228058477	-2.757401834440
C	4.908914009918	4.815578079881	-0.649025498736
C	2.725466571575	4.443221241623	-1.209908510560
C	3.398736207219	4.817491584005	-2.382752496737
H	5.576631395547	5.362555526426	-2.694096242224
C	4.764598639059	5.051235342202	-2.018732335709
N	3.655604758617	4.428745310449	-0.164691579250
C	3.328397396477	4.199890374146	1.241544561189
H	4.229290046694	3.797937159787	1.754864604125
H	2.553464433287	3.405561413213	1.314760780038
C	2.843944768044	5.478097212744	1.977940612511
H	1.881037005996	5.805309197337	1.496035633348
C	2.570370055029	5.187239926824	3.455139571976
H	2.232456686976	6.110291837025	3.973543687974
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C	-2.900243370159	1.274755467226	-3.506895328593

C	-4.771789524768	0.037917702359	-3.951378617885
C	-3.813938344185	-0.274417792079	-4.931125755466
H	-1.695915450828	0.477219314521	-5.194423730241
C	-2.649530131635	0.503089903764	-4.643761341877
N	-4.206432104704	0.996125293265	-3.090764434443
C	-4.930616602135	1.718462680736	-2.040756433845
H	-5.704436774385	1.035574066286	-1.628545876118
H	-4.253744423804	1.945630787859	-1.186808935201
C	-5.652825185972	3.014916288827	-2.510660037717
H	-6.260695545206	3.345757697648	-1.633213044786
C	-4.723656588997	4.170948472097	-2.911767586644
H	-4.065643910969	3.889823203029	-3.766581052928
H	-5.332472810850	5.047064929297	-3.223976926627
H	-4.075530862219	4.489199881226	-2.064353905983
H	3.493887129634	4.828954278896	3.964185153996
H	5.749516481323	1.097455936927	-1.477665230654
C	-4.581944657821	-0.187735492882	1.195630653358
H	-5.540289625966	0.360270031752	1.339385174474
H	-4.494334498251	-0.441000089419	0.116326984540
H	-4.628699252809	-1.139677184301	1.768667152309
O	-6.607188154919	2.748176888999	-3.544156263539
H	-6.102339545947	2.432357881050	-4.326241454158
O	3.807275994211	6.529793210877	1.912528429054
H	3.979696256733	6.711019628229	0.963009171725
O	3.854792416352	0.854683978043	0.472339161828
H	3.148114654542	0.439310564362	1.030047996061
O	-3.503969035614	1.964429637963	1.031233817796
H	-2.578948396839	2.308324628081	0.904334961438
C	9.764952981323	4.944624508254	-0.082947213675
H	9.301112114726	4.589376411170	-1.030741899964
H	9.537740531231	6.034920072533	0.000264277471
H	10.868396132989	4.859183226219	-0.204572836328
C	2.811224852043	4.934958143572	-3.764299759304
H	3.032592121167	4.041352232576	-4.395783911181
H	1.704096444810	5.049647009242	-3.743848038310
H	3.222893310979	5.815943078181	-4.306390420541
C	-3.971867415096	-1.276340291913	-6.044536474110
H	-4.568655795864	-2.162594212351	-5.728343768940
H	-4.487001530555	-0.847100894599	-6.936740816250
H	-2.983847319114	-1.649885806097	-6.392787493225
C	-11.167943228704	-3.701999285119	-5.076862930017
H	-10.923808677348	-4.675131126348	-4.585975059541
H	-12.244968992887	-3.501643352417	-4.874676864909
H	-11.065300438737	-3.864526778848	-6.173080071640
C	11.336917120841	-1.296721451443	-4.986125213671
H	11.956628537573	-2.113303529423	-5.430561445220
H	10.740025158452	-0.864500944267	-5.820041727280
H	12.044630405244	-0.506073539755	-4.646546629769
C	4.201610551015	-4.621272962795	-4.258875179653
H	4.796664242572	-4.038910207355	-4.997304135123
H	4.762079253316	-5.567751357427	-4.068537073521
H	3.248057194330	-4.908246716665	-4.755988481706
C	-1.498024504325	-3.355344294839	5.334886365277
H	-1.550697523145	-4.237570784588	4.651573954151
H	-0.433500787818	-3.029264588081	5.360581925447
H	-1.749425862176	-3.729023638140	6.352745296273

C	-8.102097525830	0.668328895911	7.574156647609
H	-7.238407384544	0.059814750515	7.925489652428
H	-7.715484636889	1.700484686624	7.395470424240
H	-8.821256618867	0.739517799825	8.420966949415

## BA

C	6.953705908784	4.137828299301	-0.248894028497
C	7.066014114067	4.968372185013	-1.373725436848
C	8.460868092047	5.055187229387	-1.690899378979
C	9.172386767857	4.292503798549	-0.765514027387
N	8.244781320485	3.740945467671	0.117974497680
H	8.908161527370	5.635514490574	-2.512815701438
C	10.651470706076	4.070910228682	-0.645666789008
H	11.070539301462	4.440839257412	0.321395049465
H	10.946858413492	2.998105148847	-0.737028942293
H	11.173170409456	4.621527832287	-1.456615482046
C	8.584450105299	2.786572700817	1.169935631362
H	9.589089495723	3.055668612327	1.570229171787
H	7.878171955879	2.917829575263	2.020338778844
C	8.594062211846	1.313530094188	0.711649959705
H	7.556458926577	1.000751312578	0.443753695293
H	9.185235874377	1.238733369711	-0.230525540970
C	9.169451342920	0.369718001653	1.781497449534
H	10.230368032949	0.658503345892	1.986379700846
H	8.626153830911	0.526420794703	2.745024284503
C	9.117623295257	-1.128270603337	1.421112123033
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C	7.465582226123	0.256378554305	6.275203433284
H	8.555489485044	0.485392493783	6.305077307234
H	7.064649278524	0.815694458435	5.401257505013
C	6.826352649142	0.849436849695	7.560729298826
H	6.869341814781	0.130931032792	8.412949731034
H	7.412440026967	1.737965329165	7.911252543603
C	5.401452071423	1.367884913767	7.402616393744
C	4.583900287030	1.607660726782	8.655949914833
H	3.712282893124	2.260564949604	8.437355632983
H	4.210072571838	0.623334676816	9.026714896615
H	5.201686128938	2.037949007670	9.475211149151
O	4.942563335438	1.594358978438	6.280154421693
C	5.671609961478	-4.293997433133	4.742344662555
H	4.584116690737	-4.110913697362	4.928777571058
H	5.890440897837	-5.266605749868	5.236369974120
C	5.918889154220	-4.473543438244	3.207714431485
H	5.477042743438	-3.617700211277	2.644305712288
H	7.016112553099	-4.405894373370	3.032989492854
C	5.446391285831	-5.786679060101	2.647487691304

C	6.184969936922	-6.951948260633	2.394981053073
N	4.105706816478	-6.055455741475	2.341340379164
C	5.259949969443	-7.932096466092	1.907773710322
C	3.984835231425	-7.366734951712	1.873854546686
H	5.498074163879	-8.968307511365	1.620772489015
C	3.052852126435	-5.050532125783	2.324907270357
H	2.065392420402	-5.565319657332	2.361045244885
H	3.106012006405	-4.441355333518	3.257137258164
C	2.697731820695	-8.011077015199	1.427450604693
H	2.865146702579	-9.108330794098	1.486917987296
H	1.865643264803	-7.795301603974	2.139472835383
C	2.207223281590	-7.655630258871	-0.002808578422
H	3.013137650233	-7.177005462008	-0.609435990062
H	1.954109520205	-8.580346621430	-0.580416862674
C	0.961170772713	-6.772949948408	-0.081285340206
C	0.510421892437	-6.320353604101	-1.475883944022
C	0.222698219865	-4.790002341791	-1.517778494638
H	1.192654533478	-4.254233390303	-1.584183181268
H	-0.211138798570	-4.498171837579	-0.533564281423
C	-0.660154650255	-4.319717832996	-2.635917221740
C	-0.348880661140	-3.698063829287	-3.850960143317
N	-2.052944068892	-4.464299010597	-2.576355648680
C	-1.594860392466	-3.456938330749	-4.527646014735
C	-2.635606391086	-3.929353512832	-3.725272509014
H	-1.709235350391	-3.003874988880	-5.523924951335
C	-2.773612827012	-4.947275414459	-1.406872538514
H	-2.329093084762	-5.907134272089	-1.056148601124
H	-3.813271783233	-5.200239580777	-1.717778668804
H	1.243663801160	-6.610803562856	-2.261680571241
H	-0.423106197884	-6.892249101476	-1.700241565028
O	0.318466227624	-6.447089087614	0.913751104632
C	-4.126764168288	-3.922523283454	-3.935786647742
H	-4.534631078528	-4.964284488432	-3.924132628280
H	-4.633005753883	-3.408076997281	-3.082463466673
C	-4.585865524118	-3.245904230174	-5.253674833001
H	-4.214595174849	-3.848085443090	-6.115488186872
H	-4.080571314511	-2.256672620061	-5.348073962584
C	-6.080216974796	-3.100697338052	-5.357157860896
C	-7.029479952619	-4.047650334496	-5.765942002646
N	-6.773276085131	-1.955772297861	-4.940565683563
C	-8.319926109781	-3.450558833258	-5.584826112837
C	-8.144795484116	-2.164963608350	-5.073004870533
H	-9.292595986371	-3.913979284633	-5.812142382807
C	-9.170187809103	-1.130069355376	-4.710796775929
H	-9.042580393017	-0.174116438046	-5.273897990805
H	-10.182602553314	-1.515516032872	-4.956195328485
H	-9.168948425276	-0.872532705052	-3.624200740121
C	-6.164889620364	-0.723271442248	-4.450706934328
H	-5.161788454527	-0.615143542214	-4.923977196308
H	-6.764724205806	0.140403581125	-4.821396226545
C	-6.028342575321	-0.638386139027	-2.917941405391
H	-7.042231372247	-0.607780481199	-2.457002131889
H	-5.551244125037	-1.572214326952	-2.537989422786
C	-5.189610385762	0.571962289549	-2.470507253762
H	-5.560657288663	1.499761193408	-2.974330813039
H	-4.141120365331	0.431893036675	-2.831616439150

