

The Hydration of Copper (II): New Insights from Density Functional Theory and the COSMO Solvation Model

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Supporting Information Available: Cartesian coordinates and absolute energies for all $[\text{Cu}(\text{H}_2\text{O})_n]^{2+}$ complexes optimized at the B3LYP/LACV3P+/6-311++G(d,p) level of theory. This material is available free of charge via the Internet at <http://pubs.acs.org>.

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

4w E = -501.408888

Cu	-3.9976828013	2.5574841849	1.9428501040
O	-2.0496754404	2.8838714589	1.9473316435
H	-1.5855893213	3.5423346517	1.4061510789
H	-1.3983248980	2.4102185271	2.4887102382
O	-4.3221822144	4.5071304240	1.9405646926
H	-4.9654389221	4.9728511294	1.3827190361
H	-3.8680332300	5.1566068704	2.5007393345
O	-5.9457147420	2.2313191318	1.9419994749
H	-6.4084381061	1.5737953224	1.3986342042
H	-6.5984059689	2.7031276668	2.4833686777
O	-3.6716529820	0.6080484712	1.9410726076
H	-3.0294785985	0.1423544701	1.3818480007
H	-4.1268966134	-0.0418227074	2.4998440141

5w-a E = -577.917692

Cu	-0.0198268873	0.0188781347	0.0533553059
O	1.4552448995	0.6373040111	-1.0732085867
H	1.8475291922	0.0347665256	-1.7557315603
H	1.6170206061	1.5621700083	-1.3083377135
O	0.0355978048	1.7083854499	1.1023782907
H	-0.7220190897	2.2820145547	1.2944152586
H	0.8248579150	2.0895327351	1.5175754658
O	0.0685644789	-1.7097594808	-0.8571520648
H	0.7482792239	-1.8696490947	-1.5603526135
H	-0.2283161989	-2.5492674236	-0.4778002059
O	-1.6437468730	-0.5531028945	1.0526686109
H	-1.7564894319	-0.5256804394	2.0152265173
H	-2.4569397883	-0.9030886665	0.6565733602
O	2.0675585922	-1.4591641784	-2.6489594549
H	2.9169137796	-1.9181009312	-2.5487101279
H	1.8787984719	-1.4666732682	-3.6010173690

5w-b E = -577.914764

Cu	0.0651997604	-0.0447559785	0.0712771125
O	1.5466428243	0.5902554688	-1.1634377843
H	2.4856635772	0.5479877987	-0.9279192861
H	1.4684742159	0.9726779129	-2.0506989052
O	-0.1925091470	1.8311544756	0.6873189242
H	0.3265035074	2.5934227729	0.3925066298
H	-0.9216359391	2.1436119901	1.2424495378
O	1.3913732041	-0.6668954083	1.6876569967
H	1.7873435976	-1.5418844508	1.8065928167
H	1.6985184940	-0.1260693283	2.4290943552
O	0.0471138201	-1.7908104248	-0.8864476289
H	0.6285095465	-2.0306822109	-1.6225330722
H	-0.6187831067	-2.4844946602	-0.7733088755
O	-1.6596857633	-0.5659171517	1.0078142399
H	-1.6849710287	-0.9541471280	1.8953995808
H	-2.5689290459	-0.4818640943	0.6824850385

6w-a E = -654.423128

Cu	0.0015293567	0.0049079982	-0.0076713157
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O	1.4474205024	0.6435128447	-1.1817841713
H	1.8681211966	0.0218536737	-1.8257329776
H	1.5213231316	1.5519912011	-1.5064793461
O	0.0296395701	1.6791660001	1.0277972881
H	-0.6753542044	1.8537485970	1.6988002613
H	0.8367286675	2.1556214504	1.2681315193
O	0.1697498365	-1.7813375560	-0.8190172191
H	0.8450447452	-1.9395621724	-1.5235249908
H	-0.0209979089	-2.6089085348	-0.3553690488
O	-1.6407903729	-0.5216412280	0.9424719895
H	-2.0313351445	0.0825598584	1.6206659656
H	-2.3341693455	-1.0786620207	0.5614745196
O	2.1515293614	-1.5204580971	-2.6500236662
H	3.0207398837	-1.9346256923	-2.5319173314
O	-2.1466549756	1.5324189113	2.6357701476
H	-2.8964170566	2.1343353580	2.5072065738
H	-2.0729459317	1.4107503329	3.5953717909
H	1.9597124675	-1.5857688274	-3.5987215107

6w-b E = -654.418147

O	-3.6663751453	0.4722911682	0.5524012621
H	-3.9603822588	0.3940201662	-0.3844914090
H	-3.0057401977	-0.2026859938	0.7553530103
O	-5.8597537116	2.1622753079	0.3878361071
H	-6.0441255438	3.1088898778	0.3058303219
H	-5.7187702549	1.7850036430	-0.5153058519
O	-6.2464766452	2.0296860899	3.1219911996
H	-7.1716811115	2.0679883424	2.8387901900
H	-6.2254428282	1.9530137257	4.0862791026
O	-3.8100676842	0.5687103283	3.4277870693
H	-3.9707973750	-0.3008369790	3.8221655613
H	-3.0378787898	0.9705645982	3.8519185088
O	-5.0141450507	0.7788110002	-1.7984743805
H	-4.6002404802	1.2119512966	-2.5608197838
H	-5.5724822598	0.0788885597	-2.1710316737
Cu	-4.7464260395	1.4788953460	1.8887783184
O	-3.4219998699	3.2115987393	2.2429059427
H	-2.6360774321	3.4235115282	1.7206911124
H	-3.6073269349	3.9937909207	2.7808213683

6w-c E = -654.409044

Cu	0.0037114307	0.0046035299	-0.0089457176
O	-0.0713914663	-0.2292596480	-2.0388719971
H	-0.8675618301	-0.1560964177	-2.5836952381
H	0.6839314415	-0.4285744782	-2.6096340286
O	0.3537658010	1.9811963549	-0.2499643547
H	0.4145822220	2.4413206619	-1.0981660504
H	0.4721070000	2.6220306085	0.4642909347
O	2.2245609070	-0.3856641314	-0.0450430994
H	2.9268952584	0.2707485184	-0.1454335041
H	2.6675941871	-1.2407641187	0.0364627464
O	-0.3453994443	-1.9724921249	0.2295955636
H	-0.4647176213	-2.6115159894	-0.4860587515
H	-0.4086880465	-2.4341042036	1.0767773602
O	0.0781447075	0.2384386072	2.0211137223
H	-0.6773652629	0.4375155796	2.5916838110

H	0.8740638163	0.1654805492	2.5663024689
O	-2.2167542600	0.3960935710	0.0261807443
H	-2.6595017994	1.2513623750	-0.0554109438
H	-2.9194054119	-0.2599346118	0.1267167186

8w-a E = -807.423510

Cu	0.0019833091	0.0053642421	-0.0077907621
O	1.5565155900	0.5919849646	-1.0322567407
H	1.9923634659	0.0312485100	-1.7072536863
H	1.9545692123	1.4819208670	-0.9333914369
O	-0.0509654383	1.7328718460	0.8997949101
H	-0.7089755913	1.9499782666	1.5925666381
H	0.5924752683	2.4495486466	0.7207070539
O	0.0329382633	-1.7098011225	-0.9393281437
H	0.7027413842	-1.9340197806	-1.6183968315
H	-0.5988480187	-2.4333389986	-0.7465163480
O	-1.5316073869	-0.5940666825	1.0406669023
H	-1.9780708801	-0.0270664147	1.7034710707
H	-1.9404776974	-1.4777281330	0.9292898274
O	-2.0423796215	-3.1408349251	0.1542939398
H	-1.8901326842	-3.9116751470	0.7203633092
O	2.1628443855	-1.5304182398	-2.6622692704
H	2.9691444468	-2.0509839809	-2.5330593897
O	2.0469054607	3.1502948487	-0.1690677074
H	1.8985031472	3.9191516247	-0.7388611807
O	-2.1585117304	1.5403695051	2.6475031267
H	-2.9682612400	2.0554308697	2.5177859572
H	-2.8344593799	-3.3516963627	-0.3613762308
H	-2.0252973059	1.5060848947	3.6060995418
H	2.8353938425	3.3630801127	0.3513521735
H	2.0322854098	-1.4906026239	-3.6210277578

