

Supporting Information for

Computational Design of Next Generation Atom Transfer Radical Polymerization Ligands

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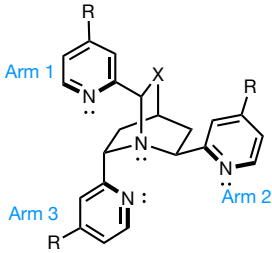
*Email: michael.sherburn@anu.edu.au michelle.coote@anu.edu.au

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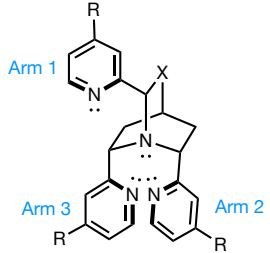
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Table S1. Copper(I)-nitrogen distances in the Cu^I/L complex for the four possible donor nitrogens.

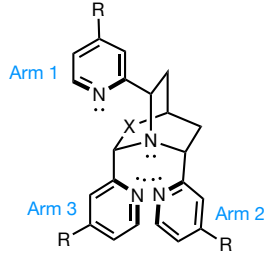
The mean of the distances between copper and the nitrogen donors in each arm is also given. Distances are highlighted according to their relative favorability, with red being less favorable and green being most favorable. The axial distances have a different scale to the individual arm distances and also to the mean arm distances (so that there are three separate scales).



L1



L2

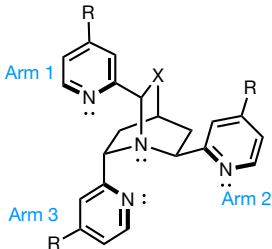


L3

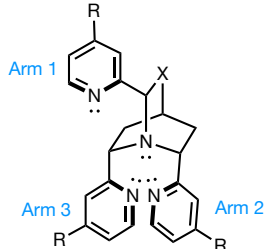
R		X = O					X = CH ₂				
		Axial (Å)	Arm 1 (Å)	Arm 2 (Å)	Arm 3 (Å)	Mean Arm (Å)	Axial (Å)	Arm 1 (Å)	Arm 2 (Å)	Arm 3 (Å)	Mean Arm (Å)
	1a	2.12	2.13	2.11	2.13	2.13	2.12	2.10	2.10	2.10	2.10
	2a	2.23	1.98	3.37	1.98	2.44	2.12	2.08	2.20	2.16	2.15
	3a	2.13	2.09	2.16	2.23	2.16	2.12	2.08	2.20	2.16	2.15
	1b	2.13	2.13	2.11	2.13	2.12	2.13	2.10	2.10	2.10	2.10
	2b	2.23	1.98	3.30	1.98	2.42	2.12	2.08	2.19	2.16	2.14
	3b	2.13	2.08	2.14	2.24	2.16	2.12	2.08	2.19	2.16	2.14
	1c	2.13	2.12	2.11	2.12	2.12	2.13	2.09	2.09	2.09	2.09
	2c	2.21	1.99	3.30	1.99	2.43	2.19	1.98	3.16	1.98	2.37
	3c	2.13	2.06	2.08	2.45	2.20	2.19	1.98	3.16	1.98	2.37
	1d	2.12	2.13	2.11	2.13	2.12	2.13	2.10	2.10	2.10	2.10
	2d	2.12	2.10	2.44	2.09	2.21	2.12	2.08	2.18	2.16	2.14
	3d	2.13	2.08	2.14	2.23	2.15	2.12	2.08	2.18	2.16	2.14
	1e	2.14	2.12	2.10	2.12	2.11	2.14	2.09	2.09	2.09	2.09
	2e	2.28	1.95	3.41	1.95	2.44	2.13	2.06	2.14	2.27	2.16
	3e	2.15	2.03	2.04	2.59	2.22	2.13	2.06	2.14	2.27	2.16
	1f	2.14	2.12	2.10	2.12	2.11	2.14	2.09	2.09	2.09	2.09
	2f	2.21	1.99	3.26	1.99	2.41	2.20	1.98	3.12	1.98	2.36
	3f	2.14	2.05	2.07	2.42	2.18	2.20	1.98	3.12	1.98	2.36

Table S2. Copper(II)-nitrogen distances in the theoretical Cu^{II}/L complex for the four possible donor nitrogens.

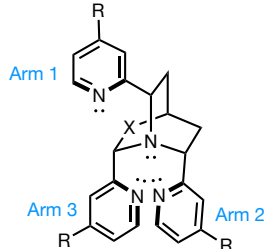
The mean of the distances between copper and the nitrogen donors in each arm is also given. Distances are highlighted according to their relative favorability, with red being less favorable and green being most favorable. The axial distances have a different scale to the individual arm distances and also to the mean arm distances (so that there are three separate scales).



L1



L2



L3

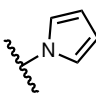
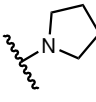
R		X = O					X = CH ₂				
		Axial (Å)	Arm 1 (Å)	Arm 2 (Å)	Arm 3 (Å)	Mean Arm (Å)	Axial (Å)	Arm 1 (Å)	Arm 2 (Å)	Arm 3 (Å)	Mean Arm (Å)
	1a	1.93	2.07	2.06	2.07	2.07	1.93	2.05	2.05	2.05	2.05
	2a	1.96	2.01	2.03	2.15	2.07	1.96	1.99	2.01	2.15	2.05
	3a	1.96	1.99	2.00	2.18	2.06	1.96	1.99	2.01	2.15	2.05
	1b	1.93	2.06	2.05	2.06	2.06	1.93	2.05	2.05	2.05	2.05
	2b	1.96	2.00	2.02	2.13	2.05	1.97	1.98	2.00	2.13	2.04
	3b	1.97	1.98	1.99	2.16	2.05	1.97	1.98	2.00	2.13	2.04
	1c	1.92	2.06	2.05	2.06	2.06	1.93	2.05	2.05	2.05	2.05
	2c	1.96	2.01	2.02	2.13	2.05	1.97	1.98	2.00	2.12	2.04
	3c	1.97	1.99	2.00	2.15	2.04	1.97	1.98	2.00	2.12	2.04
	1d	1.93	2.05	2.04	2.05	2.05	1.93	2.04	2.04	2.04	2.04
	2d	1.97	1.99	2.01	2.11	2.04	1.98	1.97	1.99	2.11	2.02
	3d	1.98	1.97	1.98	2.14	2.03	1.98	1.97	1.99	2.11	2.02
	1e	1.93	2.05	2.04	2.05	2.04	1.93	2.04	2.04	2.04	2.04
	2e	1.98	1.99	2.00	2.09	2.03	1.99	1.97	1.98	2.09	2.01
	3e	1.99	1.97	1.97	2.11	2.02	1.99	1.97	1.98	2.09	2.01
	1f	1.93	2.04	2.04	2.05	2.04	1.93	2.03	2.03	2.03	2.03
	2f	1.98	1.99	1.99	2.09	2.02	1.99	1.97	1.98	2.09	2.01
	3f	1.99	1.97	1.97	2.11	2.02	1.99	1.97	1.98	2.09	2.01

Table S3. Copper(II)-nitrogen distances in the BrCu^{II}/L complex for the four possible donor nitrogens.

The mean of the distances between copper and the nitrogen donors in each arm is also given. Distances are highlighted according to their relative favorability, with red being less favorable and green being most favorable. The axial distances have a different scale to the individual arm distances and also to the mean arm distances (so that there are three separate scales).