C	-5.183146726984	0.792809703089	-0.945350466633
H	-4.337554266584	1.471006810553	-0.672723959814
H	-4.961193108289	-0.176917284182	-0.438140499339
C	-6.495578281728	1.380065515462	-0.399403432976
H	-6.657604262579	2.393318493039	-0.838844351223
H	-7.364530361020	0.761950172670	-0.712966337409
C	-6.501834535434	1.484913628891	1.137094546399
H	-6.496121072591	0.469105848125	1.591186121840
H	-5.558585280711	1.958791938066	1.490058797626
C	3.011715417400	0.976368012135	-5.010980281809
C	0.853248914824	1.687991498389	-4.778311112811
C	0.859985586929	0.679234264293	-5.755140123262
H	2.582664921228	-0.537031877043	-6.578368839719
C	2.215152654812	0.243212473061	-5.894069413655
N	2.167176357757	1.847713099496	-4.321186443455
C	2.591565512606	2.815489527770	-3.316150963881
H	3.650104712773	2.590459261074	-3.052220385853
H	2.018325736723	2.664668581954	-2.375016690124
C	-2.231891127551	5.370407128304	0.483518039447
C	-4.131512197304	5.364299335230	1.759267467227
C	-3.897798716085	6.686080787320	1.353804678959
H	-2.240574753803	7.549162827957	0.066727958398
C	-2.703647405987	6.678607563000	0.557049835712
N	-3.112499020991	4.567547200680	1.212725608014
C	-2.802083283476	3.194947474670	1.606506213593
H	-2.568539852606	2.578926465697	0.708843964298
C	2.493313109369	4.273157903000	-3.749942287239
C	2.254483191794	5.274528757867	-2.780666515188
C	2.654347181470	4.653598005709	-5.100089541869
C	2.178296026689	6.624441823861	-3.149825165375
H	2.119783747708	4.987998803230	-1.720737407962
C	2.576774800534	6.003909752541	-5.474986425265
H	2.829431745959	3.878539838238	-5.867995482952
C	2.336542013047	7.002068681946	-4.502575245260
H	1.989069471281	7.410636539776	-2.398037912207
H	2.702523629433	6.290572313881	-6.532560939719
C	3.082049875041	-4.121002054909	1.111695358090
C	2.217317159858	-3.007590725927	1.073112363174
C	3.950193535525	-4.350070746978	0.020937276903
C	2.209830024197	-2.135269440860	-0.035042735204
H	1.526904210168	-2.795583707864	1.910434646719
C	3.937281201311	-3.490638593681	-1.094362003071
H	4.653405877604	-5.201587329220	0.049416028237
C	3.066749241008	-2.390243813214	-1.129510576849
H	4.623020636534	-3.674837167207	-1.940877986982
H	3.039693061986	-1.725677550862	-2.005431472471
C	-2.826077569878	-3.972295574033	-0.233362684763
C	-2.997686510525	-4.476505375342	1.075667654165
C	-2.716987219163	-2.577347310777	-0.418332745127
C	-3.087139450038	-3.608875731716	2.170547444155
H	-3.041804722364	-5.568662338772	1.239682259818
C	-2.804132291291	-1.703289873114	0.677586042139
H	-2.538128757268	-2.172511817809	-1.431079665143
C	-3.004957584121	-2.210573385137	1.981088450435
H	-3.212640984752	-3.999071777684	3.195463371226
H	-2.696157193858	-0.617407334414	0.524982934613

H	-3.723616471674	2.739704978173	2.032243589547
C	-1.660639204506	3.073436118508	2.610967627833
C	-1.528848998888	3.984371904465	3.684434926405
C	-0.722371752277	2.027093764796	2.480009672096
C	-0.478542467928	3.848476525446	4.604776108105
H	-2.247237503719	4.818506040487	3.788656741513
C	0.336523303352	1.898767721063	3.390563137193
H	-0.791954629084	1.302913322566	1.650263255872
C	0.471802996858	2.812234915190	4.459491390492
H	-0.365079671166	4.556436605942	5.444560532532
H	1.066110326427	1.083116849019	3.257820461376
C	2.232336043784	8.457976854897	-4.844627475840
C	1.291141416085	-0.943253854278	-0.007637065482
C	-3.098385718846	-1.332359819289	3.190136533297
C	1.616810682821	2.728618033887	5.431083246338
O	2.406953438089	8.700871886723	-6.176981694939
H	2.319570973929	9.676642658992	-6.284292981967
O	1.451753748338	-0.136321028655	-1.077896734595
H	0.851854260739	0.669818695446	-0.992376798137
O	2.551352452824	1.837586057828	5.038727831140
H	3.335359754246	1.868764891111	5.666746021171
O	-3.231584456466	-0.005720034807	2.876658912883
H	-3.183918946531	0.481898513284	3.732683152827
O	2.013202225451	9.348626021556	-4.037122287074
O	1.704567831155	3.402222900477	6.453523496446
O	-3.074399377810	-1.729316878833	4.344824357758
O	0.494752361318	-0.726642800172	0.901025461916
C	-6.749266737168	-5.437876071586	-6.273388607146
H	-5.723409079287	-5.531531517979	-6.695573463834
H	-6.839952409636	-6.210666998227	-5.472251597886
H	-7.463123167191	-5.728589351054	-7.076912314193
C	1.020502665753	-3.324324914390	-4.355742808051
H	1.178789522817	-2.219406489437	-4.357870734683
H	1.829874523204	-3.768975603008	-3.736611942379
H	1.179529089964	-3.670684637774	-5.402951725941
C	7.658583053851	-7.159513250070	2.624460666580
H	7.865626909841	-7.683540456620	3.588000832490
H	8.109844609706	-7.781893147051	1.819159337607
H	8.219908306135	-6.199363543305	2.654328300876
C	9.278663962953	-1.999913260437	7.643870506852
H	8.957117368335	-1.872839595735	8.706013632182
H	9.980723007402	-2.862574102120	7.625643228295
H	9.868782609680	-1.091827295915	7.379951262530
C	-10.973592063731	2.761605618441	3.248096956096
H	-11.808172257686	2.757047045939	2.505108858424
H	-11.104515449695	1.859175211547	3.888141999896
H	-11.139720104131	3.647616343324	3.900136612931
C	-4.767974726707	7.881010611707	1.641371041136
H	-5.453246189629	8.121933325534	0.793461191884
H	-5.405812866414	7.727723130848	2.540137003653
H	-4.154944550994	8.792257628665	1.823727748397
C	-0.335627658115	0.139904425085	-6.494755061741
H	-0.897099915829	-0.613390323689	-5.891336311382
H	-1.063126200870	0.938635152639	-6.768837354769
H	-0.030366487462	-0.362985951290	-7.438151194731
C	6.752895703008	-2.140109955068	-5.269391786609



H	6.930526803409	-1.574749930970	-6.216056929907
H	7.377589924492	-3.059484339831	-5.326686044264
H	5.687080985883	-2.464209283588	-5.285910285435

### [Cu(H<sub>2</sub>O)<sup>5</sup>]<sup>2+</sup>

Cu	0.062351457602	-0.044061602990	0.068621530372
O	1.550658763260	0.776269316751	-1.120923676694
H	2.486927982390	0.528974794413	-0.924777227407
H	1.500637778238	0.917989600679	-2.096803135172
O	-0.154539243163	1.847634352773	0.829496376553
H	0.366886719758	2.563644501494	0.392219807813
H	-1.009201861148	2.257229124433	1.102998650918
O	1.410428208584	-0.670950350150	1.700261374537
H	1.822637545075	-1.554413852959	1.827496172707
H	1.716126297099	-0.133149956274	2.464432194785
O	0.152717957215	-1.878618210568	-0.847627502975
H	0.492402581975	-2.045355147829	-1.758550230738
H	-0.626286083994	-2.474402602116	-0.730123014346
O	-1.688828584661	-0.736097992615	0.938766204272
H	-1.680933235647	-0.932661090511	1.906814446316
H	-2.603157766584	-0.430441300531	0.725947711059