8w-b E = -807.415401246740

Cu	0.1600880065	-0.0965845212	0.1960101602
O	1.6065972962	0.5615981603	-0.9744647545
H	1.8658794732	0.0951907901	-1.7947186878
H	1.8776130815	1.5028531247	-0.9765303163
O	0.0226684783	1.7035694667	1.0262247677
H	0.5455586331	2.4535716621	0.6720229450
H	-0.8250411560	2.0010427968	1.4139322206
O	1.2894579583	-1.2014957128	1.7850955219
H	1.7380409314	-2.0436415490	1.6340916694
H	1.7231356961	-0.7986925434	2.5484481838
O	0.0286244926	-1.7439757515	-0.9460879190
H	-0.8097815504	-2.2116069716	-1.0543075275
H	0.5574330379	-1.8109797048	-1.7723925414
O	-1.5210060141	-0.6677367533	1.1314902414
H	-2.0833362790	0.0430856413	1.5177262732
H	-1.3839397513	-1.3438777047	1.8105080977
O	1.8214720201	-1.3315638005	-2.9781791950
H	2.6123880416	-1.8872317025	-3.0383564531
O	1.8516310888	3.2342181365	-0.3519064619
H	1.6072537608	3.9465804527	-0.9602432860
O	-2.5596460893	1.7030054735	2.0565793540
H	-3.3209250648	2.1124601560	1.6194024959
H	-2.7011608582	1.8490030361	3.0035011724

H 2.6430103546 3.5494701552 0.1086651315
H 1.5472554272 -1.1742098065 -3.8935073408

9w-a E = -883.911080

Cu -0.0214300161 -0.0380801664 -0.0047872104
O 1.5770442291 0.5266491533 -0.9643231588
H 1.9818304549 0.0068318568 -1.6845833778
H 1.9128045156 1.4540641714 -0.8848614972
O -0.1132120500 1.7231493280 0.8208780175
H -0.7332452565 1.9505207221 1.5395600224
H 0.5643924324 2.4158238794 0.6211810591
O 4.0473978118 3.8754320632 1.1393444201
H 4.9670785392 3.7783029176 0.8654519356
H 4.0406790506 4.5449252511 1.8336548102
O -0.0238518084 -1.7395596860 -0.9653160140
H 0.6528539520 -1.9660186984 -1.6376627938
H -0.6432658766 -2.4687380697 -0.7594416101
O -1.5206243696 -0.6502243185 1.0882084994
H -1.9874649640 -0.0581671206 1.7151760908
H -1.9582752896 -1.5156796127 0.9551329560
O -2.0863092090 -3.1783457363 0.1599404999
H -1.9335472877 -3.9514592230 0.7223708123
O 2.0929980210 -1.5959060620 -2.6900643173
H 2.8909111447 -2.1316286206 -2.5740990360
O 1.9273894263 3.0703397727 -0.2398772190
H 1.7326849101 3.7859049877 -0.8596602269
O -2.2153204983 1.4967592685 2.6288711226
H -3.0319861269 1.9970268075 2.4880563381
H -2.8826734090 -3.3840996667 -0.3506766241
H -2.0907756767 1.4706862136 3.5884888807
H 2.7263684279 3.3690032238 0.2775436282
H 1.9493071972 -1.5514954489 -3.6464058398

9w-b E = -883.909467

Cu 0.1652585927 -0.0982501620 0.1867029256
O 1.7133907736 0.5244381065 -0.8925111784
H 1.9530462056 0.0568035859 -1.7187160895
H 1.9198631879 1.4805333741 -0.9406704031
O -0.2168159396 1.7876317555 0.7131016806
H -0.8665494747 2.0088848961 1.4077473931
H 0.4186066372 2.5107541669 0.5476274354
O 1.5093821270 -0.7214490395 1.8350493843
H 1.2492714613 -1.2140486197 2.6222342824
H 2.4730778217 -0.7338750905 1.8040614316
O 0.0585218271 -1.7450513496 -0.9306049768
H 0.6055297905 -1.8773873833 -1.7285269540
H -0.6846406059 -2.3756931004 -0.8704443343
O -1.4319283357 -0.6997031501 1.2041643004
H -1.9881616932 -0.0421785847 1.6705981658
H -1.9566414693 -1.4620852618 0.8847935656
O -2.2676684121 -2.9929824464 -0.1038504367
H -2.2267430452 -3.8354689948 0.3710288440
O 1.9570563751 -1.3579687410 -2.9082058518
H 2.7552055692 -1.9051295903 -2.9304696821
O 1.8613748739 3.2398265925 -0.3901393908
H 1.6451395818 3.9308911431 -1.0323254245

O	-2.3690592764	1.5835340078	2.4431923280
H	-3.1908322671	2.0383476410	2.2097273820
H	-3.0580465558	-3.0495273698	-0.6594065829
H	-2.3107389835	1.6360405336	3.4075797997
H	2.6272453919	3.5729791044	0.0986310857
H	1.7259088293	-1.2033486213	-3.8351891386

10w-a E = -960.397723

Cu	-0.0317642884	-0.0642916232	-0.0082472172
O	1.5194133966	0.5309543532	-1.0288550155
H	1.8740068693	-0.0147550686	-1.7719159160
H	1.8506265105	1.4495817007	-1.0021191284
O	-0.1872895499	1.6839226444	0.8426519654
H	-0.7881991837	1.8163711653	1.6150688965
H	0.4564970963	2.4042823098	0.6978340302
O	-0.0790675831	-1.7071021132	-1.0575897620
H	0.6137824336	-1.8891400949	-1.7381501471
H	-0.6088803444	-2.485220688	-0.7967582441
O	-1.3809681366	-0.7652560532	1.2110784020
H	-1.8279292523	-0.1714223343	1.8625076325
H	-1.8263226524	-1.6229352574	1.0682957996
O	-1.9563816593	-3.2883085531	0.2264848260
H	-1.7386475038	-4.0636913478	0.7628957667
O	1.9705570790	-1.4630241107	-2.7527925540
H	2.7978676971	-2.0111934096	-2.6684058799
O	1.8881865050	3.1621684212	-0.2403660590
H	1.6888859083	3.9238419888	-0.8029720251
O	-2.0415326761	1.3211606803	2.7372572484
H	-2.9243018516	1.7759516041	2.6591964446
H	-2.7741976464	-3.5167987480	-0.2375428337
H	-1.8267646661	1.3124496686	3.6793064090
H	2.6859044232	3.4058986110	0.2501887242
H	1.8001382777	-1.3793661901	-3.7002272183
O	-4.4025812550	2.5099099940	2.4740977343
H	-5.2486139014	2.1179465250	2.7203800652
H	-4.5479455636	3.4624115920	2.4318121614
O	4.1643166453	-2.9360403869	-2.4733316015
H	4.2144023960	-3.8869826977	-2.6257127472
H	5.0696695739	-2.6068796945	-2.5196120075

10w-b E = -960.395785

O	1.7139101754	0.4781313899	-0.8316473719
H	1.9635982240	0.0117677289	-1.6526856454
H	1.8816814868	1.4499372573	-0.8869631492
O	0.0045006493	1.6875365361	1.0037937947
H	-0.7965232050	1.9904567483	1.4685368632
H	0.5254859551	2.4274691574	0.6142213977
O	3.8853891616	4.1575653625	0.7901359234
H	4.7739100443	4.1906430883	0.4167188784
H	3.8601810538	4.8242937370	1.4865659452
O	-0.1663293190	-1.6062469671	-1.1040337786
H	0.5136526767	-1.8507043773	-1.7614309164
H	-0.7989554227	-2.3292478084	-0.9318339264
O	-1.5024380681	-0.6839090653	1.1885152087
H	-2.0643258829	-0.0024747768	1.6119014320
H	-2.0295322489	-1.4438587727	0.8692768292

O	-2.3271754632	-3.0045358446	-0.0875039497
H	-2.2721155458	-3.8362442695	0.4036283067
O	1.9869354983	-1.4624858277	-2.8171242714
H	2.7645126883	-2.0361232904	-2.7721110756
O	1.7539699887	3.1356543934	-0.4317681109
H	1.4716679076	3.7799034102	-1.0934079896
O	-2.4756201302	1.6453692180	2.3017398965
H	-3.2608714058	2.1165204497	1.9898229977
H	-3.1180898743	-3.0826240068	-0.6393433818
H	-2.4977488245	1.7185908807	3.2663260756
H	2.5493495583	3.5327552160	0.0160655417
H	1.8178497519	-1.3301131132	-3.7604724872
Cu	0.1358620810	-0.1302414883	0.2049712235
O	1.4704176245	-1.1594739155	1.6508574363
H	2.4171628136	-0.9825935986	1.7013098483
H	1.2127808478	-1.5428948083	2.4973670760