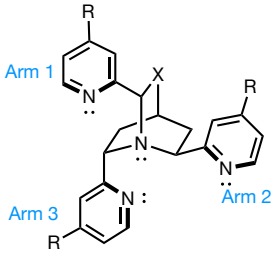
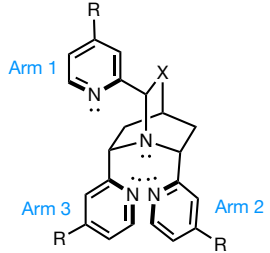
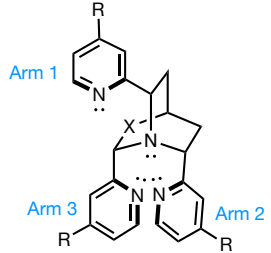
																	
L1						L2						L3					
R		X = O					X = CH ₂					X = CH ₂					
		Axial (Å)	Arm 1 (Å)	Arm 2 (Å)	Arm 3 (Å)	Mean Arm (Å)	Axial (Å)	Arm 1 (Å)	Arm 2 (Å)	Arm 3 (Å)	Mean Arm (Å)	Axial (Å)	Arm 1 (Å)	Arm 2 (Å)	Arm 3 (Å)	Mean Arm (Å)	
	1a	2.06	2.15	2.14	2.15	2.15	2.06	2.13	2.13	2.13	2.13	2.06	2.13	2.13	2.13	2.13	
	2a	2.05	2.13	2.20	2.24	2.19	2.05	2.10	2.16	2.24	2.16	2.05	2.10	2.16	2.24	2.16	
	3a	2.06	2.10	2.14	2.31	2.18	2.05	2.10	2.16	2.24	2.16	2.05	2.10	2.16	2.24	2.16	
	1b	2.06	2.14	2.13	2.14	2.14	2.06	2.12	2.12	2.12	2.12	2.06	2.12	2.12	2.12	2.12	
	2b	2.05	2.11	2.18	2.24	2.18	2.06	2.09	2.14	2.24	2.15	2.06	2.09	2.14	2.24	2.15	
	3b	2.06	2.09	2.12	2.31	2.17	2.06	2.09	2.14	2.24	2.15	2.06	2.09	2.14	2.24	2.15	
	1c	2.06	2.14	2.13	2.14	2.14	2.06	2.12	2.12	2.12	2.12	2.06	2.12	2.12	2.12	2.12	
	2c	2.05	2.12	2.18	2.24	2.18	2.06	2.09	2.14	2.23	2.15	2.06	2.09	2.14	2.23	2.15	
	3c	2.06	2.09	2.12	2.29	2.17	2.06	2.09	2.14	2.23	2.15	2.06	2.09	2.14	2.23	2.15	
	1d	2.07	2.13	2.12	2.14	2.13	2.07	2.12	2.12	2.12	2.12	2.07	2.12	2.12	2.12	2.12	
	2d	2.05	2.09	2.15	2.35	2.20	2.05	2.06	2.12	2.34	2.17	2.05	2.06	2.12	2.34	2.17	
	3d	2.06	2.06	2.10	2.43	2.20	2.05	2.06	2.12	2.34	2.17	2.05	2.06	2.12	2.34	2.17	
	1e	2.07	2.12	2.12	2.13	2.12	2.07	2.11	2.11	2.11	2.11	2.07	2.11	2.11	2.11	2.11	
	2e	2.05	2.07	2.14	2.34	2.19	2.07	2.06	2.10	2.24	2.13	2.07	2.06	2.10	2.24	2.13	
	3e	2.06	2.05	2.09	2.40	2.18	2.07	2.06	2.10	2.24	2.13	2.07	2.06	2.10	2.24	2.13	
	1f	2.07	2.12	2.11	2.13	2.12	2.07	2.11	2.11	2.11	2.11	2.07	2.11	2.11	2.11	2.11	
	2f	2.05	2.07	2.12	2.39	2.19	2.06	2.05	2.11	2.11	2.09	2.06	2.05	2.11	2.11	2.09	
	3f	2.06	2.05	2.09	2.41	2.18	2.06	2.05	2.11	2.11	2.09	2.06	2.05	2.11	2.11	2.09	

Table S4. Raw energetics data for species involved in the manuscript.

Unless otherwise noted, units are in Hartrees. Gas phase at wB97XD/SDD-6-31G(d); solution phase at wB97XD/Def2-TZVP SMD in acetonitrile and G(sol) includes phase change term.

Species	Ee(gas)	ZPVE(gas)	TC(gas)	TS(gas)	S(gas, J/mol/K)	H(gas)	G(gas)	Ee(sol)	G(sol)
Br-	-2573.990194	0.000000	0.002360	0.018536	163.2	-2573.987834	-2574.006370	-2574.399307	-2574.412474
BrMMA	-2920.225179	0.139244	0.010608	0.046445	409.0	-2920.075327	-2920.121772	-2920.665180	-2919.698008
Cu1+	-197.011679	0.000000	0.002361	0.018215	160.4	-197.009318	-197.027533	-1640.381693	-1581.394538
MMA•	-346.258553	0.134903	0.009918	0.044810	394.6	-346.113732	-346.158542	-346.399213	-286.431096
CH2_1a	-1683.558249	0.416612	0.028262	0.091883	809.1	-1683.113375	-1683.205258	-1684.190658	-1647.251270
CH2_1b	-2449.000923	0.379094	0.024205	0.081102	714.2	-2448.597624	-2448.678726	-2449.456565	-2414.510453
CH2_1c	-1696.979374	0.600010	0.032430	0.099507	876.3	-1696.346934	-1696.446441	-1697.571802	-1659.635870
CH2_1d	-1070.255268	0.408305	0.020521	0.070904	624.4	-1069.826442	-1069.897346	-1070.621313	-1030.668688
CH2_1e	-1472.066591	0.632442	0.033548	0.099942	880.1	-1471.400601	-1471.500543	-1472.583367	-1436.646752
CH2_1f	-1704.293736	0.744279	0.035564	0.106018	933.6	-1703.513893	-1703.619911	-1704.881390	-1665.948835
CH2_2a	-1683.540981	0.417170	0.027921	0.088015	775.1	-1683.095890	-1683.183905	-1684.180903	-1629.237988
CH2_2b	-2448.978849	0.379399	0.024009	0.078584	692.0	-2448.575441	-2448.654025	-2449.445648	-2396.497214
CH2_2c	-1696.960782	0.599886	0.032152	0.096641	851.0	-1696.328744	-1696.425385	-1697.562580	-1641.624060
CH2_2d	-1070.233253	0.408378	0.020358	0.069058	608.1	-1069.804517	-1069.873575	-1070.611844	-1012.657535
CH2_2e	-1472.042953	0.632032	0.033016	0.096063	845.9	-1471.377905	-1471.473968	-1472.572633	-1418.632671
CH2_2f	-1704.272178	0.744790	0.034961	0.101689	895.5	-1703.492427	-1703.594116	-1704.872240	-1647.935959
CH2_Br_Cu2+_1a	-4454.734087	0.421857	0.031222	0.095228	838.6	-4454.281008	-4454.376236	-5898.954118	-5892.015115
CH2_Br_Cu2+_1b	-5220.199377	0.384933	0.027063	0.084615	745.1	-5219.787381	-5219.871996	-6664.232079	-6659.286622
CH2_Br_Cu2+_1c	-4468.187467	0.605221	0.035582	0.104573	920.9	-4467.546664	-4467.651237	-5912.348152	-5903.414134
CH2_Br_Cu2+_1d	-3841.469463	0.414581	0.023292	0.074511	656.1	-3841.031590	-3841.106101	-5285.405514	-5283.453724
CH2_Br_Cu2+_1e	-4243.304588	0.637685	0.036784	0.105378	928.0	-4242.630119	-4242.735497	-5687.378300	-5681.443885
CH2_Br_Cu2+_1f	-4475.534922	0.750576	0.038488	0.110477	972.9	-4474.745858	-4474.856335	-5919.676726	-5911.745706
CH2_Br_Cu2+_2a	-4454.719046	0.422093	0.031272	0.096778	852.2	-4454.265681	-4454.362459	-5898.941956	-5886.004453
CH2_Br_Cu2+_2b	-5220.184155	0.385043	0.027130	0.086189	759.0	-5219.771982	-5219.858171	-6664.219925	-6653.275975
CH2_Br_Cu2+_2c	-4468.175487	0.605380	0.035452	0.104546	920.6	-4467.534655	-4467.639201	-5912.337652	-5898.403737
CH2_Br_Cu2+_2d	-3841.453768	0.414566	0.023386	0.076084	670.0	-3841.015816	-3841.091900	-5285.393161	-5269.442850
CH2_Br_Cu2+_2e	-4243.288734	0.637888	0.036737	0.106929	941.6	-4242.614109	-4242.721038	-5687.367129	-5675.434312
CH2_Br_Cu2+_2f	-4475.522139	0.750852	0.038121	0.108575	956.1	-4474.733166	-4474.841741	-5919.669299	-5904.736745
CH2_Br_Cu2+_4a	-3893.194876	0.447700	0.026125	0.080959	712.9	-3892.721051	-3892.802010	-5337.171386	-5334.223211
CH2_Br_Cu2+_4b	-3893.104436	0.446722	0.026275	0.080607	709.8	-3892.631439	-3892.712046	-5337.072687	-5333.124010
CH2_Br_Cu2+_4c	-3725.513917	0.352521	0.021734	0.071485	629.5	-3725.139662	-3725.211147	-5169.620234	-5159.666976
CH2_Cu1+_1a	-1880.774101	0.419452	0.029461	0.090264	794.9	-1880.325188	-1880.415452	-3324.689203	-3302.746997