### [Cu(H<sub>2</sub>O)<sub>6</sub>]<sup>2+</sup>

Cu	-0.004419254942	-0.087305738948	-0.007205583753
O	-0.234492572380	-0.369019441966	-2.073502817194
H	-1.128594728865	-0.026131723099	-2.315504404877
H	0.381662301241	0.223824649450	-2.566474540137
O	0.448033000614	1.916539081236	-0.290148352074
H	-0.125363568632	2.277303236337	-1.008934768631
H	0.180445875122	2.435758639872	0.506442262359
O	2.297109069385	-0.604068053105	-0.121684567149
H	2.776859747395	0.001317222618	0.487382855693
H	2.400606986739	-1.478781901304	0.316246888750
O	-0.440851618248	-2.099514586486	0.257303475386
H	-0.074115456395	-2.620117383288	-0.497202308331
H	0.054657322388	-2.444445968599	1.038512118337
O	0.179608284259	0.092896996099	2.072957796938
H	-0.263317104046	0.916673130089	2.388238832333
H	1.132818666628	0.243784412350	2.281633884710
O	-2.303658061328	0.470347090625	0.126076024955
H	-2.402335173726	1.355507295890	-0.291304692578
H	-2.806082086210	-0.114182326770	-0.484931720737

### 3-H<sub>2</sub>O

O	-0.364120290237	3.112901996930	1.372424705754
H	0.491435983906	2.680305464626	1.170560254402
H	-0.937417610391	2.830683071413	0.601323083671
O	-0.630108490041	5.455714600477	-0.142324294796
H	-0.353768064902	4.785690384454	0.548754685990
H	-1.286224246934	6.000250971992	0.339865740207
O	-1.797847589720	3.065389043615	-1.032870354689
H	-2.758902864181	3.164960239583	-0.872566479957

H	-1.461927177502	4.007392316909	-0.986812730581
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#### 4-H<sub>2</sub>O

O	0.898046302826	3.652364809909	1.303762346649
H	0.829791349310	3.752673108264	2.274931105432
H	0.386854511134	2.800427878531	1.122055576013
O	-0.754933465720	5.350755453764	-0.091430523344
H	-0.066646893411	4.824720325577	0.427853701659
H	-1.209827569289	5.874380842254	0.599402748547
O	-2.289985835519	3.201296678277	-0.846572518549
H	-2.082160295913	3.112979877502	-1.799488997528
H	-1.810199904651	4.052951999434	-0.593069048369
O	-0.743421150121	1.532536996297	0.685835081345
H	-1.359084838064	1.289962655234	1.407325961549
H	-1.338744660582	2.047296464956	0.052152426595

#### A2P-Cu(II)

C	7.728473099704	0.821319208015	-2.292070595695
C	8.740389986630	1.483041801821	-3.023277315743
C	9.739401523789	1.867590163729	-2.084933752407
C	9.337447045476	1.452667819925	-0.807582342796
N	8.104680175831	0.812332967319	-0.946485488257
H	10.667232730845	2.416936827871	-2.305222538815
C	10.021829647828	1.669289913245	0.507223066647
H	10.337722937772	0.723222036488	1.004371204278
H	10.935782110524	2.278690247392	0.350281245300
H	9.379215704548	2.221517304195	1.233133553587
C	7.406196393637	0.071629710407	0.106829138777
H	7.729958695105	0.481712099867	1.089088327384
H	6.315051875317	0.287766643807	0.034360292658
C	7.645906231340	-1.455892505001	0.062074086648
H	6.977818641764	-1.929678516452	0.822382913664
H	7.306472889795	-1.841826353017	-0.928923843720
C	9.105176801811	-1.870207690238	0.321081651745
H	9.774853057771	-1.316067899754	-0.379649165744
H	9.393763358110	-1.541160792786	1.347785422941
C	9.402404555473	-3.376440404359	0.186450360478
H	10.443128094133	-3.553959642566	0.547698807847
H	8.745966179748	-3.960811012359	0.877482831671
C	9.281927846377	-3.935438301038	-1.245382115071
H	8.213244718308	-3.991533541634	-1.566452637967
H	9.775713519219	-3.236178601871	-1.962847069444
C	9.930627819107	-5.328103306341	-1.370471917128
H	9.462784932037	-6.037216990118	-0.651587396209
H	11.006701818567	-5.293546122165	-1.090779319990
C	6.372482123135	0.396882455039	-2.772146417114
H	5.990804888163	-0.489552196526	-2.214439739629
H	6.442815071887	0.076888117438	-3.836131234964
C	5.330457913553	1.565476306822	-2.674734486357
H	5.252525816129	1.905241486397	-1.617167707453
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H	1.121388623310	-2.221434824902	-2.551003451343
H	0.854083018303	-1.865756643505	-4.302534863096
C	-0.941618761785	-2.184340888697	-3.154259993737
C	-1.790862346619	-2.459852869797	-4.361592632513
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C	-2.548135630807	-1.145629205089	-4.854302978263
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C	-8.411619300549	-2.132727672458	-6.393293946596
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H	4.056457762475	0.011073545680	-0.861274380726
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C	2.449423525199	1.327176199281	-0.181514078536
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O	-3.466977237486	-2.183277237439	0.073418881904
H	-3.532375606225	-2.125522912425	-0.905289017049
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H	8.264325759533	0.957427657230	-5.090263752718
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H	1.204529045527	0.271786999255	-6.409562253483
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H	1.559939461968	2.020324730622	-6.489516482818
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C	5.097835397039	-9.772914280569	-2.864908058916
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Cu	-0.975027737711	-1.949516196502	-0.221277735140
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## BA-Cu(II)

C	5.411757292665	2.169560314471	-1.968578252392
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C	6.238531891026	2.777757721168	-4.004563693763
C	7.324197257197	2.518493326531	-3.167172210691
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H	8.395683984436	0.026396438102	1.271728487891
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H	10.272469729068	-4.367509521110	0.143525832708
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C	0.224033702874	3.232482260659	2.928052114402
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C	-1.210548247888	3.323920084398	2.366166077843
H	-1.534892331806	4.379136251684	2.234119310088
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C	-1.445316182191	2.574003865826	1.068933223402
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H	-2.156415928136	3.190428796653	-0.845721005464
H	-3.023446672801	3.966215009741	0.516345723704
C	-3.696639093401	1.929339879196	0.065367606125
H	-3.234050953311	0.967429480668	-0.264059789648
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H	-9.169960035517	3.362909279838	-1.529489231548
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C	-10.683116524200	2.049846886988	-2.220024061234
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H	-10.745418120162	3.647256731185	-3.770369993810
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C	-14.041636173678	0.457310040085	-2.415641956057
H	-14.782540002210	1.130954708980	-1.915813975065
H	-13.869462622439	-0.373933590326	-1.699807081544
C	-14.724217586361	-0.112245910796	-3.677887740935
H	-15.697948931982	-0.579391117152	-3.385505263618

H	-15.015286606922	0.689806925729	-4.392792714169
C	-13.940649795753	-1.191844034019	-4.432120697547
C	-14.440520401820	-1.519834671504	-5.831392517261
H	-13.965028707140	-2.448837718112	-6.206678850044
H	-15.549138987478	-1.617098141236	-5.861077373044
H	-14.180569473970	-0.681243620615	-6.519909627145
O	-12.976134937828	-1.763797332689	-3.936914966090
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C	11.386950879676	-5.072202595741	-2.202807798733
C	9.238945490144	-5.259288214099	-2.926669125728
C	11.416722949447	-5.727342518693	-3.463894105462
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H	9.732423373193	-6.296214582465	-4.841392950599
C	12.564009055489	-4.702210901788	-1.340531997010
H	13.311928291422	-4.187427052204	-1.989479364840
H	12.276309288414	-3.962753842613	-0.562202499071
C	13.281443623980	-5.893933825519	-0.663602392075
H	13.532802356117	-6.690940033499	-1.402056598969
H	14.272789879673	-5.557973211249	-0.268057571737
C	12.536271082665	-6.520059726401	0.521549255909
C	13.071373243261	-7.855421262608	1.015163881961
H	12.628722534983	-8.110264391058	1.999551573295
H	12.799162916634	-8.652122657607	0.283153201144
H	14.182573774500	-7.856253302430	1.081512268879
O	11.575343030179	-5.972411401336	1.050885050609
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H	7.442179891168	-5.117181975976	-5.124796792536
C	5.752525688684	-4.142989192961	-4.248623978381
C	4.691618752226	-5.049651174687	-4.433768328363
N	5.203757174085	-2.899703943966	-3.918033014023
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C	3.814110404484	-2.999992317845	-3.900686980090
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H	6.944862882625	-1.856017897983	-3.370943533770
C	2.923407129047	-1.833711016555	-3.555382188619
H	3.225078953208	-1.384985944484	-2.576714684484
H	3.033479037899	-1.000915202048	-4.293234657133
C	1.449791463064	-2.247103150969	-3.477020932750
H	1.074208289771	-2.611575151130	-4.464075071354
H	1.339642740775	-3.139907114716	-2.808023242998
C	0.478705820051	-1.214874531022	-2.940013603949
C	-0.995256736555	-1.567401830471	-3.053146408421
C	-1.970393790836	-0.773175314333	-2.150283967398
H	-2.070960955494	0.265150094860	-2.540865009950
H	-1.516423390766	-0.675201823003	-1.134383731666
C	-3.344723414982	-1.375692616681	-2.062053943495
C	-4.476827667684	-1.104201461702	-2.847203625334
N	-3.671936656422	-2.401061175472	-1.165172464362
C	-5.509193299534	-1.980910585125	-2.390519266762
C	-5.005559878851	-2.763162258712	-1.344284440045