10w-c E = -960.385801

Cu	-0.0037285806	0.0013027810	-0.0098551169
O	1.7005635170	0.5493817618	-0.9290337327
H	2.0091168783	0.0625510499	-1.7166806319
H	1.9594097890	1.4899321374	-0.9564399993
O	-0.1881512664	1.8422502023	0.7852898607
H	-0.7232695064	1.9721230911	1.5908159452
H	0.5570923497	2.4704081614	0.7378270808
O	1.4063814028	-0.8039132029	1.6429195726
H	1.1410870095	-1.2501947149	2.4547613521
H	2.3696489014	-0.7761231361	1.6427372031
O	-0.0579729246	-1.7008878635	-1.0831946843
H	0.7133202483	-1.9702757486	-1.6163536712
H	-0.5671674863	-2.4686468999	-0.7614874464
O	-1.4713192990	-0.6850411205	1.1839889026
H	-2.0193840157	-0.0585771196	1.6933617182
H	-1.9699034263	-1.4853426828	0.9326480580
O	-1.4208975123	0.8204542489	-1.6500563946
H	-1.7488624537	0.3456491202	-2.4218539975
H	-1.7938014235	1.7081406518	-1.6904149749
O	-2.0564813892	-3.2016564385	0.1423974430
H	-1.9350418047	-3.9515867613	0.7411975953
O	2.2109835546	-1.5362109670	-2.7002406782
H	3.0462115007	-2.0077318564	-2.5753134499
O	2.0431939101	3.2074913967	-0.1720862638
H	1.8635842860	3.9919471810	-0.7087473121
O	-2.2200698936	1.5476263583	2.6693804884
H	-3.0058920961	2.0959107054	2.5374260590
H	-2.8136388273	-3.4383806903	-0.4110428902
H	-2.1173064552	1.4770188408	3.6285810996
H	2.8539387306	3.4121432294	0.3141901213
H	2.0591053145	-1.5365934074	-3.6555174543

10w-d E = -960.395407

Cu	0.2524844244	0.3847913072	-0.0509644737
O	0.6197892615	-0.0637894125	1.8826700414
O	2.2101451348	0.4431109090	-0.3872049331
O	-0.0120887266	0.1160971773	-2.0159232320
O	-1.6948053825	0.0911554284	0.2454549754

H	0.0021584214	0.1174133592	2.6212463904
H	1.5395376216	-0.0232657996	2.2059456045
H	2.5736629106	0.1976199421	-1.2614544217
H	2.8465693733	0.2570753195	0.3335312598
H	-0.8638670077	-0.2013624505	-2.3765886461
H	0.7329084439	-0.0614041723	-2.6223422140
H	-2.1430950990	0.8048815410	0.7605778835
H	-2.2367717007	-0.1459908209	-0.5329654750
O	-0.0277449697	2.5506920475	0.3230273397
O	-2.3718962896	2.1205734633	1.8723871060
O	-1.2058859156	0.5611256452	3.9507617375
H	-3.1843493727	2.6367663510	1.9525816295
H	-2.1615792382	1.7730764069	2.7591206610
H	-1.7357969088	-0.1872975249	4.2598767972
H	-0.8651919678	0.9789059913	4.7542079975
H	-0.7907625666	2.8356941816	0.8522206445
H	0.3952899302	3.3307295051	-0.0518532169
O	2.5336209401	-0.1671374646	-3.0741703880
H	2.8780146464	0.5156828590	-3.6671666786
H	2.8905608145	-1.0026767158	-3.4065165118
O	-2.6444274352	-0.6334506229	-2.3015620076
H	-2.9276692370	-1.5474535458	-2.4457727439
H	-3.2503334218	-0.0892618160	-2.8238357713
O	3.4261508167	-0.0203764428	2.0343365681
H	3.9630889436	0.6792219933	2.4320928492
H	3.8736634819	-0.8490024379	2.2565010979

10w-e E = -960.381206

Cu	0.3484407268	-0.0074063791	-0.0095626328
O	0.5257503341	0.1031876123	2.0033340531
O	2.3890098468	0.0843652730	-0.0776597572
O	0.4012425313	-0.1017308848	-2.0312248786
O	-1.6491037076	-0.0693079980	0.1276485902
H	-0.0259775936	0.7496976993	2.5009332146
H	0.3592930693	-0.7718898936	2.3820662726
H	2.9191812651	-0.1316332437	-0.8548756593
H	2.9598383435	0.1330841156	0.6995108239
H	-0.1183441259	-0.7486032460	-2.5600722401
H	0.2442056715	0.7817275779	-2.3939166578
H	-2.1769917800	0.7481869933	0.2347172687
H	-2.1541761038	-0.8220176807	-0.2453762779
O	0.2467684510	-2.2718037703	0.3085726377
O	-2.2946057513	-2.4983952855	-0.9102012858
O	-1.1266349108	-1.9510873728	-3.4814796583
H	-3.0480866154	-3.0756531506	-0.7286886637
H	-2.1357875029	-2.5249475672	-1.8709150889
H	-1.6887253078	-1.6002740495	-4.1872659530
H	-0.6178999402	-2.6611320923	-3.8988366523
H	-0.5905353332	-2.6791759184	0.0191278402
H	0.9213937358	-2.9609252435	0.3054438096
O	0.1669893402	2.2359328522	-0.4167235281
O	-2.3317371470	2.4916348363	0.7839811972
O	-1.0984045193	1.9530322606	3.3552289893
H	-3.0881023334	3.0683982655	0.6142139632
H	-2.1570637504	2.5173709564	1.7418453555
H	-1.6625432719	1.5875122321	4.0519137484

H	-0.6188540638	2.6787785835	3.7802887346
H	-0.6667412217	2.6475945383	-0.1192064937
H	0.8524061166	2.9141936047	-0.3985169715

11w-4coord E = -1036.883000

Cu	3.5927042121	-6.5757777203	-0.2130974635
O	5.1842259565	-6.0518459501	-1.2142613320
H	5.5766321868	-6.6617549780	-1.8862897960
H	5.5003989287	-5.1299103239	-1.2639637189
O	3.3602946879	-4.7571138331	0.4588915029
H	2.7518039814	-4.5856157331	1.2186008990
H	4.0100250297	-4.0478970025	0.2921947541
O	3.5778993465	-8.2952545043	-1.1273625253
H	4.3131528901	-8.5540086326	-1.7267409975
H	3.0468858232	-9.0433576819	-0.7688153716
O	2.2478019730	-7.2116668249	1.0383047779
H	1.7565489434	-6.5921556198	1.6227800212
H	1.8554413199	-8.1106986335	0.9465156017
O	1.7956387064	-9.7407445373	0.2755156969
H	2.0426043477	-10.4664990785	0.8629113453
O	5.7619843158	-8.1721534807	-2.7207147466
H	6.5976714657	-8.6816512425	-2.5457695764
O	5.4779508205	-3.3489978389	-0.6489843254
H	5.2900941583	-2.6423734953	-1.2824272829
O	1.5120298314	-4.9859367879	2.3740358439
H	0.6257269722	-4.5505559738	2.2585429915
H	0.9539473000	-10.0205115912	-0.1724053657
H	1.7273762520	-4.9092014202	3.3125385904
H	6.2512025479	-3.0497453039	-0.1505044359
H	5.6407467281	-8.1776779411	-3.6790168005
O	-0.8727220118	-3.8479809721	2.0227539798
H	-1.7093776131	-4.2095214317	2.3373108216
H	-1.0284669392	-2.9108738615	1.8572298216
O	7.9895942130	-9.5377953313	-2.1982385256
H	8.0736222332	-10.4976288182	-2.2357046840
H	8.8864529012	-9.1861333383	-2.2404086421
O	-0.4732081696	-10.4226086557	-0.9469703708
H	-0.5363604468	-10.8889038060	-1.7885295966
H	-1.3278587409	-10.5302631287	-0.5137665686

11w-5coord E = -1036.881148

Cu	3.8284461411	-6.7043351368	0.0967856690
O	5.3349640776	-6.0524719350	-1.0182800649
H	5.5988816251	-6.5607153037	-1.8099730972
H	5.4281752685	-5.0792331602	-1.1475872616
O	3.6038532778	-4.8558618227	0.8078596654
H	2.7877010285	-4.5889790502	1.2690564260
H	4.0442317311	-4.1059959865	0.3473890412
O	3.5623944614	-8.2563742625	-1.1239041109
H	4.2534209340	-8.5388493269	-1.7491727406
H	2.9563373519	-8.9854615096	-0.8632303673
O	2.2883415028	-7.3248149658	1.1810382456
H	1.6688496393	-6.6707352265	1.5579595395
H	1.8337688584	-8.1573889386	0.9069883829
O	1.6035577723	-9.6772377747	0.0693416200
H	1.7512120310	-10.4925435021	0.5653462970