CH2_Cu1+_1b	-2646.236348	0.382518	0.025313	0.079716	702.0	-2645.828517	-2645.908233	-4089.962554	-4070.013948
CH2_Cu1+_1c	-1894.222120	0.602992	0.033716	0.100254	882.8	-1893.585412	-1893.685666	-3338.076477	-3314.140006
CH2_Cu1+_1d	-1267.505123	0.412121	0.021554	0.069526	612.2	-1267.071448	-1267.140974	-2711.133590	-2694.178553
CH2_Cu1+_1e	-1669.335073	0.634948	0.035012	0.100601	885.9	-1668.665113	-1668.765714	-3113.100145	-3092.162725
CH2_Cu1+_1f	-1901.564727	0.748163	0.036655	0.105284	927.1	-1900.779909	-1900.885193	-3345.398035	-3322.463655
CH2_Cu1+_2a	-1880.758874	0.419587	0.029593	0.092125	811.2	-1880.309694	-1880.401819	-3324.675164	-3281.734687
CH2_Cu1+_2b	-2646.221152	0.382517	0.025471	0.081681	719.3	-2645.813164	-2645.894845	-4089.948549	-4049.001750
CH2_Cu1+_2c	-1894.212327	0.603622	0.033401	0.098068	863.6	-1893.575304	-1893.673372	-3338.067693	-3294.129351
CH2_Cu1+_2d	-1267.489332	0.412072	0.021752	0.071502	629.6	-1267.055508	-1267.127010	-2711.119162	-2665.165903
CH2_Cu1+_2e	-1669.319830	0.635177	0.034866	0.100561	885.5	-1668.649787	-1668.750348	-3113.087667	-3071.150353
CH2_Cu1+_2f	-1901.553362	0.748932	0.036228	0.103141	908.3	-1900.768202	-1900.871343	-3345.391031	-3300.454935
CH2_Cu1+_4a	-1319.241093	0.446133	0.023916	0.074190	653.3	-1318.771044	-1318.845234	-2762.904004	-2744.951269
CH2_Cu1+_4b	-1319.161111	0.444585	0.024349	0.075266	662.8	-1318.692177	-1318.767443	-2762.818760	-2743.866668
CH2_Cu1+_4c	-1151.514299	0.349322	0.019923	0.065715	578.7	-1151.145054	-1151.210769	-2595.327548	-2570.370331
CH2_Cu2+_1a	-1880.404504	0.420375	0.029060	0.089585	788.9	-1879.955069	-1880.044654	-3324.491058	-3293.548574
CH2_Cu2+_1b	-2645.889565	0.384493	0.024756	0.078603	692.2	-2645.480316	-2645.558919	-4089.773754	-4060.824592
CH2_Cu2+_1c	-1893.897312	0.604689	0.033384	0.098869	870.6	-1893.259239	-1893.358108	-3337.890759	-3304.953235
CH2_Cu2+_1d	-1267.167461	0.414200	0.021051	0.068669	604.7	-1266.732210	-1266.800879	-2710.950287	-2684.994896
CH2_Cu2+_1e	-1669.036823	0.637953	0.034311	0.098719	869.3	-1668.364559	-1668.463278	-3112.929455	-3082.990854
CH2_Cu2+_1f	-1901.272632	0.750957	0.036034	0.103804	914.1	-1900.485641	-1900.589445	-3345.228343	-3313.293104
CH2_Cu2+_2a	-1880.388774	0.420699	0.029059	0.090615	798.0	-1879.939016	-1880.029631	-3324.479127	-3275.537674
CH2_Cu2+_2b	-2645.874577	0.384481	0.024772	0.079617	701.1	-2645.465324	-2645.544941	-4089.762321	-4042.814157
CH2_Cu2+_2c	-1893.883465	0.605043	0.033335	0.099691	877.9	-1893.245087	-1893.344778	-3337.879781	-3287.943128
CH2_Cu2+_2d	-1267.151977	0.414168	0.021064	0.069609	613.0	-1266.716745	-1266.786354	-2710.938471	-2658.984007
CH2_Cu2+_2e	-1669.023431	0.637826	0.034266	0.099476	876.0	-1668.351339	-1668.450815	-3112.919419	-3064.981620
CH2_Cu2+_2f	-1901.259422	0.750894	0.035981	0.104501	920.2	-1900.472547	-1900.577048	-3345.218468	-3294.283979
CH2_Cu2+_4a	-1318.912908	0.446584	0.024284	0.077363	681.3	-1318.442040	-1318.519403	-2762.721479	-2735.771550
CH2_Cu2+_4b	-1318.830886	0.446523	0.024278	0.077331	681.0	-1318.360085	-1318.437416	-2762.633730	-2734.683774
CH2_Cu2+_4c	-1151.566707	0.353605	0.019218	0.064593	568.8	-1151.193884	-1151.258477	-2595.199468	-2561.241834
O_1a	-1719.436896	0.391909	0.028136	0.091889	809.2	-1719.016851	-1719.108740	-1720.092330	-1618.153074
O_1b	-2484.880029	0.354711	0.024015	0.080807	711.6	-2484.501303	-2484.582110	-2485.359166	-2385.412949
O_1c	-1732.859553	0.575313	0.032207	0.099097	872.6	-1732.252033	-1732.351130	-1733.473702	-1630.537583
O_1d	-1106.135189	0.383609	0.020431	0.071514	629.8	-1105.731149	-1105.802663	-1106.525241	-1001.573315
O_1e	-1507.946169	0.607794	0.033434	0.100076	881.3	-1507.304941	-1507.405017	-1508.486784	-1407.550417
O_1f	-1740.172601	0.719422	0.035422	0.106994	942.2	-1739.417757	-1739.524751	-1740.784206	-1636.852769
O_2a	-1719.430216	0.392338	0.027747	0.087947	774.5	-1719.010131	-1719.098078	-1720.089435	-1600.146626
O_2b	-2484.870567	0.354788	0.023765	0.078011	687.0	-2484.492014	-2484.570025	-2485.356502	-2367.407739