H	-6.533883011648	-2.036615563483	-2.790996753107
C	-2.789902057720	-2.889675884213	-0.105045027164
H	-1.746070377616	-2.909293633032	-0.494583144596
H	-3.044288988242	-3.951858358751	0.110951606886
H	-1.274336694140	-1.431566736712	-4.128576069715
H	-1.103453192304	-2.666518784052	-2.891517697106
O	0.883251817453	-0.157464427103	-2.420565869148
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H	-5.193996184502	-4.057636926778	0.399834827768
H	-6.708911442787	-3.422406205264	-0.243788361255
C	-5.955258958036	-5.157853411166	-1.347431153092
H	-4.973215826268	-5.668740166225	-1.480607294291
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N	-8.275724685913	-6.168955921760	-1.004577126000
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H	-8.089300642347	-8.404637388763	1.435934907801
C	-10.349562332166	-7.442733844041	-0.273718707757
H	-10.617777794441	-7.894560330321	-1.258539302121
H	-10.613703858925	-8.183648635541	0.508813952383
H	-11.011947194763	-6.556629574530	-0.131471206517
C	-8.959584643663	-5.358015589396	-2.015019361932
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C	-9.429538984475	-3.982851652782	-1.496661716304
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H	-8.583999423065	-3.507242526339	-0.945724339844
C	-9.889258925161	-3.031985233646	-2.616884515827
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C	-10.084624333738	-1.572488405517	-2.159836538533
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C	-11.252944509851	-1.352641666163	-1.186569232199
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C	-11.469298384961	0.115219689015	-0.759090261588
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C	-2.843535287188	-2.051364340888	1.188680094282
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H	-3.867688809715	-2.117715671711	1.629955897070
C	-1.790486717916	-2.472225267761	2.228241726565
H	-1.946338999934	-3.540546230035	2.512766922312
H	-0.780349011322	-2.432610955318	1.750981343269
C	-1.801506031894	-1.594667480653	3.489797718382
H	-2.787674087974	-1.632230943764	4.005465287571
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H	-1.604036519412	-0.524403362659	3.243116167482
C	6.018795000640	-0.781331765741	-5.056309847790
H	4.999875735825	-0.720610972136	-5.505687575425
H	6.271650839252	0.260716604920	-4.748121367851
C	7.026203108127	-1.256175044701	-6.123167982848
H	6.816943565841	-0.700755306756	-7.066907648359

H	6.843719876839	-2.328552616661	-6.374848123822
C	8.499616888567	-1.035980896754	-5.740366567504
H	9.185063727305	-1.387836682004	-6.542361367725
H	8.712614561609	0.043764242899	-5.568088917445
H	8.792755485701	-1.577714130937	-4.810311372566
C	3.239484136946	3.667227841657	0.766281286222
C	1.290510262579	3.704248251718	1.965089804387
C	1.289620967058	4.839149013229	1.136482901654
H	2.857766465807	5.561383954331	-0.334710023181
C	2.506186015695	4.793693360043	0.373294174638
N	2.489229074130	3.007020718220	1.735952449609
C	2.981525891825	1.839205755281	2.477660833520
H	3.488476177329	1.165093568078	1.750834525386
H	2.105771049525	1.268872943659	2.860165403023
C	3.948042690543	2.174147928156	3.637394093019
H	4.416201964072	1.214900549981	3.967309947940
H	4.781423056786	2.793399417935	3.232619327839
C	3.326778357592	2.884451188078	4.857568622590
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H	2.770875334957	3.791629998194	4.519386446476
C	2.428207347691	1.991718975182	5.729015880658
H	2.020281562678	2.555249052075	6.596571036297
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H	2.994877023777	1.123805860481	6.136650882039
C	-4.798254844181	2.329308586671	-0.878791798057
C	-6.777193582779	2.164599189883	-1.992982718586
C	-6.066275095416	3.243051842083	-2.554631961895
H	-4.035068790676	4.073921871710	-2.048386795043
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N	-5.997987877595	1.627191276762	-0.964685117270
C	-6.367217527958	0.508792069399	-0.095140333097
H	-7.108433299231	-0.112945486688	-0.640030696398
H	-5.477237013242	-0.149600605437	0.029115532886
C	-6.916487484383	0.928033594571	1.285569908897
H	-6.189349172201	1.617143423387	1.775569955201
H	-7.846071952839	1.530913429984	1.149169430561
C	-7.192935293210	-0.265297269242	2.223843250897
H	-6.257069248717	-0.867758858326	2.334427964897
H	-7.409931502392	0.131413116477	3.242667504166
C	-8.347116414755	-1.183341755113	1.789649624531
H	-8.165580086839	-1.663624251298	0.801319610608
H	-8.508790762940	-2.003713562074	2.522886107716
H	-9.304573376805	-0.618452914950	1.713056240294
C	3.632017692137	2.756676042316	-3.786624166185
H	2.948038287838	1.927487560988	-3.484086258437
H	3.186126649517	3.729842419235	-3.459813169879
H	3.623680940135	2.778465529606	-4.897995013958
C	0.269452521506	5.948948076225	1.059478650196
H	-0.606023985024	5.704293918387	0.411603398929
H	-0.126832824392	6.229516820162	2.060704694153
H	0.728979214883	6.865395785763	0.630382835881
C	-6.529005676543	4.130506041653	-3.679300553850
H	-6.961616018396	3.548400926504	-4.525194344573
H	-7.313418145963	4.854541560434	-3.354687626084
H	-5.687760786909	4.729554338304	-4.089386963801
C	-13.495055858861	2.886209266611	-4.553462274580

H	-13.147119100143	3.884969492776	-4.893561911405
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H	-14.520886196610	3.019989495223	-4.140808363824
C	12.642520187395	-6.205430318140	-4.191005727980
H	12.987254168495	-7.203493290967	-3.829142498746
H	12.445564516804	-6.312154628891	-5.279339595732
H	13.502025677050	-5.507364746483	-4.073249033369
C	4.814603639510	-6.511643680141	-4.768087289991
H	5.670837684181	-6.716380586404	-5.449591060814
H	4.967798765205	-7.144217813872	-3.860983316326
H	3.897234399293	-6.888721519137	-5.270250909700
C	-4.579477995153	-0.085551863987	-3.952379052698
H	-5.614873494507	-0.037659666178	-4.351617827219
H	-4.321777666384	0.941411487927	-3.603564855570
H	-3.912244330885	-0.321354359255	-4.814317873842
C	-5.345739183190	-7.257036737421	1.035363146334
H	-4.491753578624	-7.156926473484	0.327354681406
H	-5.158888093972	-6.545641721849	1.875729930605
H	-5.297823686235	-8.279956700483	1.467832416409
Cu	0.376478457567	1.076317948379	-0.857078871873
O	1.075428432656	-0.616648256911	0.551956749879
H	1.966740291725	-1.005416493803	0.678581086290
H	0.755810019653	-0.421316364227	1.459197012631
O	0.943016254926	2.975486497452	-1.570734680907
H	1.545794735678	2.996837571495	-2.347461636050
H	1.377350214722	3.593465912794	-0.910620406445

## DAP-Cu(II)

C	15.934222965111	6.939302918442	1.656388335113
C	16.578511261080	8.072377164784	1.089119928375
C	17.942691196869	7.992928196044	1.459886026987
C	18.126114389705	6.840072908794	2.245527639301
N	16.890772335436	6.202742972358	2.355004098300
H	18.736483055403	8.708815387054	1.198651734449
C	19.378303863036	6.361693645157	2.908573003289
H	19.259245701349	6.253890596926	4.012652407619
H	19.729516938653	5.377274924591	2.522064466838
H	20.192437742926	7.095043872381	2.734619183903
C	16.647445496315	4.930374939149	3.051828461115
H	17.433255892922	4.819093981006	3.831878377013
H	15.682996981544	4.998062666561	3.601543141609
C	16.608773278350	3.670584148568	2.162451365130
H	16.271377154907	2.841966680594	2.831134357310
H	15.791504631257	3.784625515919	1.411621755363
C	17.929049053622	3.291590493294	1.464005864379
H	18.173608438612	4.046383337781	0.677978882240
H	18.760748857880	3.342979701445	2.206438305308
C	17.937074400930	1.874312937021	0.852815857915
H	18.952092339056	1.661402894505	0.441532063316
H	17.787672464870	1.132232157344	1.676880213697
C	16.879968056090	1.620027347044	-0.236397294622
H	15.863826834104	1.851106631619	0.156049784572
H	17.034076515732	2.319184927040	-1.092701324841
C	16.893139815826	0.157081167950	-0.734217795733
H	17.004104588700	-0.530308360603	0.133584565262