O	5.7419343121	-8.0931314008	-2.8567157751
H	6.5659846566	-8.5918905484	-2.7710876661
O	5.1839533940	-3.3711222466	-0.7956072598
H	4.8373404232	-2.7936441721	-1.4874136627
O	1.1641929304	-4.9715901318	2.1597883884
H	0.3437059213	-4.5665526707	1.8469494665
H	0.7454713328	-9.8001945996	-0.4153036902
H	1.1661789072	-4.8426536123	3.1184204665
H	5.9567867717	-2.8883210937	-0.3982854884
H	5.5661249525	-8.0466268965	-3.8066256394
O	-0.7145737062	-9.9312952459	-1.2332291828
H	-0.8116097246	-10.2642752541	-2.1330457240
H	-1.5723576177	-10.0514431306	-0.8090657556
O	7.2639508539	-2.1100244506	0.3005962204
H	8.1391087778	-2.0337835111	-0.0971332685
H	7.2044079446	-1.4073690779	0.9584985858
O	5.2786837289	-7.5732161671	1.5447313141
H	5.0495860107	-7.9347441304	2.4087123645
H	6.2039472917	-7.3057574461	1.5901918766

12w-coord4 E = -1113.367667

Cu	3.6062998034	-6.5666032518	-0.1765579333
O	5.2268673582	-6.0400747512	-1.1212789585
H	5.6020290367	-6.6128845811	-1.8280571819
H	5.5014464061	-5.0957722731	-1.1541710276
O	3.3542396384	-4.7409885630	0.4571322945
H	2.7583664720	-4.5545879086	1.2172598278
H	4.0236103687	-4.0456234712	0.2664343917
O	3.5850980402	-8.2771290487	-1.1102503973
H	4.3166899367	-8.5251227979	-1.7194346227
H	3.0526841212	-9.0286772135	-0.7635568869
O	2.2555390643	-7.2076016461	1.0697435396
H	1.7515265029	-6.5794792870	1.6354855278
H	1.8514841624	-8.0984150146	0.9621425289
O	1.7895856012	-9.7343297647	0.2712378893
H	2.0308918790	-10.4644043559	0.8551569838
O	5.7431295925	-8.1420899483	-2.7240325164
H	6.5711661953	-8.6686210710	-2.5764931452
O	5.4271958205	-3.3998233939	-0.6212692794
H	5.2391501471	-2.7242181301	-1.2851762883
O	1.4737524904	-4.9902656327	2.3743234932
H	0.5878871707	-4.5670353276	2.2300911129
H	0.9516744528	-10.0088823923	-0.1838849647
H	1.6611598424	-4.9084008143	3.3179839330
H	6.1974711436	-3.0613832610	-0.0949551986
H	5.6041956348	-8.1239435210	-3.6794474591
O	-0.9185832388	-3.8816437614	1.9304476961
H	-1.7597629210	-4.2246058454	2.2534842195
H	-1.0748788767	-2.9589064408	1.6985401199
O	7.9643482774	-9.5650191245	-2.2809556408
H	8.0300338240	-10.5252288950	-2.3379451574
H	8.8669046649	-9.2290197621	-2.3265021879
O	-0.4779605396	-10.4106316573	-0.9711153590
H	-0.5379727633	-10.8703362384	-1.8166057639
H	-1.3357711712	-10.5175870901	-0.5440772940
O	7.4935574556	-2.5173933289	0.8296635463

H 8.4246097386 -2.6018637665 0.5940228747
H 7.4464579225 -1.8280597072 1.5020107204

12w-coord5 E -1113.365387

Cu 3.8327446460 -6.6628451479 0.1616553546
O 5.3427379614 -6.0491490420 -0.9657937138
H 5.5349364433 -6.5556910946 -1.7866257280
H 5.4472848688 -5.0777986649 -1.0889158656
O 3.6669954288 -4.8328797066 0.9266271531
H 2.8312230042 -4.5780398944 1.3720638702
H 4.1004600205 -4.0836366563 0.4632771566
O 3.5167566467 -8.1734807849 -1.0991191363
H 4.1924651425 -8.3863680334 -1.7811093146
H 2.9641911955 -8.9369723295 -0.8552536809
O 2.2805166536 -7.2380378261 1.2606387961
H 1.7116772188 -6.5333076620 1.6533276321
H 1.7622112922 -8.0168136445 0.9816818834
O 1.4872006129 -9.6517311856 0.1083598261
H 1.5949403611 -10.4487252663 0.6450120341
O 5.5447460686 -7.9838381560 -2.8616624120
H 6.3774461250 -8.5193874985 -2.8147746499
O 5.2633198805 -3.3593628014 -0.7046953406
H 4.9392646614 -2.7450626218 -1.3747552870
O 1.2602186542 -4.9409158728 2.2127409850
H 0.4167140615 -4.5399263490 1.8792891869
H 0.6838596442 -9.7952368702 -0.4101310515
H 1.2621462086 -4.8025377478 3.1684554872
H 6.0654501643 -2.9332635096 -0.3060250385
H 5.3313889244 -7.8969606656 -3.7991211154
O -1.0145209574 -3.8796691287 1.2714406753
H -1.8927184155 -4.2549839226 1.4047494554
H -1.1489959395 -2.9441993140 1.0803045050
O 7.8052758357 -9.4091871570 -2.6557150321
H 7.8551986277 -10.3699186812 -2.7221584707
H 8.6820195031 -9.0788498413 -2.8838250661
O 7.4419720167 -2.2669680832 0.4044246383
H 8.3031758846 -2.1854900841 -0.0213071716
H 7.4342365800 -1.6238361887 1.1227515647
O 5.2634529389 -7.6276430045 1.5686657580
H 5.0662263596 -7.8705309745 2.4804967456
H 6.2108949123 -7.4553566637 1.5227100650

12w-coord6 E = -1113.355051

Cu 3.5920112573 -6.5538690994 -0.1587432985
O 5.2334251327 -5.9837175017 -1.1694376704
H 5.5258992888 -6.4871496209 -1.9497776670
H 5.4350664576 -5.0254514603 -1.2391367608
O 3.3389174461 -4.6653062608 0.4755489201
H 2.8530603345 -4.4915727839 1.3007908348
H 4.0549550948 -4.0129090594 0.3123135240
O 3.5740646632 -8.3337781791 -1.0928244103
H 4.3548960741 -8.6279083487 -1.5940302951
H 3.0902880459 -9.0786552173 -0.6748088967
O 2.2258966459 -7.2314842471 1.1475869906
H 1.6307530239 -6.6043806998 1.5947299442
H 1.7983760433 -8.0980340349 0.9700466235

O	1.7479283522	-9.7698637744	0.3197129916
H	1.9298781869	-10.4831229644	0.9439415595
O	5.7964258300	-8.1907576484	-2.7954721786
H	6.6709327431	-8.5815423229	-2.6654160922
O	5.4330134657	-3.3257994219	-0.6196042834
H	5.2266182704	-2.5976617973	-1.2186113422
O	1.3783746247	-4.9107236749	2.4597220770
H	0.5749071795	-4.3962378261	2.3048331140
H	0.9470436251	-10.0499942666	-0.1910938481
H	1.4963069644	-4.9172651183	3.4190960466
H	6.2476720282	-3.0521109652	-0.1275467605
H	5.6030098366	-8.3055420355	-3.7356386057
O	-0.4250494893	-10.4579425359	-1.1070275465
H	-0.4346706530	-11.1374252536	-1.7914719090
H	-1.3287599910	-10.4023680556	-0.7749481086
O	7.6431381695	-2.6398905794	0.7525482407
H	8.5321665058	-2.6164129764	0.3793545523
H	7.6499655047	-2.0238381327	1.4944373919
O	5.1263703997	-7.1613534989	1.4768958020
H	4.9402170050	-7.5589455538	2.3342767598
H	6.0740176116	-6.9915269668	1.4435354297
O	2.0607410979	-5.9712678932	-1.8074575774
H	1.6966767177	-6.5731962702	-2.4656804919
H	1.6398274098	-5.1155869608	-1.9431640073