O_2c	-1732.849542	0.575554	0.032009	0.096959	853.8	-1732.241979	-1732.338938	-1733.471571	-1612.533512
O_2d	-1106.123957	0.383816	0.020124	0.068519	603.4	-1105.720017	-1105.788536	-1106.521800	-983.567186
O_2e	-1507.934178	0.607596	0.032711	0.095523	841.2	-1507.293871	-1507.389394	-1508.483837	-1389.543640
O_2f	-1740.162990	0.719911	0.034850	0.101617	894.8	-1739.408229	-1739.509846	-1740.783568	-1618.847326
O_3a	-1719.429440	0.392090	0.027916	0.088972	783.5	-1719.009434	-1719.098406	-1720.088865	-1582.146912
O_3b	-2484.870228	0.354799	0.023861	0.078828	694.2	-2484.491568	-2484.570396	-2485.355857	-2349.407815
O_3c	-1732.850703	0.575712	0.031881	0.096322	848.2	-1732.243110	-1732.339432	-1733.471009	-1594.532441
O_3d	-1106.124121	0.384101	0.020145	0.068871	606.5	-1105.719875	-1105.788746	-1106.521254	-965.566971
O_3e	-1507.934420	0.607886	0.032790	0.095803	843.6	-1507.293744	-1507.389547	-1508.482444	-1371.542448
O_3f	-1740.163463	0.720342	0.034809	0.101683	895.4	-1739.408312	-1739.509995	-1740.782177	-1600.846042
O_Br_Cu2+_1a	-4490.610431	0.396759	0.031115	0.096370	848.6	-4490.182557	-4490.278927	-5934.849862	-5869.912108
O_Br_Cu2+_1b	-5256.076831	0.359973	0.026929	0.085640	754.1	-5255.689929	-5255.775569	-6700.128638	-6637.184340
O_Br_Cu2+_1c	-4504.065905	0.580322	0.035416	0.105464	928.7	-4503.450167	-4503.555631	-5948.245179	-5882.312218
O_Br_Cu2+_1d	-3877.347500	0.389622	0.023192	0.075630	666.0	-3876.934686	-3877.010316	-5321.302750	-5253.352179
O_Br_Cu2+_1e	-4279.184202	0.612661	0.036594	0.106219	935.4	-4278.534947	-4278.641166	-5723.276733	-5659.343349
O_Br_Cu2+_1f	-4511.414677	0.725658	0.038326	0.111361	980.6	-4510.650693	-4510.762054	-5955.575220	-5888.645246
O_Br_Cu2+_2a	-4490.592541	0.396876	0.031203	0.097000	854.2	-4490.164462	-4490.261462	-5934.834816	-5862.897604
O_Br_Cu2+_2b	-5256.058798	0.360149	0.027015	0.086200	759.1	-5255.671634	-5255.757834	-6700.113690	-6630.169866
O_Br_Cu2+_2c	-4504.051188	0.580746	0.035289	0.104578	920.9	-4503.435153	-4503.539731	-5948.232286	-5875.298566
O_Br_Cu2+_2d	-3877.328948	0.389688	0.023270	0.076028	669.5	-3876.915990	-3876.992018	-5321.287562	-5246.337311
O_Br_Cu2+_2e	-4279.165750	0.613140	0.036282	0.104388	919.2	-4278.516328	-4278.620716	-5723.264215	-5652.329312
O_Br_Cu2+_2f	-4511.398728	0.726032	0.038051	0.109016	960.0	-4510.634645	-4510.743661	-5955.564898	-5881.632854
O_Br_Cu2+_3a	-4490.599336	0.396855	0.031209	0.097122	855.3	-4490.171272	-4490.268394	-5934.841786	-5856.904690
O_Br_Cu2+_3b	-5256.065669	0.359872	0.027048	0.086492	761.6	-5255.678749	-5255.765241	-6700.120682	-6624.177117
O_Br_Cu2+_3c	-4504.058363	0.580570	0.035220	0.103934	915.2	-4503.442573	-4503.546507	-5948.240300	-5869.306005
O_Br_Cu2+_3d	-3877.335592	0.389616	0.023283	0.076187	670.9	-3876.922693	-3876.998880	-5321.294217	-5240.344112
O_Br_Cu2+_3e	-4279.172668	0.613149	0.036284	0.104614	921.2	-4278.523235	-4278.627849	-5723.271367	-5646.336688
O_Br_Cu2+_3f	-4511.406146	0.726184	0.037977	0.108507	955.5	-4510.641985	-4510.750492	-5955.572453	-5875.639974
O_Br_Cu2+_4a	-3929.073638	0.421965	0.026529	0.083871	738.6	-3928.625144	-3928.709015	-5373.067259	-5312.121592
O_Br_Cu2+_4b	-3928.982569	0.421862	0.026147	0.081669	719.2	-3928.534560	-3928.616229	-5372.969896	-5311.022409
O_Br_Cu2+_4c	-3761.398950	0.328062	0.021542	0.072280	636.5	-3761.049346	-3761.121626	-5205.522581	-5136.570310
O_Cu1+_1a	-1916.652026	0.394677	0.029366	0.091459	805.4	-1916.227983	-1916.319442	-3360.587943	-3274.647027
O_Cu1+_1b	-2682.115531	0.357675	0.025240	0.080937	712.7	-2681.732616	-2681.813553	-4125.862238	-4041.914926
O_Cu1+_1c	-1930.102192	0.577849	0.033747	0.100965	889.1	-1929.490596	-1929.591561	-3373.976564	-3287.040773
O_Cu1+_1d	-1303.384862	0.387270	0.021491	0.070766	623.2	-1302.976101	-1303.046867	-2747.033892	-2658.080158
O_Cu1+_1e	-1705.216623	0.610287	0.034924	0.101726	895.8	-1704.571412	-1704.673138	-3149.001750	-3064.065543
O_Cu1+_1f	-1937.446419	0.723262	0.036615	0.106609	938.8	-1936.686542	-1936.793151	-3381.299728	-3293.366713

O_Cu1+_2a	-1916.636984	0.395175	0.029172	0.090793	799.5	-1916.212637	-1916.303430	-3360.573842	-3252.632454
O_Cu1+_2b	-2682.100026	0.358218	0.025082	0.081089	714.1	-2681.716726	-2681.797815	-4125.848974	-4019.901972
O_Cu1+_2c	-1930.092431	0.578696	0.033305	0.098506	867.4	-1929.480430	-1929.578936	-3373.967813	-3265.030005
O_Cu1+_2d	-1303.366392	0.387308	0.021666	0.072112	635.0	-1302.957418	-1303.029530	-2747.017365	-2636.064802
O_Cu1+_2e	-1705.203507	0.611205	0.034390	0.099335	874.7	-1704.557912	-1704.657247	-3148.992350	-3042.054286
O_Cu1+_2f	-1937.434705	0.724353	0.035951	0.102425	902.0	-1936.674401	-1936.776826	-3381.292510	-3271.355975
O_Cu1+_3a	-1916.641755	0.394536	0.029474	0.092063	810.7	-1916.217745	-1916.309808	-3360.578406	-3234.637986
O_Cu1+_3b	-2682.105374	0.357692	0.025270	0.081175	714.8	-2681.722412	-2681.803587	-4125.852739	-4001.905635
O_Cu1+_3c	-1930.095885	0.578523	0.033338	0.098080	863.7	-1929.484024	-1929.582104	-3373.970006	-3247.031739
O_Cu1+_3D	-1303.373941	0.387384	0.021532	0.070969	625.0	-1302.965025	-1303.035994	-2747.023771	-2618.070199
O_Cu1+_3e	-1705.207007	0.610681	0.034685	0.101024	889.6	-1704.561641	-1704.662665	-3148.994106	-3024.057436
O_Cu1+_3f	-1937.439187	0.723937	0.036182	0.103575	912.1	-1936.679068	-1936.782643	-3381.294949	-3253.359333
O_Cu1+_4a	-1355.121653	0.420209	0.023671	0.075369	663.7	-1354.677773	-1354.753142	-2798.803318	-2716.852007
O_Cu1+_4b	-1355.039460	0.419839	0.024219	0.076305	671.9	-1354.595402	-1354.671707	-2798.717114	-2715.766191
O_Cu1+_4c	-1187.401153	0.325006	0.019766	0.066688	587.3	-1187.056381	-1187.123069	-2631.233089	-2541.277002
O_Cu2+_1a	-1916.274075	0.395511	0.028872	0.090389	796.0	-1915.849692	-1915.940081	-3360.383026	-3265.441534
O_Cu2+_1b	-2681.760559	0.359519	0.024589	0.079490	700.0	-2681.376451	-2681.455941	-4125.666640	-4032.718532
O_Cu2+_1c	-1929.770001	0.579878	0.033207	0.099773	878.6	-1929.156916	-1929.256689	-3373.784034	-3277.847592
O_Cu2+_1d	-1303.038798	0.389180	0.020898	0.069546	612.4	-1302.628720	-1302.698266	-2746.843739	-2648.889378
O_Cu2+_1e	-1704.910797	0.613170	0.034093	0.099353	874.9	-1704.263534	-1704.362887	-3148.824321	-3054.886572
O_Cu2+_1f	-1937.146789	0.725885	0.035869	0.104712	922.1	-1936.385035	-1936.489747	-3381.123267	-3284.189101
O_Cu2+_2a	-1916.254251	0.395482	0.028938	0.090513	797.1	-1915.829831	-1915.920344	-3360.367791	-3246.426357
O_Cu2+_2b	-2681.741580	0.359573	0.024610	0.079419	699.4	-2681.357397	-2681.436816	-4125.652022	-4013.703822
O_Cu2+_2c	-1929.752373	0.579961	0.033211	0.099653	877.5	-1929.139201	-1929.238854	-3373.770156	-3258.833589
O_Cu2+_2d	-1303.019277	0.389174	0.020920	0.069405	611.2	-1302.609183	-1302.678588	-2746.828843	-2629.874319
O_Cu2+_2e	-1704.893557	0.613056	0.034137	0.099417	875.5	-1704.246364	-1704.345781	-3148.811440	-3035.873711
O_Cu2+_2f	-1937.129944	0.726170	0.035784	0.104148	917.1	-1936.367990	-1936.472138	-3381.110736	-3265.176091
O_Cu2+_3a	-1916.264038	0.395720	0.028864	0.090327	795.4	-1915.839454	-1915.929781	-3360.376278	-3228.434732
O_Cu2+_3b	-2681.751216	0.359502	0.024588	0.079352	698.8	-2681.367126	-2681.446478	-4125.660312	-3995.712067
O_Cu2+_3c	-1929.761772	0.579921	0.033186	0.099604	877.1	-1929.148665	-1929.248269	-3373.778491	-3240.841900
O_Cu2+_3d	-1303.028842	0.389061	0.020898	0.069352	610.7	-1302.618883	-1302.688235	-2746.836882	-2611.882327
O_Cu2+_3e	-1704.902755	0.612982	0.034104	0.099211	873.6	-1704.255669	-1704.354880	-3148.819467	-3017.881565
O_Cu2+_3f	-1937.138955	0.725865	0.035826	0.104292	918.4	-1936.377264	-1936.481556	-3381.118636	-3247.184093
O_Cu2+_4a	-1354.785575	0.421773	0.023295	0.075134	661.6	-1354.340507	-1354.415641	-2798.614148	-2707.662978
O_Cu2+_4b	-1354.708694	0.421865	0.023899	0.076182	670.9	-1354.262930	-1354.339112	-2798.532795	-2706.582069
O_Cu2+_4c	-1187.447003	0.329130	0.019012	0.065378	575.7	-1187.098861	-1187.164239	-2631.098817	-2532.142174