H	17.764117022964	-0.044093365207	-1.396598858573
C	14.473178426226	6.626126838747	1.644226568934
H	14.293703494852	5.544557812356	1.444733859365
H	14.004367210963	7.175892894248	0.799291611044
C	13.730539792412	7.049414125855	2.972675180062
H	14.134569424121	6.444168353875	3.817037809167
H	14.008242954383	8.102428368942	3.196088800443
C	9.046478127600	5.062366862967	2.880461416946
H	9.383147227199	4.096150531973	3.314345889603
H	8.224587902613	5.421726355910	3.544364808651
C	8.462502177771	4.800160775209	1.450849962348
H	9.261991392999	4.402671206887	0.787451930669
H	8.109777818585	5.767238207702	1.024724838028
C	7.314920821136	3.792488963863	1.493354974036
C	5.936635482249	4.349413601824	1.866514706403
H	5.624166511319	5.049968007125	1.051997984536
H	6.046439414412	5.009841306100	2.760776092833
C	4.872344863796	3.263443549221	2.132944271310
H	4.731614354927	2.665412581083	1.201960093666
H	5.296101395384	2.541619932190	2.866279650093
O	7.492961032434	2.594014598519	1.283355308603
C	0.287680824077	5.512083095097	2.343037017080
H	0.181618184097	6.476248817299	2.894765761674
H	0.376710741232	5.801080941641	1.271773483695
C	-1.006445873395	4.686612281688	2.537154173201
H	-1.144085522042	4.501588087086	3.631711795029
H	-0.848816508124	3.672040681334	2.092951961516
C	-2.229049963563	5.340040397475	1.951315117494
C	-2.359119173701	6.562075907483	1.281589944522
N	-3.502339066962	4.772633314726	2.034845376285
C	-3.735485957940	6.750063972821	0.949550374204
H	-1.546392776976	7.272315746063	1.069067209496
C	-4.429482968516	5.622098815669	1.425761556269
C	-5.893409055928	5.301413202168	1.305489720188
H	-6.490241184985	6.160245528165	1.694142601864
H	-6.162017073184	4.434526627969	1.948497073813
C	-6.368665433049	4.985068683871	-0.140061845148
H	-6.679703759868	5.905420638701	-0.683874918817
H	-5.519125503166	4.568543507200	-0.738271025529
C	-7.467296874535	3.907209617361	-0.213798970014
C	-8.481149922363	4.044840784383	-1.336486789324
H	-9.114404421897	3.137261092106	-1.409499413646
H	-9.132409191807	4.928595506205	-1.137863640634
H	-7.979052062400	4.244370369804	-2.310919416448
O	-7.491224716305	2.973484175119	0.580077053285
N	15.673651234864	-0.239585530134	-1.450919144028
C	15.383273489727	0.062312235688	-2.777153686616
C	14.590408604260	-0.914967236609	-0.881869533377
C	14.081878720682	-0.425606708948	-3.062707877651
C	13.602116785582	-1.034483441141	-1.872802067833
H	12.626641351656	-1.524362616889	-1.732651404242
C	16.325807690046	0.766958667659	-3.717240666308
H	15.770130308582	1.600913907618	-4.208529404205
H	17.163132118281	1.241823215756	-3.162237576506
C	16.912759678666	-0.125691302144	-4.836041098450
H	16.111042055937	-0.667555864765	-5.390583503527

H	17.402619474281	0.517122270646	-5.610139062729
C	17.977553404780	-1.131627128789	-4.378768873780
C	18.348177456036	-2.212346563656	-5.383449248904
H	19.277228633956	-2.730641761348	-5.070037856301
H	17.522121094349	-2.960466740681	-5.435426236155
H	18.465527033956	-1.800102084417	-6.410765607286
O	18.509093577476	-1.063418794921	-3.276747333424
C	14.565373875862	-1.416745167896	0.529193434274
H	15.521314762695	-1.946476224977	0.758977508498
H	13.767879419596	-2.189082910430	0.599088414804
C	14.334241510816	-0.354237485965	1.669198383690
H	14.683383373012	-0.818990791459	2.616861266575
H	15.013506867366	0.511188445104	1.506594316019
C	12.932735075435	0.162050389650	1.817420462978
C	12.288291891392	1.185968974173	1.091904852174
N	11.994769913834	-0.383648214726	2.708028393054
C	10.945177109908	1.251698609789	1.569806471382
C	10.782605055609	0.289990819145	2.573481136401
H	10.143793156510	1.915353414595	1.208224287539
C	12.253872403610	-1.390828751540	3.745208121483
H	11.354093450405	-2.040968576036	3.816476935153
H	13.070685725352	-2.061320398001	3.397460927132
C	9.526862405592	-0.018305172144	3.344782825114
H	9.736325670477	-0.490969972631	4.329548901154
H	9.023241163383	0.944051735322	3.590977288766
C	8.519424519708	-0.880781995339	2.555913469621
H	8.406008211582	-0.484672324694	1.516521818513
H	8.883696328777	-1.929227006019	2.412951206214
C	7.128532500676	-0.933639481529	3.176247058875
C	6.012956697402	-1.580587965780	2.336612643227
C	5.014928757488	-0.467163442709	1.901676986261
H	5.554979792064	0.244916217934	1.235249931539
H	4.757657640237	0.115332560286	2.812594278618
C	3.778910518369	-0.955177153637	1.201217660735
C	3.612968346872	-1.264228968138	-0.154308997935
N	2.580971207913	-1.248966792173	1.870550728499
C	2.251669488736	-1.750847482101	-0.315795421203
C	1.636222676028	-1.731164122166	0.972187640144
H	1.908784836983	-2.370600876955	-1.163398141484
C	2.345100742448	-1.046786551423	3.305834729109
H	3.193369818226	-1.497864024354	3.869067263131
H	1.447445587305	-1.642727713690	3.584042852681
H	6.415034862620	-2.116429349960	1.447909063558
H	5.492423940524	-2.330777119342	2.975694278374
O	6.864945524399	-0.421219033913	4.257828626992
C	0.315353956551	-2.329388821407	1.396154999900
H	0.489560757187	-3.086952918489	2.198440582270
H	-0.344925777983	-1.557758332748	1.860026483218
C	-0.452268220563	-3.024989938847	0.239296070096
H	0.198411803874	-3.832711627774	-0.172702615133
H	-0.586556052606	-2.291542634859	-0.588869372903
C	-1.772022324591	-3.622987984811	0.639504087878
C	-2.010500577825	-4.815481905446	1.342254515030
N	-3.012829949238	-3.041763328519	0.346312141933
C	-3.428479114180	-4.938571564222	1.478902373305
C	-4.032173630730	-3.840706380834	0.863047849555

H	-3.967717680066	-5.762834369887	1.969806426183
C	-5.486864608450	-3.512460896457	0.708905106860
H	-5.813089441705	-3.484784283855	-0.358194117203
H	-6.097174531253	-4.290470270411	1.212607938289
H	-5.766443963944	-2.532443559598	1.163334714465
C	-3.214095209407	-1.764855433389	-0.326096175137
H	-2.457781722212	-1.662115016170	-1.140560643477
H	-4.202108235891	-1.784892217533	-0.838172406203
C	-3.128070484754	-0.547687100035	0.617504706326
H	-3.987900412955	-0.580820042100	1.325870442398
H	-2.212236659188	-0.649351140876	1.248546187276
C	-3.078875000193	0.799505240709	-0.121928211075
H	-4.008840397767	0.942792784547	-0.724085750704
H	-2.236481160438	0.763513006724	-0.857759398485
C	-2.864925778334	2.014441037081	0.801938999565
H	-2.672877469146	2.919484764822	0.177523744292
H	-1.928432511763	1.849143328356	1.393330530209
C	-4.037405051945	2.302470526410	1.755698645098
H	-4.977077268520	2.448470799726	1.172570663197
H	-4.234763560646	1.419775780458	2.408923684061
C	-3.817019144243	3.504146869602	2.698987119609
H	-4.722474234702	3.645099789801	3.331484549730
H	-2.988067202038	3.281028778441	3.406652144676
C	2.166128689245	0.412526951957	3.806456131380
H	3.118787510809	0.965993913685	3.635691993330
C	1.908268005912	0.390902511818	5.325937440029
H	0.957381338336	-0.137372955272	5.571536740381
H	2.730763491824	-0.117429577926	5.877713070358
C	12.572258460410	-0.799494303262	5.140825968546
H	11.907475102726	0.077785530199	5.313287335671
H	12.296221630489	-1.557722016110	5.913930208735
C	14.036561212849	-0.357496061547	5.381727407351
H	14.391827277533	0.186781772114	4.471740408315
C	14.974265172929	-1.561867631819	5.610706304101
H	14.685851130774	-2.125570060676	6.528183187282
H	14.957456024834	-2.283042862983	4.760564754474
C	12.234947871428	6.978662930528	2.927390321043
C	10.142366703552	6.088851662230	2.901994680978
C	10.003265035368	7.493317178393	2.830101106554
H	11.585241280099	9.103407854255	2.811607181665
C	11.317761404584	8.036071419010	2.842434423250
N	11.502931028111	5.789787435835	2.952317666299
C	12.100449655057	4.459902132938	3.061761847644
H	13.018224934211	4.433035793868	2.435631208651
H	11.412483692490	3.710757603267	2.609439129786
C	12.501122659821	3.996750930331	4.488504309077
H	13.021728956457	4.852888920120	4.987149764692
C	11.286504202628	3.621599646653	5.363660872223
H	11.623135736020	3.289046984559	6.370814044546
H	10.593100904177	4.480498823786	5.514856297439
C	3.572301538495	3.772290168198	2.697407365993
C	1.535530444996	4.810930479488	2.811195319324
C	1.945774265352	4.546696099878	4.127371704829
H	3.846252485754	3.575890532041	4.891300190380
C	3.220284458995	3.894686816994	4.042889224522
N	2.533010081541	4.333370625515	1.946568142650