16w-a E = -1419.290545

Cu	-0.6645741820	-2.6869958158	-3.2782253446
O	-1.1740065246	-3.2745278384	-5.0645263142
H	-2.0730181487	-3.6245582541	-5.2352318557
H	-0.7136863298	-2.8671855907	-5.8464904886
O	0.7525910570	-1.5818286818	-4.0321653170
H	1.5111917646	-1.2969216391	-3.4815850479
H	0.9185727494	-1.6232764778	-5.0112759640
O	-2.3466348730	-3.3229775503	-2.5238951656
H	-2.9769734267	-3.8344468677	-3.0726152263
H	-2.3977463609	-3.4821938630	-1.5443304721
O	0.1079006497	-2.5662589904	-1.4939517812
H	0.8667450196	-1.9711044476	-1.3210624966
H	-0.4763727602	-2.7586680301	-0.7119550877
O	-1.8528668725	-3.3440733664	0.0491328600
H	-1.7536709423	-4.1622285717	0.5916545663
O	-3.6335085060	-4.3646521655	-4.6777052337
H	-3.7442706953	-5.3082067316	-4.8456688114
O	0.5145171043	-2.0058581610	-6.6051475923
H	0.2673090346	-1.2564556478	-7.1982284192
O	2.2862392316	-0.9849886236	-1.8657806038
H	2.3460265851	-0.0635579019	-1.5864174483
H	-2.3365841058	-2.7237633637	0.6455066831
H	3.1759661885	-1.3819074156	-1.6991258602
H	1.1481403192	-2.5349625903	-7.1461806043
H	-4.4780711223	-3.9341275619	-4.9573564507
O	4.6917845891	-2.1233226804	-1.4535604297
H	5.4927612346	-1.9431910808	-1.9581172385
H	4.9733799352	-2.5659695179	-0.6452658136
O	-5.9069988212	-3.1305684004	-5.4284685468
H	-6.2070356134	-3.0059343439	-6.3356903851

H	-6.6739457314	-2.9786322328	-4.8652603462
O	-1.8087111270	-5.3509745573	1.8501908333
H	-1.4639307451	-6.2415177338	1.9650691911
H	-2.2184362017	-5.0779391853	2.6878925125
O	-3.0992898037	-1.9515655142	1.9868367879
H	-3.6179284835	-1.1492346302	2.0978661052
H	-3.2288617489	-2.5024113314	2.7771297546
O	2.2003073507	-3.1306984022	-8.3813287314
H	2.6274310958	-3.9775577996	-8.5417149034
H	2.1865952028	-2.6416648421	-9.2212443005
O	0.0626824225	-0.1806827933	-8.5380102595
H	-0.2413182222	0.7290812600	-8.6125834621
H	0.6187867362	-0.3703684963	-9.3122957994
O	1.8282815132	-1.2648456212	-10.5528291241
H	2.6105225478	-0.7691545292	-10.8277420739
H	1.4076798939	-1.5561991882	-11.3721677079
O	-3.1439979038	-3.9949958606	4.0253116737
H	-2.6492855477	-3.8136422049	4.8349373534
H	-3.9925893325	-4.3523451811	4.3172612704

16w-b E = -1419.289717

Cu	0.2407152986	-0.0173335243	0.0380905638
O	0.5141404257	0.1655477412	2.0305985988
O	2.2081652029	-0.1825561979	-0.2588595616
O	-0.0050314497	0.0698177838	-1.9599213621
O	-1.7466651007	-0.0006678620	0.2956134294
H	-0.1840121011	0.6439988598	2.5241907632
H	0.7401627175	-0.6715526075	2.4903886411
H	2.6077855794	0.4339280188	-0.8972262087
H	2.8733173548	-0.6263700083	0.3112435340
H	-0.1516013341	-0.7578787688	-2.4759826020
H	0.7138010104	0.5891786927	-2.3725916452
H	-2.1702538074	0.8867026280	0.2906569173
H	-2.2301825058	-0.6197080778	-0.2915068142
O	-0.0239495300	-2.4308658029	0.2425264641
O	3.7300567451	-1.8397488145	1.2708861896
O	-2.5171547859	-2.2152527706	-1.1079960362
O	-0.5525720695	-2.3119102765	-3.1608334056
O	1.2272920403	-3.8515212702	-1.7400945141
O	1.3213668109	-2.3804869031	2.5917554769
O	3.7645647010	-3.2141898987	-1.2522904764
H	4.5330406165	-1.6662819961	1.7770688164
H	3.0538004443	-2.1605225837	1.9020373250
H	-3.3859853477	-2.6340456894	-1.1206934027
H	-2.1161229746	-2.3472884052	-1.9877204929
H	-0.6605196846	-2.4052138400	-4.1160514063
H	0.1349723688	-2.9539640421	-2.8769991088
H	2.1979426441	-3.6579843241	-1.6547059705
H	1.1458505628	-4.8126993058	-1.7629098140
H	1.1765847355	-2.9634718338	3.3467903373
H	0.7414001885	-2.6849030677	1.8588752247
H	4.5638530772	-3.6514763181	-1.5663610390
H	3.9429549689	-2.8752398636	-0.3590360549
H	-0.9710832531	-2.5888970859	0.0761945201
H	0.4461943725	-2.9879332179	-0.4209825324
O	0.3775552084	2.4197248181	-0.0173174233

O	-2.3764186494	2.6044194155	0.6950549757
O	-1.1365534841	2.1070864861	3.1811657164
O	1.0642016592	3.7489336588	2.5291030922
H	-3.1631157244	3.1282726739	0.4990541969
H	-2.2444058055	2.6077276050	1.6613458321
H	-1.5481305933	2.0752272677	4.0547667757
H	-0.4273301019	2.7782903804	3.2199054777
H	1.9032922163	3.5754196284	2.9761892385
H	0.9934117758	4.7126763625	2.4916780614
H	-0.5413002998	2.7450006318	-0.0445773921
H	0.7593641943	2.8270693956	0.7812900291
O	2.1005121470	1.8153191439	-2.1305639424
H	1.6173707765	2.4557534408	-1.5788176258
H	2.5953541444	2.3042826124	-2.7989185933

17w-4coord E = -1495.769702

Cu	-0.7150347961	-2.6937272565	-3.3044093975
O	-1.2449414382	-3.2972363091	-5.0795265220
H	-2.1470066550	-3.6417781073	-5.2386055111
H	-0.7917925050	-2.8905247124	-5.8681108201
O	0.6748952064	-1.5740517751	-4.0847667996
H	1.4514281537	-1.3025263117	-3.5532860485
H	0.8207085846	-1.6285902366	-5.0696145143
O	-2.3834334152	-3.3328058095	-2.5201600488
H	-3.0199516843	-3.8485671481	-3.0569525143
H	-2.4192906902	-3.4896466562	-1.5405321939
O	0.0897184486	-2.5716061846	-1.5335224923
H	0.8546813036	-1.9796039808	-1.3760368120
H	-0.4795376838	-2.7608998646	-0.7402226749
O	-1.8452278765	-3.3424730775	0.0487584488
H	-1.7362701717	-4.1560839199	0.5955992212
O	-3.7041794490	-4.3880254084	-4.6426142755
H	-3.8094811662	-5.3325656016	-4.8076568379
O	0.4106597957	-2.0323772762	-6.6361775768
H	0.1596307008	-1.2919927349	-7.2431615650
O	2.2714480841	-1.0050728750	-1.9521446074
H	2.3495091009	-0.0841005083	-1.6761514787
H	-2.3130972168	-2.7157164160	0.6503789327
H	3.1610438982	-1.4114694943	-1.8127403777
H	1.0654518977	-2.5543908225	-7.1652200114
H	-4.5583344487	-3.9669646788	-4.9059478260
O	4.6754525151	-2.1766996578	-1.6203813765
H	5.4519824017	-2.0326586554	-2.1728116952
H	4.9910829003	-2.6028072681	-0.8157919876
O	-6.0103806321	-3.1830698628	-5.3487732243
H	-6.3108832359	-3.0222799330	-6.2500346677
H	-6.7794205617	-3.0613258368	-4.7809044790
O	-1.7605894396	-5.3315152630	1.8710284235
H	-1.4215841878	-6.2243378488	1.9856650526
H	-2.1430541883	-5.0460338520	2.7172434105
O	-3.0323794303	-1.9212739185	2.0046996405
H	-3.5668597598	-1.1287668658	2.1109386527
H	-3.1430673152	-2.4632479481	2.8040782601
O	2.1872720811	-3.1020857784	-8.3217328911
H	2.4598155838	-3.9910020268	-8.5677569007
H	2.1886746394	-2.5559652070	-9.1321427318