Appendix S1. Optimized gas-phase geometries

Br-

-1 1

Br 1.6583 -2.49421 -1.96203

BrMMA

O 1

C 1.659444919 -1.4825440192 -0.1299467561
C 0.4276253046 -2.2045971698 0.3948386882
C 2.907913843 -1.7951342839 0.6882883329
C 1.3902080009 0.0220973251 -0.2259483647
O 2.5110575709 0.7201251059 -0.4280147188
O 0.2965986481 0.5204392448 -0.1160973861
C 2.3345660428 2.1291243097 -0.5752709372
Br 1.9761900883 -2.0715583891 -2.0061578982
H 0.2350955063 -1.8794270352 1.423264771
H 0.5955229041 -3.2844190764 0.3931177327
H -0.4540629177 -1.9725968301 -0.2036694342
H 2.7593169751 -1.4401450824 1.7152691739
H 3.7921784347 -1.3074101296 0.2768953658
H 3.0746411452 -2.8750402618 0.7181464604
H 3.333082796 2.53368641 -0.735428692
H 1.8853550164 2.5552531697 0.3249606442
H 1.6911957224 2.3433567122 -1.4319069819

CH2_Br_Cu2+_1d

1 2

C -0.0000000006 0.0000000005 3.7390461579
C -1.1452888661 0.8771434713 3.2034614589
C -0.1869840962 -1.4304209871 3.2034614589
C -1.2711346894 0.5943502767 1.6890422128
N -0.0000000006 0.0000000005 1.1946491826
C 1.1502897818 0.8036597946 1.6890422128
C 0.120844906 -1.3980100697 1.6890422128
H -0.0000000006 0.0000000005 4.8310426381
H -0.922415301 1.9337557646 3.3908861914
H -2.0865000907 0.6461739659 3.7106431159
H -1.2134739668 -1.7657129645 3.3908861914
H 0.4836469752 -2.1300490652 3.7106431159
C -0.7010352429 -2.3165602748 0.8067588992
C -1.2229078056 -3.5250126733 1.2463908232
C -1.9013118897 -4.3315897098 0.3358710948
H -1.0961765888 -3.8392990135 2.2765716526
C -1.4869756912 -2.6838243651 -1.3424286231
C -2.0378660767 -3.9059998893 -0.9792261867
H -2.3164870742 -5.2822511165 0.6542203616
H -1.5495887983 -2.2951185741 -2.3540788075
H -2.5586076419 -4.5051826582 -1.7168820461
N -0.835281412 -1.9122784405 -0.4668736052
H 1.1706622287 -1.6734818646 1.528932561
C -1.6556824272 1.765394467 0.8067588992
C -2.4412966222 2.821575563 1.2463908232
C -1.5807722352 2.6296709063 -1.3424286231
C -2.8006107839 3.8123792522 0.3358710948
H -2.7768421853 2.86896628 2.2765716526
C -2.3637620943 3.7178437368 -0.9792261867
H -1.212836592 2.4895425522 -2.3540788075
H -3.4163201203 4.6472622123 0.6542203616

H -2.622298811 4.4684105456 -1.7168820461
N -1.2384410039 1.6795141426 -0.4668736052
C 2.3567176685 0.5511658093 0.8067588992
C 3.6642044261 0.7034371118 1.2463908232
C 4.7019226719 0.5192104592 0.3358710948
H 3.8730187724 0.9703327351 2.2765716526
C 3.0677479247 0.0541534604 -1.3424286231
C 4.4016281692 0.188156154 -0.9792261867
H 5.7328071927 0.6349889057 0.6542203616
H 2.7624253887 -0.1944239764 -2.3540788075
H 5.1809064512 0.0367721142 -1.7168820461
N 2.0737224142 0.2327642994 -0.4668736052
H 0.8639466928 1.8505641629 1.528932561
H -2.0346089232 -0.1770822967 1.528932561
Cu -0.0000000006 0.0000000005 -0.8667250165
Br -0.0000000006 0.0000000005 -3.2115211018
C 1.3322729606 0.5532775174 3.2034614589
H 1.6028531138 1.4838751009 3.7106431159
H 2.1358892661 -0.1680427985 3.3908861914

CH2_Br_Cu2+_4a

1 2

C -0.0000000006 0. -3.5249835508
C 0.0687605681 1.4439815432 -2.9890395769
C 1.2161444141 -0.7815391708 -2.9890395769
C 0.4053449439 1.3427733342 -1.4816321933
N -0.0000000006 0. -0.9884182788
C -1.3655482917 -0.3203476478 -1.4816321933
C 0.9602033461 -1.0224256863 -1.4816321933
H -0.0000000006 0. -4.6169985425
H -0.8869968319 1.9529116614 -3.1567305526
H 0.8402348736 2.0140522849 -3.5145944508
H 2.1347695252 -0.2082940416 -3.1567305526
H 1.3241030056 -1.7346908886 -3.5145944508
C 2.1237831484 -1.0039322749 -0.5284886756
N 1.9667264614 -0.5479337221 0.7024172514
H 0.4535345601 -1.9866509438 -1.3540122253
C -0.1924607212 2.3412162966 -0.5284886756
N -0.3769644098 3.6708179107 -0.6937114972
N -0.5088387086 1.9772019395 0.7024172514
C -1.9313224288 -1.3372840216 -0.5284886756
N -2.9905393592 -2.16186971 -0.6937114972
N -1.4578877545 -1.4292682172 0.7024172514
H -1.9472574667 0.6005530209 -1.3540122253
H 1.4937229049 1.386097923 -1.3540122253
Cu -0.0000000006 0. 1.1811806438
C -1.2849049839 -0.6624423723 -2.9890395769
H -2.1643378809 -0.2793613962 -3.5145944508
H -1.247772695 -1.7446176197 -3.1567305526
N 3.3675037674 -1.5089482006 -0.6937114972
C 3.1473953477 -0.7526894616 1.3628095112
C 4.0284169458 -1.3472256764 0.5083543746
C 3.9289790799 -2.141259633 -1.8783018198
H 3.2649330975 -0.4696918181 2.3976768009
H 5.0502088556 -1.669769715 0.6361981535
H 3.1966361464 -2.8134517681 -2.3290138731
H 4.7955064555 -2.730681928 -1.5782545779
H 4.2435430269 -1.3945301684 -2.6113244687

C -3.1809401342 -2.8150985744 0.5083543746
 C -2.2255458696 -2.3493795965 1.3628095112
 C -3.8188747791 -2.3319658781 -1.8783018198
 H -3.9711674203 -3.5387243063 0.6361981535
 H -2.0392315961 -2.5926690955 2.3976768009
 H -4.0348387776 -1.3616422258 -2.3290138731
 H -4.762593148 -2.7876894509 -1.5782545779
 H -3.3294700665 -2.9777509796 -2.6113244687
 C -0.8474768134 4.1623242509 0.5083543746
 C -0.1101043025 4.4732255112 -1.8783018198
 H -1.0790414369 5.2084940214 0.6361981535
 H 0.8382026295 4.175093994 -2.3290138731
 H -0.0329133092 5.5183713791 -1.5782545779
 H -0.9140729621 4.3722811481 -2.6113244687
 C -0.9218494798 3.1020690582 1.3628095112
 H -1.2257015031 3.0623609137 2.3976768009
 Br -0.0000000006 0. 3.5108244484