C	2.463050267906	4.358590529449	0.490415846871
H	2.097911447344	5.356031798707	0.154832578821
H	3.498320886693	4.269925981524	0.088077102457
C	1.575614095032	3.259698843366	-0.168923269190
H	0.519692889044	3.409466811024	0.160646683263
C	1.638936786797	3.400524804966	-1.696491027838
H	2.673297968207	3.234168069919	-2.077669797281
H	0.975232328266	2.659637956976	-2.191952370020
H	10.713580258467	2.779835884021	4.907848402700
H	1.319703159547	4.414266355355	-2.024287027688
H	1.835796114451	1.427598839554	5.722247119510
H	16.031039096053	-1.232873088404	5.732211464932
N	13.488532327523	2.918172089711	4.316557126574
H	13.644841451500	2.423767277566	5.218273377120
H	13.094987567292	2.197870669560	3.684887309111
N	14.057888147544	0.639532023611	6.473751291415
H	13.629533595338	0.242541743682	7.327457779362
H	15.034644310360	0.852620502623	6.734689079218
N	1.140322953358	1.151915725323	3.036563030443
H	0.203773458436	0.741988028582	3.200362939163
H	1.090846001388	2.116335662361	3.416851449742
N	1.959553518375	1.884818420088	0.263704675255
H	2.993963046809	1.808655958762	0.254217601656
H	1.679389220015	1.704544267467	1.273520449275
C	15.920845758700	9.150156338010	0.273146825454
H	15.356451217933	8.735822874795	-0.594042370311
H	15.194886614590	9.749314558717	0.871489936176
H	16.674565838945	9.858716519340	-0.130290307917
C	8.710610244754	8.258638051842	2.747340025376
H	8.315025690464	8.313349247994	1.704517770748
H	7.908991680406	7.804638582400	3.374219113233
H	8.842854591916	9.306655204080	3.092529882282
C	1.210963253981	4.912618268473	5.391654859336
H	0.559193074276	5.803683841813	5.254729609598
H	0.556188368620	4.088704368446	5.763902168695
H	1.921321858493	5.148824053211	6.213999830792
C	-4.335426754333	7.926562289171	0.227685703325
H	-4.390616598152	7.765680987302	-0.875467750408
H	-5.370895931139	8.144389258555	0.573259161950
H	-3.733660490071	8.847658532358	0.387957956853
C	13.360871972364	-0.329950794672	-4.379251096503
H	13.567158755999	0.628877034627	-4.906952656166
H	13.645950833394	-1.150171618491	-5.080790484092
H	12.260568086968	-0.401720166057	-4.237723326383
C	12.892468825978	2.073631641411	0.036164364866
H	13.786595258987	2.621918799758	0.415770584533
H	13.216613921254	1.506524826791	-0.865294833915
H	12.159899993602	2.839211675458	-0.299858614728
C	4.673554455105	-1.218238406012	-1.222322920538
H	5.442940677958	-0.440534535298	-1.018617469523
H	5.213223929723	-2.191233091616	-1.303818323399
H	4.243356347174	-1.008355004629	-2.226060435712
C	-0.973722661418	-5.779287237187	1.855353163218
H	-0.033680511245	-5.749952239553	1.258817399397
H	-0.693782344745	-5.576497822621	2.916938870265
H	-1.347432462992	-6.826279870007	1.823409786623

Cu	1.402142492621	0.155263539191	-0.649259047018
O	0.094847612099	-0.082889327699	-2.367717599243
H	-0.088039691012	-0.948708125009	-2.791595900980
H	-0.660924823750	0.489065932052	-2.621980166118

### HAMC-Cu(II)

C	-0.616511695097	4.838484096914	1.573384906998
C	-1.733028137869	4.895047892643	0.724283733998
C	-2.890732249914	4.653667045328	1.543742990266
C	-2.464092755291	4.490871121125	2.870024459073
N	-1.076547464665	4.586323833904	2.874205915786
H	-3.943174019210	4.722377038683	1.224446656250
C	-3.294651189780	4.381339470557	4.115285798523
H	-3.117342579508	3.448359448303	4.697697439201
H	-3.118769337022	5.235185323950	4.811135861661
H	-4.371139907879	4.403554811871	3.844800462816
C	-0.248165307975	4.435767076899	4.076710168158
H	0.759379706644	4.845568257934	3.846903908132
H	-0.665934302507	5.089988343564	4.876143344395
C	-0.119927674885	2.993712070784	4.615410333314
H	0.533598716652	3.043412417173	5.519613869993
H	-1.112034486388	2.653418867219	4.990747287211
C	0.448622135054	1.963493234438	3.624189119141
H	-0.219057304506	1.895755052099	2.732881271764
H	1.429648380572	2.336364202997	3.243152698516
C	0.677069430493	0.558910615092	4.228341000974
H	1.222831610665	-0.071050931432	3.482889482729
H	1.375439126062	0.657996059401	5.092921838779
C	-0.579377952839	-0.196214980757	4.710488365603
H	-0.269043473436	-1.008159995337	5.406276512356
H	-1.222922135749	0.473214417831	5.327929903262
C	-1.448445047344	-0.826831977007	3.595961536532
H	-0.847650626850	-1.541849518575	2.989456738521
H	-1.798317185197	-0.056109923828	2.873601082372
C	0.826680843112	4.981908182749	1.162318086474
H	1.488141368570	5.204226539549	2.029673734908
H	0.920177270011	5.865691704388	0.489429833450
C	1.337873222159	3.726908386087	0.388470381015
H	1.427238432390	2.871668701368	1.096291176611
H	0.525225293302	3.449525002053	-0.321363437682
C	6.263120754207	3.822931367678	-0.963814159567
H	6.534826045655	2.884184754316	-0.432512202504
H	6.640102097685	3.680093744776	-2.000134074942
C	7.090420668422	4.992183559926	-0.355743406677
H	6.848873765658	5.176778842867	0.715695453446
H	6.862656752288	5.937970270836	-0.903233262771
C	8.582819861594	4.690973022309	-0.536831392513
C	9.487452504515	4.767072458763	0.682797731216
H	9.046802811901	4.080717599995	1.449078009564
H	9.381144126543	5.784307079954	1.135537685097
C	10.969409546884	4.436499149946	0.396535023206
H	11.032885878337	3.425073124000	-0.063894673308
H	11.336749710379	5.134623148788	-0.388327278136
O	9.000686957353	4.356250177694	-1.646986190006



C	13.528316026299	3.156870878175	4.617499562688
H	13.782314235937	3.848481447872	5.452476097192
H	12.753449637230	2.465303301162	5.024039829181
C	14.800698308402	2.349024830994	4.245384732644
H	15.513585885524	3.038228225254	3.726299369522
H	14.531307556742	1.586853286069	3.475771177714
C	15.482117372163	1.690938461220	5.410405872692
C	15.134213501973	1.683025163832	6.770647741314
N	16.687305970253	0.995047353571	5.280591858750
C	16.137179246563	0.974085915358	7.485828504091
H	14.248760928726	2.165772639388	7.209253245901
C	17.098633800838	0.550703940933	6.534420215293
C	18.338537266288	-0.261402929211	6.766476418204
H	18.905563544453	0.183187244697	7.618309923121
H	19.023291382936	-0.210536652466	5.891251628014
C	18.073211507130	-1.758474326867	7.079849810237
H	17.824893905024	-1.919951790802	8.153339681951
H	17.174150367478	-2.116572291635	6.516952463589
C	19.218268387321	-2.691854486912	6.637589294452
C	19.395258716708	-3.970879682629	7.438790495978
H	20.101230757036	-4.658115835358	6.929571565821
H	19.798843288581	-3.719607810788	8.448061021607
H	18.418918284917	-4.478589073684	7.612089943621
O	19.917250051447	-2.421563445061	5.669276570547
N	-2.606161915981	-1.541645814924	4.140714010427
C	-3.736065029984	-0.897002708787	4.666375608072
C	-2.602401036077	-2.876896158636	4.563150424565
C	-4.463933170826	-1.830355973163	5.418750173131
C	-3.741860648279	-3.065837273363	5.347989855259
H	-4.041782700761	-4.021648585543	5.804643999181
C	-4.137827302388	0.490930724737	4.247412670672
H	-4.547725192810	1.051483286760	5.118869647167
H	-3.258394691934	1.075571272930	3.897619081549
C	-5.234847555367	0.520241920174	3.124642509205
H	-6.209839867251	0.214192058598	3.563279960324
H	-5.344620858951	1.563910201283	2.747816458333
C	-4.897706446867	-0.394076542260	1.949627390837
C	-5.574563917795	-1.737027753834	1.896506268769
H	-5.247513952650	-2.321569657828	1.013205027842
H	-5.341272366661	-2.293357409970	2.837534316472
H	-6.682031590260	-1.611871430407	1.883699509708
O	-4.074234677255	-0.069508038192	1.079196310464
C	-1.609585668725	-3.914816039315	4.112402071931
H	-1.611521198406	-3.966746137126	2.995535271418
H	-1.999558146063	-4.902304330631	4.443521684731
C	-0.135333265275	-3.786408581869	4.623134881534
H	0.301640921343	-2.817252940602	4.290188349640
H	-0.159263644875	-3.737401755418	5.734699102379
C	0.778272018049	-4.907755071433	4.224880926063
C	1.210816743373	-6.011737929912	4.991461246469
N	1.357467461744	-5.011693893316	2.956438913172
C	2.072524888738	-6.779215047070	4.156688934787
C	2.156894330588	-6.153734053141	2.905297263446
H	2.598876443634	-7.703354161150	4.440998359877
C	1.065173500880	-4.145177976018	1.814330514234
H	0.974489514613	-4.796286509044	0.917246276481