O	-0.0158127983	-0.2505122731	-8.5883174376
H	-0.2824869270	0.6699544243	-8.6664699059
H	0.6269395606	-0.4353995221	-9.2999687515
O	1.9336130704	-1.2041682346	-10.3736610234
H	2.7213234052	-0.6720568875	-10.5376795539
H	1.6113507369	-1.4886471578	-11.2585706514
O	-3.0208250793	-3.9417701866	4.0696862250
H	-2.4978497790	-3.7494629936	4.8592104120
H	-3.8585115621	-4.2932078534	4.3978020880
O	1.0178817855	-2.0119772588	-12.8078691429
H	1.4243555506	-2.6677724939	-13.3852889924
H	0.3769572328	-1.5374266786	-13.3480620406

17w-5coord E = -1495.768529

Cu	-0.3390332799	-3.2991183403	-3.2849947050
O	-0.9926247527	-3.6037245008	-5.1359718610
H	-1.9574848616	-3.7360101408	-5.2496870441
H	-0.6140733379	-3.0035088655	-5.8301101513
O	1.1508017830	-2.2023283299	-4.0211357222
H	1.5878676383	-1.5469236192	-3.4418501620
H	1.0702964416	-1.9029526851	-4.9612923194
O	-2.0947796085	-3.8745051344	-2.5589326544
H	-2.8727620893	-3.9639009811	-3.1431098185
H	-2.3130468767	-3.6696168362	-1.6164797654
O	0.2555835331	-2.8784100648	-1.4360663396
H	0.8497339226	-2.1067624889	-1.3300071180
H	-0.4576462562	-2.8937668443	-0.7436320720
O	-1.9435764068	-3.2190015750	-0.0037836943
H	-1.9176170379	-3.9577003619	0.6497577069
O	-3.6564211852	-4.1378979081	-4.7862642861
H	-3.9443489363	-5.0315698728	-5.0082851341
O	0.4734084624	-1.9262474470	-6.5592934496
H	0.1384332480	-1.1140236767	-7.0040377824
O	2.0598160226	-0.8488698373	-1.8258307326
H	1.9104314943	0.0834036155	-1.6306805857
H	-2.4275096248	-2.5037037927	0.4678876036
H	2.9876769088	-1.0433734397	-1.5489114238
H	1.0590655768	-2.3444785248	-7.2333003464
H	-4.3941318909	-3.5390190900	-5.0508470299
O	4.5860968122	-1.4565462570	-1.0990330004
H	5.3772209603	-1.2846244457	-1.6216116744
H	4.8867558777	-1.6350828586	-0.2010922804
O	-5.6673293623	-2.4702340848	-5.5008495199
H	-5.8849853580	-2.2213037652	-6.4060282287
H	-6.4613148110	-2.3098362649	-4.9787780529
O	-1.9951933759	-4.9754815051	2.0471631977
H	-1.9545874295	-5.9292072368	2.1658913372
H	-2.4596005598	-4.6005703051	2.8139281073
O	-3.2232941165	-1.5398067433	1.7045653185
H	-3.7470150800	-0.7330556068	1.7141745938
H	-3.3710355302	-1.9955558390	2.5502303511
O	1.9111825639	-2.8099337680	-8.6674105179
H	2.6317317186	-3.4158158650	-8.8643064369
H	1.8089227876	-2.2116030995	-9.4260308303
O	-0.2814731628	0.1178470283	-8.1770302151
H	-0.5432429030	1.0407816477	-8.1030138584

H	0.1588499397	0.0082974491	-9.0369033438
O	1.1667623069	-0.7407733215	-10.5360293524
H	1.8493098647	-0.1773177866	-10.9226740504
H	0.6141479349	-1.0202159845	-11.2773615020
O	-3.3417132723	-3.3171559433	3.9869929269
H	-2.8125008152	-3.0639022946	4.7543650622
H	-4.2003492922	-3.5804742775	4.3423425386
O	0.6980165028	-5.2786084895	-3.2583970159
H	1.3412559148	-5.5392200614	-2.5905166160
H	0.8440951689	-5.8350174602	-4.0308690870

18w-a E = -1572.254731

Cu	0.2306700975	0.0103763402	-0.0162487910
O	0.5528894733	0.1225916212	1.9614182800
O	2.1882591397	-0.2082934756	-0.3101594227
O	-0.0628610202	0.1422778434	-2.0007983304
O	-1.7559152371	-0.1025850772	0.2671621059
H	0.0766997662	0.7759207112	2.5206735993
H	0.6441563573	-0.7309146497	2.4346035322
H	2.7304605450	0.5062219170	-0.7148280282
H	2.7202357325	-0.6527794866	0.3866879130
H	-0.0165959139	-0.6719445026	-2.5549481020
H	0.3907676927	0.8827728459	-2.4505806084
H	-2.2435463705	0.7047095110	0.5352567552
H	-2.2333897815	-0.5980177317	-0.4276813895
O	-0.0399076981	-2.4408797983	0.1236833514
O	3.5236996292	-1.8415401151	1.4348892139
O	-2.4151235101	-2.1813816366	-1.4168875127
O	-0.2388299942	-2.2328316436	-3.2836254031
O	1.3705047003	-3.8571418795	-1.7663093619
O	1.0750269976	-2.4761275066	2.5850256695
O	3.8631446962	-3.3610803324	-0.9699515338
H	4.2575186456	-1.5909785060	2.0088008725
H	2.8117283985	-2.1830684153	2.0155155119
H	-3.2630710153	-2.6277901283	-1.5269736806
H	-1.9290816106	-2.2723643031	-2.2572210958
H	-0.2453166490	-2.3270568890	-4.2439625019
H	0.4187416975	-2.8731618034	-2.9303720829
H	2.3336384736	-3.7113968706	-1.5698572809
H	1.2525218943	-4.8124325243	-1.8368638343
H	0.8576410432	-3.0663425424	3.3160604205
H	0.5472676368	-2.7474629475	1.8013814479
H	4.6532177910	-3.8947856588	-1.1044042687
H	3.9284993713	-2.9471407091	-0.0918560956
H	-0.9732291482	-2.5709788448	-0.1242431405
H	0.4721237887	-3.0001557338	-0.5037043220
O	-0.0012345845	2.4917100725	-0.1134223730
O	3.5514370107	1.8813604769	-1.4155324299
O	-2.4979102703	2.3524794690	1.1963414524
O	-0.5658502464	2.2477548827	3.2610560744
O	1.3114828898	3.7644055583	1.9372407418
O	1.1526953524	2.5771238895	-2.5562292379
O	3.7622658798	2.9478775777	1.2312424295
H	4.3282464178	1.7403791514	-1.9707160697
H	2.8567864771	2.2761140777	-1.9861620257
H	-3.3525049226	2.7999967045	1.2156831289

H	-2.0994234481	2.4315244988	2.0847403468
H	-0.6866864657	2.2885678609	4.2176974185
H	0.1441754540	2.8856502570	3.0287850810
H	2.2560535331	3.4960601242	1.7943053493
H	1.3119256534	4.7270716724	2.0052907125
H	0.9523734784	3.2078048673	-3.2579536050
H	0.6465804044	2.8405138458	-1.7557794627
H	4.5960001543	3.3493837702	1.4988728965
H	3.8447348807	2.7013340188	0.2927079067
H	-0.9444782049	2.6489157715	0.0762905211
H	0.4798646264	3.0123841725	0.5699143509

18w-b E = -1572.248654

Cu	-0.7103767461	-2.6629728005	-3.2818814645
O	-1.2572152541	-3.2798130334	-5.0482389567
H	-2.1605445581	-3.6264746348	-5.1969315769
H	-0.8082747425	-2.8832024267	-5.8444483718
O	0.6765178772	-1.5524246500	-4.0807151861
H	1.4553048404	-1.2752711345	-3.5558488105
H	0.8162730676	-1.6144727927	-5.0652079723
O	-2.3809123526	-3.2697704936	-2.4797241590
H	-3.0157180312	-3.8012942600	-3.0030837253
H	-2.3971573673	-3.4225582401	-1.4957629751
O	0.1195179581	-2.5526055941	-1.5218059778
H	0.8758907726	-1.9502959289	-1.3699531042
H	-0.4492180542	-2.7411345488	-0.7246140480
O	-1.8014864206	-3.2980911424	0.0656928731
H	-1.7235696952	-4.1307790772	0.5944963680
O	-3.7093131605	-4.3715177237	-4.5815897586
H	-3.8094937007	-5.3194004037	-4.7294199039
O	0.3972146191	-2.0341910924	-6.6275794595
H	0.1465773519	-1.3016439161	-7.2432231323
O	2.2844471803	-0.9584125591	-1.9680716085
H	2.3545348456	-0.0350786635	-1.6982613035
H	-2.2474795945	-2.6700139336	0.6871299310
H	3.1773157456	-1.3560659589	-1.8276787901
H	1.0512625567	-2.5628687472	-7.1499876948
H	-4.5700170925	-3.9608516172	-4.8383322771
O	4.6992218170	-2.1117985835	-1.6284660813
H	5.4779653659	-1.9628908913	-2.1759630415
H	5.0092599943	-2.5460414229	-0.8262489814
O	-6.0371764559	-3.1918214545	-5.2642631864
H	-6.3639992499	-3.0569970084	-6.1605832601
H	-6.7879009506	-3.0517751359	-4.6767834211
O	-1.8740622865	-5.3443248191	1.7888500374
H	-1.3718432175	-6.1409867903	1.9821307930
H	-2.2602860263	-5.0228800737	2.6265607820
O	-2.9193138855	-1.9043236658	2.0556161670
H	-3.5258733153	-1.1645396916	2.1507304601
H	-3.0850037228	-2.5222286308	2.7943393809
O	2.1771372512	-3.1257908181	-8.2993586098
H	2.4420173456	-4.0187040004	-8.5385863089
H	2.1821037213	-2.5869017169	-9.1146135485
O	-0.0223325554	-0.2743777575	-8.6047448085
H	-0.2937356196	0.6432181973	-8.6989332954
H	0.6214145483	-0.4689822626	-9.3130869176