CH2_Br_Cu2+_4b

1 2
 C 0.0000000004 -0.0000000001 -3.9520381878
 C 1.4211341118 0.2812696867 -3.4137261376
 C -0.4669803611 -1.3713730861 -3.4137261376
 C 1.3886587893 -0.069516332 -1.9118405117
 N 0.0000000004 -0.0000000001 -1.4276618817
 C -0.6341264846 1.2373719542 -1.9118405117
 C -0.7545323034 -1.1678556225 -1.9118405117
 H 0.0000000004 -0.0000000001 -5.043313792
 H 1.6844434094 1.3332429001 -3.5706274824
 H 2.1660809876 -0.3292521141 -3.9312948752
 H 0.3124005169 -2.1253922336 -3.5706274824
 H -1.3681811881 -1.7112551047 -3.9312948752
 N -0.4115212759 -2.2755839205 -1.0378054746
 C -0.1093278137 -2.0450782546 0.271690978
 H -1.8113363209 -0.9311367061 -1.7602106033
 N 2.1764741221 0.7814040805 -1.0378054746
 C 1.8257536286 0.9278584627 0.271690978
 N -1.7649528448 1.4941798396 -1.0378054746
 C -1.7164258136 1.1172197915 0.271690978
 H 0.0992801194 2.034231622 -1.7602106033
 H 1.7120562029 -1.1030949163 -1.7602106033
 Cu 0.0000000004 -0.0000000001 0.7818311429
 Br 0.0000000004 -0.0000000001 3.1906318659
 C -0.9541537494 1.0901033991 -3.4137261376
 H -0.7978997982 2.0405072184 -3.9312948752
 H -1.996843925 0.7921493332 -3.5706274824
 N 2.823800844 1.6654844272 0.7890898818
 C 3.7867197079 1.9603089712 -0.1611112386
 C 3.3834619203 1.3958046211 -1.3224801041
 C 2.8867087737 2.1253616819 2.1724672015
 N -2.854252245 1.612741052 0.7890898818
 C -3.5910372217 2.2992409779 -0.1611112386
 C -2.9005332202 2.2322616647 -1.3224801041
 N 0.0304514023 -3.2782254795 0.7890898818
 C -0.1956824849 -4.2595499494 -0.1611112386
 C -0.4829286989 -3.6280662861 -1.3224801041
 C 0.3972628227 -3.5626439721 2.1724672015
 C -3.2839715951 1.4372822899 2.1724672015
 H 4.6638922191 2.5443400354 0.0704694604
 H 3.8453471564 1.3769958265 -2.2969375882
 H 2.0480432966 1.6919670381 2.7169445581

H 2.8278330385 3.2158649096 2.2008861244
 H 3.8249833624 1.7953307589 2.6233123163
 H -4.5354092155 2.766879124 0.0704694604
 H -3.1151869443 2.64167041 -2.2969375882
 H -0.1284830022 -5.3112191597 0.0704694604
 H -0.7301602108 -4.0186662369 -2.2969375882
 H 0.4412647898 -2.6196410417 2.7169445581
 H 1.3711041884 -4.0569077036 2.2008861244
 H -0.3576896351 -4.2101981401 2.6233123163
 H -2.4893080851 0.9276740033 2.7169445581
 H -4.1989372256 0.8410427936 2.2008861244
 H -3.467293726 2.4148673809 2.6233123163

CH2_Br_Cu2+_1b

1 2
 C -0.0000000001 -0.0000000001 -3.59869264
 C -0.90022945 1.1280016 -3.06318567
 C 1.4269927654 0.2156207706 -3.06318567
 C -0.61785767 1.2598305 -1.54935766
 N -0.0000000001 -0.0000000001 -1.05317464
 C -0.7821163848 -1.1649956887 -1.54935766
 C 1.3999740518 -0.0948348142 -1.54935766
 H -0.0000000001 -0.0000000001 -4.69050864
 H -1.95200673 0.88322745 -3.25023972
 H -0.68878923 2.07350227 -3.57067666
 H 1.7409007733 1.2488736892 -3.25023972
 H 2.1401002549 -0.4402421663 -3.57067666
 C 2.30289765 0.74083355 -0.66377953
 C 3.49765562 1.28183721 -1.11193348
 C 4.29181688 1.97005524 -0.19598244
 H 3.81837521 1.16916232 -2.14097646
 C 2.66576483 1.52506798 1.48299949
 C 3.87654876 2.09893015 1.12429954
 Cl 5.78774419 2.65899739 -0.71029737
 H 2.28478701 1.58134797 2.49796947
 H 4.47588804 2.62849004 1.85478857
 N 1.89885972 0.86355281 0.61059645
 H 1.69579592 -1.13871358 -1.39007157
 C -1.7930295017 1.6239510916 -0.66377953
 C -2.8589313998 2.388140015 -1.11193348
 C -2.6536300306 1.5460860727 1.48299949
 C -3.8520263271 2.7317948259 -0.19598244
 H -2.9217118777 2.7222287724 -2.14097646
 C -3.7560012131 2.3077246296 1.12429954
 H -2.5118810216 1.1880096073 2.49796947
 Cl -5.1966313857 3.6828348035 -0.71029737
 H -4.5142831706 2.5619877265 1.85478857
 N -1.6972885334 1.2126843501 0.61059645
 C -0.5098681514 -2.3647846446 -0.66377953
 C -0.6387242233 -3.669977228 -1.11193348
 C -0.439790556 -4.7018500688 -0.19598244
 H -0.8966633354 -3.8913910954 -2.14097646
 C -0.0121348025 -3.0711540557 1.48299949
 C -0.12054755 -4.4066547825 1.12429954
 Cl -0.5911128073 -6.3418321965 -0.71029737
 H 0.2270940086 -2.7693575803 2.49796947
 H 0.0383951276 -5.1904777695 1.85478857
 N -0.2015711897 -2.0762371631 0.61059645
 H -1.8340528486 -0.8992455587 -1.39007157
 H 0.1382569255 2.0379591358 -1.39007157
 Cu -0.0000000001 -0.0000000001 1.01085636

Br -0.000000001 -0.000000001 3.35214936
C -0.5267633185 -1.3436223735 -3.06318567
H -1.451311028 -1.6332601066 -3.57067666
H 0.2111059536 -2.1321011421 -3.25023972

CH2_Br_Cu2+_1e

1 2
C -0.0000000001 -0.0000000004 -3.5268837726
C 1.4016504984 0.3395276012 -2.9907018268
C -0.4067857211 -1.3836287401 -2.9907018268
C 1.4021993959 0.0348721202 -1.4753243044
N -0.0000000001 -0.0000000004 -0.9850114645
C -0.7312998404 1.1969042374 -1.4753243044
C -0.6708995558 -1.2317763588 -1.4753243044
H -0.0000000001 -0.0000000004 -4.6194038264
H 1.6246847983 1.3959285422 -3.1794877182
H 2.1690907401 -0.2535735955 -3.4971809971
H 0.3965671805 -2.1049825802 -3.1794877182
H -1.3041465453 -1.751700887 -3.4971809971
C -0.2832086622 -2.4006435018 -0.5891592065
C -0.289058814 -3.7027385484 -1.0436595923
C 0.0045167851 -4.761057334 -0.1482424625
H -0.5344493001 -3.9028203922 -2.0785344574
C 0.2754177216 -3.0596843263 1.5416009453
C 0.2941996131 -4.3895447357 1.1853703857
H 0.4859919195 -2.7463234782 2.5596103463
H 0.5295449755 -5.1257196469 1.9422435964
N -0.0054793011 -2.068930611 0.6828275898
H -1.7420974517 -1.0627712595 -1.3105786425
C 2.2206225887 0.9550558544 -0.5891592065
C 3.351195053 1.6010369976 -1.0436595923
C 2.5120554929 1.7683609062 1.5416009453
C 4.1209382071 2.3844403172 -0.1482424625
H 3.6471662556 1.4885635247 -2.0785344574
C 3.6543574451 2.4495567061 1.1853703857
H 2.1353899389 1.794043087 2.5596103463
H 4.1742309387 3.0214592242 1.9422435964
N 1.7944861178 1.0297200911 0.6828275898
C -1.9374139267 1.4455876463 -0.5891592065
C -3.0621362393 2.1017015496 -1.0436595923
C -4.1254549925 2.3766170157 -0.1482424625
H -3.1127169558 2.4142568664 -2.0785344574
C -2.7874732148 1.291323419 1.5416009453
C -3.9485570585 1.9399880285 1.1853703857
H -2.6213818587 0.9522803901 2.5596103463
H -4.7037759144 2.1042604216 1.9422435964
N -1.7890068171 1.0392105188 0.6828275898
H -0.0493381832 2.0400862781 -1.3105786425
H 1.7914356345 -0.9773150197 -1.3105786425
Cu -0.0000000001 -0.0000000004 1.0865603904
Br -0.0000000001 -0.0000000004 3.4461032035
C -0.9948647776 1.0441011377 -2.9907018268
H -0.8649441951 2.0052744813 -3.4971809971
H -2.021251979 0.7090540369 -3.1794877182
N 5.240763323 3.0343482465 -0.5508201145
N 0.0074410041 -6.0558082968 -0.5508201145
N -5.2482043274 3.0214600492 -0.5508201145
C -6.3091365726 3.2984937661 0.4048687364
H -6.716862647 2.3726801332 0.8271167895
H -5.9528848605 3.9335198112 1.2244693647
H -7.119015828 3.8230964474 -0.1010223152