H	0.052813824947	-3.708929719490	1.962513428041
C	3.023307935595	-6.512838042712	1.731045225863
H	2.919053660690	-7.602150768739	1.518468729109
H	2.703926952983	-5.990987705333	0.801687563571
C	4.515512839108	-6.187902955972	1.985741838037
H	4.623526293391	-5.162488920645	2.418096128976
H	4.943497140695	-6.871489528646	2.753829524540
C	5.391822837559	-6.168256677507	0.727468080768
C	6.842639338884	-6.589222943598	0.957998696954
C	7.769266928022	-6.498971883245	-0.267407990031
H	7.500317048560	-5.573671681632	-0.826492000645
H	7.521265732963	-7.331455363368	-0.972440485756
C	9.241533363151	-6.504041407428	0.078733961601
C	9.931403037780	-7.143036530811	1.125234450796
N	10.190667589760	-5.819052230405	-0.695136015902
C	11.315321373920	-6.781281947208	0.990753349034
C	11.458650644278	-5.967198164378	-0.141416186258
H	12.134586144332	-7.159442318670	1.620899167517
C	9.893820465043	-5.010011661983	-1.881464043415
H	9.009213308070	-5.448058741126	-2.394583538603
H	10.739879918230	-5.117154066601	-2.598136601368
H	7.221123016341	-5.960000650858	1.800567122287
H	6.813232532231	-7.621247714838	1.379281885142
O	4.965788800564	-5.792830374349	-0.359437565929
C	12.701854480594	-5.326867371623	-0.701140625306
H	12.658891540012	-5.310480065110	-1.814850136502
H	12.773833955163	-4.258950372806	-0.380437739255
C	13.998106315160	-6.057284437389	-0.253129938678
H	13.889276654330	-7.140887095892	-0.500397870556
H	14.069051781659	-6.002959304081	0.854688421931
C	15.258135086845	-5.550082278541	-0.893044210648
C	15.654529084432	-5.703543102147	-2.250328653366
N	16.285375037349	-4.891050895514	-0.220386454701
C	16.940302382112	-5.119880425449	-2.371976423749
C	17.325572100356	-4.627750197710	-1.114582206002
H	17.556832658026	-5.073154126713	-3.282261973248
C	18.612848639844	-3.980410060063	-0.714677387641
H	19.126710742983	-4.528170054786	0.110521766768
H	19.306075006912	-3.961054310885	-1.580594170111
H	18.482762747771	-2.927831212863	-0.369090290524
C	16.316438156897	-4.537251939581	1.202462000106
H	15.583046492336	-5.181065513269	1.735017405013
H	17.315818597830	-4.816427240830	1.610428694681
C	16.019571978308	-3.055880816446	1.511137738532
H	16.823273283303	-2.418014449306	1.073853690403
H	15.068422678352	-2.758906469809	1.011249866776
C	15.894260181443	-2.808624025435	3.027512408554
H	16.719344614362	-3.336655694754	3.567627020715
H	14.945820004465	-3.279080453761	3.373539405107
C	15.909294666084	-1.320685474283	3.441228125592
H	15.433566824671	-1.224321061978	4.446054620698
H	15.260005988617	-0.735095142144	2.744214546968
C	17.320106901377	-0.705509506064	3.496886511004
H	17.980119683130	-1.349668381490	4.122990740062
H	17.790763365325	-0.710228076052	2.484880882904
C	17.387252275647	0.750255079297	4.010266494385

H	18.452964049466	1.055580254918	4.122602224965
H	16.952906682574	1.441316011797	3.256618914517
C	9.655226471970	-3.524541336221	-1.557580710462
H	8.794292679394	-3.440269184793	-0.854656403111
H	10.538290892734	-3.143508346275	-0.993642604377
C	9.404449140842	-2.655551555069	-2.801921541016
H	10.315064046470	-2.654723951250	-3.449914533335
H	8.596518070463	-3.115115906854	-3.420506197196
C	9.000940230131	-1.200916933449	-2.482607894597
H	8.827584766808	-0.651925305396	-3.436949195502
H	8.027116752896	-1.196081041984	-1.936793082359
C	2.071366222625	-3.006240166978	1.543649969016
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H	3.080299003580	-3.429218757415	1.326728196141
C	1.618769252161	-2.092319588979	0.380554671601
H	2.349105455906	-1.252047825465	0.291170922251
H	0.643429552231	-1.610965149818	0.646824813238
C	1.474786415206	-2.817075338874	-0.974529078715
H	2.466889280048	-3.234718208643	-1.276329436217
H	0.814152501164	-3.704884040104	-0.846682367292
C	2.574013370690	3.881982692166	-0.449428683588
C	4.772945748434	3.984836639734	-1.053741554420
C	4.018867173025	4.296136977771	-2.195538314921
H	1.767309639092	4.450123061502	-2.447896099264
C	2.637105543573	4.213325324207	-1.813261265432
N	3.881081696016	3.747263063940	0.004630729949
C	4.241096701741	3.370364833843	1.378207073043
H	3.571020519236	3.929668235408	2.069927335437
H	5.265186811036	3.754434129551	1.579883496377
C	4.180346426391	1.863361816120	1.715313711502
H	4.316990018192	1.783422411226	2.821312117089
H	3.155275876553	1.470451981483	1.511991004999
C	5.234560761010	0.992546996993	1.012651078989
H	5.008635136700	0.925820182267	-0.079083032259
H	6.229067069757	1.494245360307	1.083008222768
C	5.383819711059	-0.419495989319	1.605528067914
H	5.620513663529	-0.333828854742	2.693192586601
H	4.422939773320	-0.982597597691	1.552968700903
C	11.894307951717	4.551986591971	1.575429343619
C	13.003618814673	3.990901991681	3.483078895555
C	13.392226418687	5.303988544504	3.139088087719
H	12.763628590717	6.589746675594	1.392463969959
C	12.692332358537	5.640297115805	1.945099029698
N	12.088230365771	3.546114970792	2.525114953768
C	11.423996218785	2.240370942170	2.525829162288
H	11.267070884284	1.941017389710	3.586537565466
H	10.405215333370	2.356752585867	2.092134621842
C	12.162802434324	1.120039274768	1.760538330038
H	12.168895544269	1.365949397883	0.673648040318
H	13.234251105304	1.099184783532	2.068410969119
C	11.530561093600	-0.270531385805	1.979879925100
H	10.429029070206	-0.204549055274	1.806119357927
H	11.920066110019	-0.965226240096	1.200528837188
C	11.805341489724	-0.886454643443	3.368520638010
H	11.530200748034	-0.167018077799	4.175058859907
H	12.898612654048	-1.069633752528	3.483257580952