O	1.9319957622	-1.2521239986	-10.3750236386
H	2.7178915903	-0.7206660471	-10.5473193231
H	1.6113708776	-1.5519595219	-11.2557744146
O	-3.1152256569	-3.9976083981	3.9155314399
H	-2.6172686547	-3.8647664099	4.7538609755
H	-3.9836375403	-4.3283050651	4.1729148652
O	-1.7035865378	-3.6122438278	6.2127104962
H	-1.3598310572	-4.2965646570	6.7971092688
H	-1.6731326119	-2.7888673285	6.7117340329
O	1.0186488125	-2.1050423993	-12.7964396201
H	1.4391548314	-2.7523002973	-13.3728313436
H	0.3560548366	-1.6549238128	-13.3314341828

18w-c (5coord) E = -1572.247451

Cu	-0.3430742234	-3.4315576842	-3.2984282879
O	-0.9981830288	-3.7941299426	-5.1377452248
H	-1.9628856326	-3.9240682881	-5.2450801882
H	-0.6204031336	-3.2053414654	-5.8464371307
O	1.1431391797	-2.3586301342	-4.0732498215
H	1.5795447139	-1.6845152973	-3.5160501608
H	1.0444189744	-2.0800791916	-5.0199865149
O	-2.1014413541	-3.9814082556	-2.5532405102
H	-2.8789245133	-4.0883871236	-3.1351946281
H	-2.3230045931	-3.7289346988	-1.6237002032
O	0.2523530695	-2.9511677619	-1.4641210261
H	0.8503034541	-2.1794660235	-1.3855948569
H	-0.4640641913	-2.9333494367	-0.7757139099
O	-1.9619937981	-3.1949047320	-0.0342639175
H	-1.9631286715	-3.8860224035	0.6694093927
O	-3.6718303594	-4.3319292410	-4.7615771365
H	-3.9340946723	-5.2412966789	-4.9485506478
O	0.4201818981	-2.1308426367	-6.5909907402
H	0.0584175894	-1.3216589143	-7.0248309790
O	2.0614701628	-0.9382100342	-1.9208811069
H	1.9186390275	-0.0003378821	-1.7488239331
H	-2.4248580152	-2.4323715007	0.3810134124
H	2.9928597336	-1.1274347134	-1.6539210967
H	1.0291761207	-2.5073970341	-7.2730005227
H	-4.4264824205	-3.7669145806	-5.0500636539
O	4.6037093408	-1.5252594049	-1.2193255909
H	5.3834986156	-1.3944624610	-1.7701505952
H	4.9250876545	-1.6786630850	-0.3239915264
O	-5.7435492125	-2.7683909310	-5.5556704479
H	-5.9296047842	-2.5203762747	-6.4679931927
H	-6.5653820263	-2.6418541969	-5.0686641822
O	-2.0792698149	-4.7889106929	2.1437990996
H	-2.0691516297	-5.7300560822	2.3419726007
H	-2.5193813120	-4.3350099408	2.8811092664
O	-3.1641240723	-1.3314509119	1.5305550263
H	-3.7090557739	-0.5422987722	1.4567146824
H	-3.3284716571	-1.7191211902	2.4066141284
O	2.0113151828	-2.7831447155	-8.6450120109
H	2.3822402959	-3.5751680623	-9.0441293562
H	1.8918420938	-2.1189801054	-9.3512541249
O	-0.3422053061	-0.0868803497	-8.1691528320
H	-0.6376230093	0.8228844893	-8.0723059854

H	0.2100791878	-0.1308110606	-8.9741321192
O	1.4154642107	-0.6046498525	-10.3118544511
H	2.1476715102	0.0051103793	-10.4589946137
H	1.0230800902	-0.7723123166	-11.1986277837
O	-3.3372024214	-2.9214645449	3.9488992317
H	-2.7897696241	-2.6247813209	4.6874644601
H	-4.2000467783	-3.1229114459	4.3331206089
O	0.3286533643	-1.0993394280	-12.7609596078
H	0.7094613889	-1.6540626162	-13.4503284848
H	-0.3703921817	-0.5863547044	-13.1802229767
O	0.6836317211	-5.4142776303	-3.2140501014
H	1.3307480138	-5.6588949178	-2.5439798789
H	0.8326264548	-5.9811109546	-3.9782989959

18w-d (6coord) E = -1572.239177

Cu	-0.5303294273	-2.9049381401	-3.3013785062
O	-1.1536744965	-3.3274846866	-5.1486429385
H	-2.1054416592	-3.4949122553	-5.2884987791
H	-0.7281900122	-2.8155518449	-5.8809044420
O	1.2445548203	-2.3199008674	-4.0481493140
H	1.6626167304	-1.6277596144	-3.4975060417
H	1.2035037275	-2.0460417533	-4.9954932964
O	-2.3978899809	-3.0879697601	-2.5654247323
H	-3.0272856967	-3.6056073771	-3.1066149396
H	-2.4503947958	-3.3102571206	-1.6005158279
O	0.1938898918	-2.7221713704	-1.4487764135
H	0.7815471290	-1.9482464172	-1.3298177741
H	-0.4757353003	-2.8000350099	-0.7239195139
O	-1.9453639682	-3.2912430477	0.0307431769
H	-1.8707892096	-4.1437011821	0.5184540879
O	-3.7608563017	-4.1210548658	-4.7059237814
H	-3.9046872616	-5.0605207943	-4.8702122632
O	0.5831108569	-1.9896959234	-6.6396396843
H	0.4611305513	-1.1534120009	-7.1406683361
O	2.0021497465	-0.7333950858	-1.9191644991
H	1.7564283153	0.1957134959	-1.8427701925
H	-2.3930951358	-2.6904414891	0.6686011708
H	2.9199336178	-0.8048876420	-1.5659924062
H	1.0466783373	-2.5794720611	-7.2795538827
H	-4.5963641643	-3.6690582731	-4.9678553439
O	4.5320483436	-0.9523047049	-0.9692397376
H	5.3411146541	-0.8529533168	-1.4825999373
H	4.8012416646	-1.0081272467	-0.0459071788
O	-6.0474217751	-2.8345778148	-5.4138364231
H	-6.3141555579	-2.6496360620	-6.3212656927
H	-6.8533577944	-2.8059879997	-4.8860538520
O	-1.8575450028	-5.4100808898	1.7134873698
H	-1.7467806915	-6.3653403110	1.6905372683
H	-2.2506032834	-5.1767582173	2.5708706642
O	-3.1221429743	-1.9804365803	2.0950755321
H	-3.6136100817	-1.1787773610	2.2974440501
H	-3.1980703688	-2.5752626252	2.8600210872
O	1.7206152887	-3.3727124047	-8.6694499271
H	2.3526855511	-4.0919632363	-8.7630814097
H	1.7894480202	-2.8161497881	-9.4632250941
O	0.3966616704	0.0637756149	-8.4410215274

H	0.3216853365	1.0216824854	-8.4893263600
H	0.7718723982	-0.2397338168	-9.2849888657
O	1.5491050754	-1.3332885035	-10.7009781398
H	2.3486085696	-0.9862480820	-11.1168708237
H	0.9459752148	-1.5326946883	-11.4281622349
O	-3.0388937030	-4.1328054993	4.0154889363
H	-2.4520395357	-4.0084697123	4.7726778738
H	-3.8657801300	-4.4706364615	4.3826022298
O	-1.2456344500	-0.5575213615	-3.2933540208
H	-2.1529797152	-0.6318721097	-2.9735987523
H	-1.2518304667	0.1463189173	-3.9513663889
O	0.0680125984	-5.1303157509	-3.0792480246
H	0.7809077822	-5.2568399963	-2.4423756625
H	0.3157176186	-5.6257448336	-3.8680601816