C -5.383170579 3.4616214274 -1.9282920659
H -5.3346435945 2.6157527586 -2.6249406231
H -6.3507580286 3.9454607806 -2.057479342
H -4.604586733 4.1859920422 -2.1978942404
C -0.3062668054 -6.3927731885 -1.9282920659
H -0.2414902518 -7.4726481768 -2.057479342
H -1.3228820825 -6.0806851063 -2.1978942404
H 0.4020134578 -5.9278132527 -2.6249406231
C 0.2979888901 -7.1131194313 0.4048687364
H 1.3036300526 -7.0033137531 0.8271167895
H -0.430085653 -7.1221094211 1.2244693647
H 0.2486092689 -8.0767967812 -0.1010223152
C 5.6894373841 2.93115176 -1.9282920659
H 5.9274688153 1.894693063 -2.1978942404
H 4.9326301364 3.312060493 -2.6249406231
H 6.5922482801 3.5271873951 -2.057479342
C 6.0111476822 3.8146256641 0.4048687364
H 6.8704065588 4.2537003326 -0.1010223152
H 5.4132325941 4.6306336187 0.8271167895
H 6.3829705133 3.1885896088 1.2244693647

CH2_Br_Cu2+_1a

1 2
C -0.0000000005 -0.0000000001 -3.5498437613
C -0.0267445601 -1.4428647044 -3.0148745541
C -1.2361852089 0.7445938201 -3.0148745541
C -0.3306622464 -1.3633460887 -1.5015808434
N -0.0000000005 -0.0000000001 -1.0025422678
C 1.3460234693 0.3953111392 -1.5015808434
C -1.0153612245 0.9680349492 -1.5015808434
H -0.0000000005 -0.0000000001 -4.6413936242
H 0.9389736866 -1.9262690473 -3.2012734617
H -0.7922047005 -2.0362691406 -3.5225392366
H -2.1376847734 0.149959457 -3.2012734617
H -1.3673584552 1.7042039654 -3.5225392366
C -2.2439963969 0.9062321163 -0.6171309978
C -3.509945081 1.2529886643 -1.065443424
C -4.5390198223 1.2268258618 -0.1374889181
H -3.7088446457 1.5427933765 -2.0898810489
C -3.0239476562 0.5385261314 1.5391800938
C -4.3252126119 0.8721189229 1.1807184105
H -2.7621423781 0.2531780563 2.553095719
H -5.1370541345 0.8560336312 1.8968524597
N -2.0182388578 0.5569636537 0.6601634928
H -0.5758734814 1.9609400186 -1.344159776
C 0.3371781632 -2.3964739436 -0.6171309978
C 0.6698525257 -3.6661959379 -1.065443424
C 1.0455965169 -2.8880785554 1.5391800938
C 1.207047548 -4.544319405 -0.1374889181
H 0.5183240652 -3.9833503699 -2.0898810489
C 1.4073291627 -4.1818034598 1.1807184105
H 1.1618125598 -2.5186744961 2.553095719
H 1.8271801952 -4.8768361964 1.8968524597
N 0.526774755 -2.0263279483 0.6601634928
C 1.9068182322 1.490241827 -0.6171309978
C 2.8400925538 2.4132072733 -1.065443424
C 3.3319722728 3.3174935429 -0.1374889181
H 3.190520579 2.4405569931 -2.0898810489
C 1.9783511378 2.3495524237 1.5391800938
C 2.9178834476 3.3096845366 1.1807184105
H 1.6003298168 2.2654964396 2.553095719

H 3.3098739377 4.0208025649 1.8968524597
 N 1.4914641013 1.4693642943 0.6601634928
 H 1.9861606114 -0.4817489456 -1.344159776
 H -1.4102871315 -1.4791910732 -1.344159776
 Cu -0.0000000005 -0.0000000001 1.0580783099
 Br -0.0000000005 -0.0000000001 3.3919835812
 C 1.2629297674 0.698270884 -3.0148745541
 H 2.1595631541 0.332065175 -3.5225392366
 H 1.1987110853 1.77630959 -3.2012734617
 N 4.328308917 4.3196067579 -0.5819342686
 O 4.7447318712 5.089304141 0.2606235119
 O 4.6463082357 4.2899200755 -1.7567819838
 N 1.5767347275 -5.9082288571 -0.5819342686
 O 2.0351007375 -6.6537104057 0.2606235119
 O 1.392025647 -6.1687810042 -1.7567819838
 N -5.9050436461 1.5886220989 -0.5819342686
 O -6.7798326102 1.5644062643 0.2606235119
 O -6.0383338843 1.8788609285 -1.7567819838

CH2_Br_Cu2+_1f

1 2
 C 0.0000000005 0.0000000003 -3.3770974474
 C -0.6780484805 1.2728191657 -2.8409702167
 C 1.4413179727 -0.049202373 -2.8409702167
 C -0.3842336394 1.3488975686 -1.3253810985
 N 0.0000000005 0.0000000003 -0.8355266827
 C -0.9760627409 -1.0072048771 -1.3253810985
 C 1.3602963818 -0.3416926908 -1.3253810985
 H 0.0000000005 0.0000000003 -4.4696721721
 H -1.7565895832 1.2259470002 -3.0303681509
 H -0.2944083789 2.1639653694 -3.346936324
 H 1.939996038 0.9082777038 -3.0303681509
 H 2.0212531728 -0.8270175487 -3.346936324
 C 2.3951440274 0.3269403785 -0.4403777541
 C 3.6556018658 0.6503293191 -0.89571952
 C 4.6027754149 1.2033314519 0.0012196525
 H 3.9143870858 0.4790302248 -1.9333204424
 C 2.8908971923 1.0397541984 1.6911442992
 C 4.1720067969 1.3945681787 1.3347128713
 N 5.8481741872 1.5303747777 -0.3991082529
 H 2.5335015115 1.1625931822 2.7090375654
 H 4.8352589506 1.7999371511 2.0881612728
 N 2.0042493422 0.5140477166 0.8321672607
 H 1.464513258 -1.4210673523 -1.1597145625
 C -1.480710686 1.9107853841 -0.4403777541
 C -2.3910026431 2.8406794223 -0.89571952
 C -2.3459021447 1.983713309 1.6911442992
 C -3.343503313 3.3844547112 0.0012196525
 H -2.3720458858 3.1504435441 -1.9333204424
 C -3.2937348675 2.9157797815 1.3347128713
 H -2.2735859848 1.6127800784 2.7090375654
 N -4.2494305274 4.2994800229 -0.3991082529
 H -3.9764207724 3.2874885095 2.0881612728
 N -1.4473030515 1.4787069875 0.8321672607
 C -0.9144333398 -2.2377257619 -0.4403777541
 C -1.2645992212 -3.4910087406 -0.89571952
 C -1.2592721004 -4.5877861624 0.0012196525
 H -1.5423411985 -3.6294737681 -1.9333204424
 C -0.5449950461 -3.0234675067 1.6911442992
 C -0.8782719279 -4.3103479594 1.3347128713
 N -1.5987436583 -5.8298547999 -0.3991082529