C	6.504207146647	-1.204420778125	0.896351813721
H	6.161896591843	-1.526913226930	-0.118650683808
H	7.389300527394	-0.552823943464	0.718373814745
C	6.944244902098	-2.462931413510	1.631106733883
C	11.038973561558	-2.193070696188	3.635281527385
H	11.209188679406	-2.527806538170	4.688081678788
H	9.940290986081	-2.038445057306	3.546872530132
C	11.455621872201	-3.365252596249	2.749368002978
C	0.879583902615	-1.998230955443	-2.138912950940
H	0.662640239478	-2.703098775708	-2.972428620316
H	-0.110049367147	-1.574625733371	-1.843999806745
C	1.766035473118	-0.877020430948	-2.710518932844
H	2.836228531158	-1.182083487237	-2.778751329034
H	1.472465068900	-0.667258111683	-3.770039778246
C	1.702016037834	0.477422636967	-2.034320239760
C	10.052067734433	-0.436583887973	-1.639624371353
H	10.196496352919	-0.945794874267	-0.662301761794
H	11.026671018465	-0.425856753824	-2.178866948724
C	9.625656055669	0.994437427423	-1.339212173110
O	8.286545672980	-2.643489417660	1.519424728584
H	8.577368832088	-3.474354038218	1.980249438847
O	10.465475957993	-4.288623997111	2.624727992033
H	10.806542063548	-5.073982581765	2.087361573281
O	10.087085885758	1.864041834811	-2.254957935588
H	9.756221328215	2.789278749285	-2.048764594713
O	2.723549706256	1.260545928714	-2.327409234153
H	2.607037414119	2.216972965861	-1.983921712444
O	6.208176323876	-3.228215815910	2.235419800022
O	12.556290559938	-3.493808877014	2.231621902527
O	8.922389444714	1.314705401547	-0.378501666193
O	0.756894856093	0.851543120789	-1.309929455005
C	14.864067240597	-6.376578721576	-3.337760263538
H	14.256943561586	-7.226713712633	-2.953183765781
H	14.158108255540	-5.674206119803	-3.842529649108
H	15.534099889910	-6.776186087268	-4.129310498536
C	9.404840908755	-8.075505617092	2.189457459161
H	8.816719888153	-7.555074668436	2.980147775226
H	8.753827308315	-8.874575249065	1.768911722896
H	10.247896376025	-8.587089322709	2.701899802004
C	0.821010498129	-6.328808254962	6.409588886776
H	0.683343074921	-5.413182065123	7.027630611663
H	-0.135484291969	-6.900699832420	6.463138681516
H	1.594989417704	-6.951433436335	6.908123207008
C	-5.774871213442	-1.598360969221	6.122573542490
H	-6.649323598551	-1.948129188714	5.523451310239
H	-5.814339338255	-2.151540246570	7.086695570784
H	-5.945889670103	-0.523529017299	6.353524279692
C	16.181356191071	0.714074656755	8.965765087045
H	15.810744748014	-0.306270497213	9.225206858470
H	17.213935783975	0.793700332930	9.374981541750
H	15.547147126521	1.438597317650	9.520407150792
C	14.377913930879	6.168506997008	3.877933153280
H	14.280090163910	6.072551411876	4.983086630301
H	15.435420443929	5.916648678155	3.626043005886
H	14.235339415865	7.241210640658	3.625597692679
C	4.536247973849	4.653363554318	-3.562559511087

H	4.614128249291	5.757279311868	-3.699402177817
H	5.546891072526	4.232548532054	-3.757608213993
H	3.859727308652	4.278738373168	-4.361713092664
C	-1.733485386564	5.175370401374	-0.756509248136
H	-0.815762334157	5.712665121083	-1.081880615044
H	-1.802314013887	4.245672232345	-1.372491052033
H	-2.602649137488	5.806562587708	-1.045401130128
Cu	-0.754128982364	1.291088005041	-0.288053669473
O	-2.230954975043	1.745904894532	0.812047400427
H	-2.463055844365	2.696959154934	1.038480213474
H	-3.044405904336	1.137181415782	0.944175990953

## PAMBA-Cu(II)

C	6.547156385160	1.958458195649	-4.780490867052
C	7.400658918675	1.203347423160	-5.614644831958
C	8.729530144400	1.421259525218	-5.149381646546
C	8.679953966244	2.295649797097	-4.055993122608
N	7.342320968080	2.627390129702	-3.846033908569
H	9.650148518455	0.990943522210	-5.571824746320
C	9.798267405409	2.832290819970	-3.217352003629
H	9.862784272823	3.945890378713	-3.251763517364
H	9.715320085278	2.543440196215	-2.142644700271
H	10.766173246893	2.437715288705	-3.589701286457
C	6.841790466846	3.390228626244	-2.703171903409
H	7.602480325819	4.156047098344	-2.431578268156
H	5.940966907075	3.963442032761	-3.023685235718
C	6.499057224761	2.514194649431	-1.478622380295
H	5.850352739384	1.669644193060	-1.810793437973
H	7.437032640338	2.045145752986	-1.098875380218
C	5.789171651137	3.299943766129	-0.361857449581
H	6.430864640169	4.154844636561	-0.034084433020
H	4.863301281833	3.762815905568	-0.781870928201
C	5.395078743101	2.461416339943	0.872064745048
H	4.751881433698	3.090371654118	1.534410561882
H	4.748581767031	1.609880642986	0.547585523157
C	6.576374413716	1.920020937875	1.699107129167
H	7.171816306624	1.183042501348	1.110909326551
H	7.278122180834	2.755876378587	1.933885603011
C	6.103163915863	1.269605708343	3.016736069247
H	5.438837680052	0.402812794718	2.798764078984
H	5.480658359297	1.984773577220	3.596076755766
C	5.059304800675	2.117364436106	-4.871196217065
H	4.628364898886	2.435513384722	-3.895655650269
H	4.604385926363	1.122764152820	-5.091262781940
C	4.554463271976	3.102110703313	-5.983057734578
H	5.088742604109	4.075302662948	-5.892166989650
H	4.850396395627	2.698388146129	-6.976665309474
C	-0.020186328901	5.031604038781	-4.815517760960
H	0.325954737080	6.089926880084	-4.845012811739
H	-0.892551890357	4.997783103577	-5.504504466511
C	-0.577919559285	4.687525684113	-3.378773915965
H	-0.627582998650	3.582923357886	-3.258935642657
H	-1.613116178833	5.094050579414	-3.306024445784
C	0.238920921687	5.285898139639	-2.254807428619

C	0.143490641677	6.785705297618	-2.023905794834
H	-0.800608311738	7.188616901593	-2.453865170287
H	0.951749533875	7.218785247944	-2.667441082197
C	0.345124082898	7.273574636549	-0.550804081770
H	0.864081943515	6.468824068615	0.021227425146
H	1.041109259271	8.138841805539	-0.550505361660
O	1.022310696857	4.600548147357	-1.570515084930
C	-4.350956950226	7.039841255521	1.362594108071
H	-4.263124939175	6.033707524208	1.836124939357
H	-4.865985377807	7.672454834058	2.119023821560
C	-5.262200983029	6.945876864692	0.081809250212
H	-4.668876253591	6.473025238911	-0.733688119963
H	-5.460494426009	7.985093467391	-0.262948151047
C	-6.577915131426	6.250793369802	0.262692318063
C	-7.814348552110	6.788342060973	0.643067356439
N	-6.752545832502	4.873206243524	0.104760716018
C	-8.764224198918	5.732628666784	0.712005621178
H	-8.005939133187	7.851653747049	0.853848488870
C	-8.085035342050	4.541590906367	0.353438168253
C	-8.638929941544	3.138955433319	0.307262871093
H	-8.973495564972	2.858923252876	1.335883242606
H	-7.849629702108	2.405554699840	0.033299194859
C	-9.841221704745	2.929139083387	-0.641530274411
H	-10.367082734703	1.979380798149	-0.366912241553
H	-10.617344522204	3.716449931776	-0.508272022967
C	-9.520497149444	2.791254223684	-2.132681669234
C	-10.699533497475	2.953244095529	-3.078451769957
H	-10.466836031441	2.536799305414	-4.080087162024
H	-11.626013907685	2.487338242260	-2.675116958721
H	-10.918651371397	4.041794516400	-3.191354157117
O	-8.388263241079	2.545878719746	-2.541364072137
N	7.184185406198	0.802361099299	3.886710013393
C	7.971586266288	1.622343357050	4.694096205582
C	7.639273543623	-0.514657501966	3.987870834565
C	8.963769429418	0.816845682118	5.303257124507
C	8.743571114299	-0.512460667294	4.853898485767
H	9.318332848628	-1.405004931610	5.144650619615
C	7.764943919715	3.103682322162	4.877495150245
H	8.747768087103	3.611332353188	4.729688161585
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C	7.238944687643	3.542778925219	6.266182654365
H	7.853978333389	3.111543230183	7.094549035521
H	7.361833884385	4.647421375923	6.392715031666
C	5.782564463792	3.226218109589	6.563971200722
C	5.182803909481	3.757207724854	7.848683766919
H	4.291289987898	4.373964820463	7.586982178644
H	4.808200360357	2.904054011480	8.459006754694
H	5.892321648292	4.354219337771	8.457529353775
O	5.102061141437	2.570896527086	5.765930998312
C	6.981184184588	-1.703253143245	3.351878601006
H	5.898238613816	-1.736704613871	3.630246967142
H	7.427069602826	-2.608158228445	3.819607044971
C	7.119492709877	-1.853227010014	1.797026669093
H	6.578413271996	-1.022848524745	1.284916876080
H	8.191127534696	-1.721143498746	1.530068052821
C	6.667947933812	-3.187080773002	1.276237412483

C	7.433405487801	-4.306283363903	0.907426186046
N	5.314547169197	-3.534846472726	1.153993584543
C	6.509869620169	-5.333934896767	0.533602780342
C	5.209313550016	-4.848388644788	0.683370208047
H	6.770167280146	-6.353721642255	0.210433611956
C	4.219421991292	-2.587805178565	1.252017801871
H	3.279502896576	-3.148586998170	1.454637075109
H	4.372023879181	-1.930283966775	2.139193187182
C	3.914420490120	-5.581397064232	0.436317995400
H	4.161825642887	-6.663263138995	0.489447376938
H	3.187152611374	-5.404210664484	1.263095993010
C	3.201333629580	-5.316469648579	-0.918985463628
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