21w-5coord E = -1801.680898

Cu	-1.1452504322	-1.8726777473	-3.2900043824
O	-1.6325805740	-2.4912034129	-5.1102157851
H	-2.2814961674	-3.2277544496	-5.1903041742
H	-0.9192020996	-2.5129297429	-5.7908497494
O	0.5062335241	-1.0504286206	-4.0272792960
H	1.2776602717	-1.0266127645	-3.4098910343
H	0.7644369880	-1.3629786309	-4.9284539899
O	-2.7092612153	-2.8499163275	-2.5476283890
H	-3.1309112908	-3.4987952425	-3.1628668512
H	-2.5788494611	-3.2285390739	-1.6449076451
O	-0.4094448069	-1.6844226801	-1.4515726296
H	0.5617420444	-1.5325615703	-1.3745520198
H	-0.7572364212	-2.3102924492	-0.7732383707
O	-1.8917019166	-3.4072946293	-0.0701704598
H	-1.5919397692	-4.2722071390	0.2838033714
O	-3.5634582790	-4.2635398093	-4.6464946998
H	-3.5343907577	-5.2393439041	-4.7469439535
O	0.5907821956	-2.0680062618	-6.4919078078
H	0.5089426377	-1.4280006864	-7.2342479437
O	2.1320113620	-1.0367420933	-1.9113671791
H	2.4151118024	-0.1408862543	-1.6202142752
H	-2.4055460613	-3.0104102746	0.6689612025
H	2.9369012728	-1.5883121997	-1.8029654910
H	1.2224809716	-2.7405056771	-6.8249691254
H	-4.4597424658	-4.0178726528	-4.9693864998
O	4.6160119034	-2.1278911834	-1.5576885192
H	5.2146686427	-1.4300989788	-1.2439913272
H	5.0138088513	-2.9725259982	-1.3267647297
O	-6.1209976165	-3.9842720648	-5.5338521791
H	-6.6592621312	-3.2992567537	-5.9411443124
H	-6.4882585609	-4.8437995768	-5.7964800459
O	-1.2023196937	-5.6316621899	1.3726245982
H	-0.9975357273	-6.5611271121	1.2346955459
H	-1.5850901648	-5.5477369592	2.2615174617
O	-3.1321113313	-2.5829133421	2.2022297367
H	-3.8580303490	-2.0006094631	2.4451766586
H	-3.0467941922	-3.2548974555	2.8980217467
O	2.3581784880	-3.6496073430	-7.8506466642
H	2.8397828846	-4.4801589040	-7.7937483368
H	2.4985816740	-3.2876161528	-8.7408956654

O	0.5945380780	-0.5644485059	-8.7553902467
H	0.2868605846	0.2904524436	-9.0702856068
H	1.1947658881	-0.9316030534	-9.4240165690
O	2.4441196414	-2.1389480675	-10.3245086300
H	3.2927621054	-1.7516963101	-10.5738808591
H	2.0972253859	-2.5431134992	-11.1299309013
O	-2.4426961283	-4.8367795037	3.8817749402
H	-1.8208546195	-4.6293540902	4.5909923811
H	-3.1277733670	-5.3808094869	4.2904212454
O	3.2908188709	1.3007162694	-1.1374672863
H	3.0148435519	2.1168448549	-0.7107070732
H	4.2263662391	1.1569963857	-0.9211549343
O	-3.9797587346	-6.9437024387	-5.0391808842
H	-4.8674334277	-7.0690647485	-5.4133459769
H	-3.4833362773	-7.7514506661	-5.2004864778
O	-6.7145025379	-6.7793517890	-6.0069009332
O	5.9920254435	0.3084665836	-0.7851088694
H	-7.3781118936	-7.1516054608	-5.4120905432
H	-6.9508683437	-7.0956551465	-6.8880788425
H	6.4448119909	0.3799172605	0.0646696535
H	6.6210366212	0.6353895221	-1.4410111972
O	-2.2706273975	0.0767391079	-3.3427690209
H	-3.0904540659	0.2369200678	-2.8639893459
H	-1.8640071737	0.9327980813	-3.5141075351

22w-6coord E = -1878.149633

Cu	-0.4798018055	-2.9716133772	-3.2728899711
O	-1.0448590657	-3.4548600783	-5.1218888793
H	-2.0076025205	-3.6208562832	-5.2439630067
H	-0.6557414490	-2.8898176335	-5.8299118164
O	1.3043694312	-2.3902922607	-3.9852915262
H	1.7560288761	-1.7553625039	-3.3824105372
H	1.2524827967	-2.0444719476	-4.9049905941
O	-2.3702932266	-3.1253012960	-2.6041507004
H	-2.9807446885	-3.6318739414	-3.1919089174
H	-2.4636668270	-3.3559123836	-1.6504833847
O	0.2069412046	-2.7816429606	-1.4097676156
H	0.8536676093	-2.0481799840	-1.2956894407
H	-0.4795461147	-2.8022305467	-0.7031885165
O	-1.9995183443	-3.2785634529	0.0329234545
H	-1.9342605394	-4.0995873199	0.5674062632
O	-3.6012512428	-4.1527868628	-4.7199383799
H	-3.7485499697	-5.1154351857	-4.8451774429
O	0.6128533329	-1.9428360080	-6.5612202447
H	0.4036314186	-1.1020832706	-7.0184106550
O	2.1884899531	-1.0387683584	-1.8303841156
H	2.2057776870	-0.0667995218	-1.7007921271
H	-2.4725450577	-2.6495945558	0.6185935581
H	3.0732538989	-1.3350982656	-1.5236705000
H	1.1311178092	-2.4497371231	-7.2244309230
H	-4.4364400929	-3.7401105830	-5.0280807145
O	4.7617535495	-1.4704280560	-1.0185687212
H	5.2077637572	-0.6298518091	-0.8263299077
H	5.2844113731	-2.1757704166	-0.6260930713
O	-6.1003973807	-3.4545444419	-5.5914990008
H	-6.5722604483	-2.7037790730	-5.9639131519

H	-6.5655666791	-4.2597603696	-5.8718793077
O	-1.9327603601	-5.2980554496	1.8758367162
H	-1.9003855495	-6.2588542382	1.8982901398
H	-2.3390566026	-4.9986673275	2.7052744337
O	-3.2226395599	-1.8283871133	2.0109872141
H	-3.8758599798	-1.1260197691	2.0833480000
H	-3.3141138297	-2.3903809732	2.7981040692
O	1.9176791621	-3.0939826663	-8.6681099342
H	2.6441999128	-3.7142683308	-8.7808241167
H	1.9216243815	-2.4973935602	-9.4344379429
O	0.2020271059	0.1629539826	-8.2933699581
H	0.0605375565	1.1140980889	-8.2907840197
H	0.6127635684	-0.0644486182	-9.1436352257
O	1.4784424803	-1.0127120244	-10.6261233992
H	2.2143325791	-0.5660195589	-11.0632324667
H	0.8732015560	-1.2665848892	-11.3345428602
O	-3.1035523247	-3.8481074819	4.0900652354
H	-2.4809315044	-3.6388136972	4.7980332303
H	-3.9004791430	-4.1656098912	4.5332043244
O	2.7384394808	1.6313972041	-1.4224751613
H	2.2861221735	2.3840361888	-1.0296203665
H	3.6661259742	1.6792095243	-1.1378211770
O	-4.3945212866	-6.7170481070	-5.2184218970
H	-5.3096372544	-6.7356768959	-5.5417881007
H	-4.1081979546	-7.6256964295	-5.0895832544
O	-7.0580705306	-6.1308928850	-6.1733258510
O	5.5491730071	1.2964032117	-0.7503217359
H	-7.8187089614	-6.4193223237	-5.6530167669
H	-7.2591502618	-6.3796145316	-7.0843928352
H	5.9141509976	1.6431672984	0.0735081643
H	6.1446572082	1.6036237438	-1.4456714327
O	0.0793970583	-5.2263660184	-3.0551818515
H	0.8090638939	-5.3691722990	-2.4420139060
H	0.3427996518	-5.6239662158	-3.8926884474
O	-1.2992979132	-0.6568173777	-3.3733057932
H	-2.2179235179	-0.7359977540	-3.0916493988
H	-1.1640179862	0.2546226765	-3.6513962880