H -0.2599155252 -2.7753732598 2.7090375654
 H -0.8588381767 -5.0874256598 2.0881612728
 N -0.5569462892 -1.9927547033 0.8321672607
 H -1.962937056 -0.5577720086 -1.1597145625
 H 0.4984237995 1.9788393616 -1.1597145625
 Cu 0.0000000005 0.0000000003 1.2356049859
 Br 0.0000000005 0.0000000003 3.596786947
 C -0.7632694907 -1.223616792 -2.8409702167
 H -1.7268447924 -1.3369478199 -3.346936324
 H -0.1834064533 -2.1342247032 -3.0303681509
 C 6.8307703027 2.1870617253 0.4642397904
 C 6.3747928887 1.2516747868 -1.734167563
 C 7.9407943471 2.5958620462 -0.5061296043
 C 7.8756002847 1.5155888642 -1.5899328302
 C -2.1034142812 -6.1465699781 -1.734167563
 C -1.5213341371 -7.0091514714 0.4642397904
 C -1.7223146963 -8.1748606531 -0.5061296043
 C -2.6252616837 -7.5782643479 -1.5899328302
 C -4.2713786061 4.894895192 -1.734167563
 C -5.3094361641 4.8220897469 0.4642397904
 C -5.2503385995 6.0626754844 -1.5899328302
 C -6.2184796493 5.5789986077 -0.5061296043
 H 7.19689516 1.4895206056 1.2299232558
 H 6.3852978321 3.0486493761 0.9721750039
 H 5.9154060867 1.9189119972 -2.4772075231
 H 6.1636384758 0.2174475871 -2.0273096559
 H 8.9152746351 2.6551943488 -0.0172753041
 H 7.7164934205 3.577804562 -0.9359693911
 H 8.3808555186 0.6062700751 -1.2479547811
 H 8.3336660647 1.8232010411 -2.5322455067
 H -1.2958765056 -6.0823479426 -2.4772075231
 H -2.8935041029 -5.4465912925 -2.0273096559
 H -2.3084848956 -6.977454339 1.2299232558
 H -0.5524411085 -7.0541548205 0.9721750039
 H -2.1581715589 -9.0484514893 -0.0172753041
 H -0.7597770692 -8.4715816105 -0.9359693911
 H -3.6653824721 -7.5611688213 -1.2479547811
 H -2.587894614 -8.1287670384 -2.5322455067
 H -4.6195295796 4.1634359461 -2.4772075231
 H -3.2701343714 5.2291437062 -2.0273096559
 H -4.888410263 5.4879337341 1.2299232558
 H -5.832856722 4.0055054452 0.9721750039
 H -5.7457714492 6.3055659981 -2.5322455067
 H -4.715473045 6.9548987469 -1.2479547811
 H -6.9567163498 4.8937770493 -0.9359693911
 H -6.7571030746 6.3932571412 -0.0172753041

CH2_Br_Cu2+_1c

1 2
 C 0.0000000004 0.0000000001 -3.4046555149
 C -0.8369026715 1.1750082354 -2.8692071141
 C 1.4360383178 0.1372748567 -2.8692071141
 C -0.5503370076 1.2903619526 -1.3546628415
 N 0.0000000004 0.0000000001 -0.861048255
 C -0.8423177266 -1.1217868058 -1.3546628415
 C 1.3926547354 -0.1685751467 -1.3546628415
 H 0.0000000004 0.0000000001 -4.4966961667
 H -1.9001512999 0.9877952066 -3.0578820884
 H -0.5729408361 2.1075524059 -3.3764426179
 H 1.8055313932 1.1516816939 -3.0578820884
 H 2.1116643419 -0.5575948836 -3.3764426179

C 2.337855524 0.6185617315 -0.4681020033
 C 3.5515636858 1.1030693688 -0.918720134
 C 4.4020174883 1.7589922296 -0.0166150823
 H 3.832325723 0.9956539349 -1.9592402874
 C 2.7374772802 1.3935431238 1.6675068797
 C 3.971921022 1.9003531931 1.3072313363
 N 5.6305060896 2.2542402715 -0.432190116
 H 2.366694304 1.4681088716 2.6850146391
 H 4.5982716471 2.3677169173 2.0565640371
 N 1.9329678477 0.7624181305 0.8041541349
 H 1.6321671871 -1.2270279262 -1.1935320249
 C -1.7046179347 1.7153614082 -0.4681020033
 C -2.7310679378 2.5242096904 -0.918720134
 C -2.5755823859 1.6739533047 1.6675068797
 C -3.7243406994 2.9327628578 -0.0166150823
 H -2.7784244618 2.821064464 -1.9592402874
 C -3.6317146517 2.4896079101 1.3072313363
 H -2.4547667297 1.3155629541 2.6850146391
 N -4.7674823855 3.7490411737 -0.432190116
 H -4.3496388223 2.7983616009 2.0565640371
 N -1.6267573925 1.2927901953 0.8041541349
 C -0.6332375882 -2.3339231395 -0.4681020033
 C -0.8204957469 -3.627279059 -0.918720134
 C -0.6776767878 -4.6917550872 -0.0166150823
 H -1.05390126 -3.8167183987 -1.9592402874
 C -0.161894893 -3.0674964284 1.6675068797
 C -0.3402063691 -4.389961103 1.3072313363
 N -0.8630237029 -6.003281445 -0.432190116
 H 0.0880724269 -2.7836718256 2.6850146391
 H -0.2486328236 -5.1660785181 2.0565640371
 N -0.306210454 -2.0552083256 0.8041541349
 H -1.8787209482 -0.7999842837 -1.1935320249
 H 0.2465537624 2.0270122101 -1.1935320249
 Cu 0.0000000004 0.0000000001 1.2064993133
 Br 0.0000000004 0.0000000001 3.5545000248
 C -0.5991356451 -1.3122830919 -2.8692071141
 H -1.5387235046 -1.5499575222 -3.3764426179
 H 0.0946199079 -2.1394769004 -3.0578820884
 C 6.3266182921 3.3019333595 0.1591328882
 C 6.3736566447 1.7910074928 -1.5118946678
 C 7.4798066704 3.4958421018 -0.5392661758
 C 7.5148618706 2.5302728874 -1.592854942
 C -1.6357703347 -6.4152523152 -1.5118946678
 C -0.3037509745 -7.1299788403 0.1591328882
 C -0.7124152669 -8.2256236424 -0.5392661758
 C -1.5661503357 -7.7731977292 -1.592854942
 C -4.7378863088 4.6242448226 -1.5118946678
 C -6.0228673163 3.828045481 0.1591328882
 C -5.9487115337 5.2429248419 -1.592854942
 C -6.7673914023 4.7297815408 -0.5392661758
 H 5.9079213809 3.8507074435 0.988488712
 H 6.0534368854 0.9323706696 -2.0816233977
 H 8.2221117859 4.2526983596 -0.331072232
 H 8.3046559136 2.3926759012 -2.3171919312
 H -3.8341751277 4.7762447879 -2.0816233977
 H -6.2887711584 3.1910562775 0.988488712
 H -6.2244460696 5.99570504 -2.3171919312
 H -7.7940007064 4.9942084993 -0.331072232
 H -2.2192617565 -5.7086154573 -2.0816233977
 H 0.3808497787 -7.0417637207 0.988488712
 H -0.4281110784 -9.2469068587 -0.331072232

H -2.0802098428 -8.388380941 -2.3171919312

CH2_Br_Cu2+_4c

-2 2
 C -0.0000000005 -0.0000000003 3.72938951
 C 1.40188847 0.34446862 3.19034991
 C -0.9992628118 1.0418367183 3.19034991
 C 1.27047134 0.6021099 1.66944174
 N -0.0000000005 -0.0000000003 1.19459411
 C -0.1137932013 -1.4013154061 1.66944174
 C -1.1566781403 0.7992055052 1.66944174
 H -0.0000000005 -0.0000000003 4.82759512
 H 2.09586714 -0.48538739 3.37695064
 H 1.80305035 1.23291231 3.69450897
 H -0.6275757607 2.0577678812 3.37695064
 H -1.9692585572 0.9450312524 3.69450897
 C -1.25937445 2.01421147 0.80004616
 N -0.91247254 1.85533122 -0.50722632
 H -2.02398266 0.14775653 1.50306381
 C 2.3740455261 0.0835445306 0.80004616
 N 2.0630002384 -0.137441211 -0.50722632
 C -1.1146710777 -2.0977560016 0.80004616
 N -1.1505277 -1.7178900099 -0.50722632
 H 0.8840304204 -1.8266986654 1.50306381
 H 1.139952238 1.6789421345 1.50306381
 Cu -0.0000000005 -0.0000000003 -0.92809082
 Br -0.0000000005 -0.0000000003 -3.40574044
 C -0.4026256598 -1.3863053392 3.19034991
 H 0.1662082056 -2.1779435633 3.69450897
 H -1.4682913809 -1.5723804921 3.37695064
 C 3.19956332 -0.56559661 -1.10957608
 C 4.24965317 -0.61692107 -0.19867248
 C 3.71162495 -0.19987479 1.0476538
 C -2.0896026931 -2.4881048121 -1.10957608
 C -2.6590959043 -3.3718470684 -0.19867248
 C -2.0289091212 -3.1144241019 1.0476538
 C -1.1099606285 3.0537014211 -1.10957608
 C -1.5905572673 3.9887681375 -0.19867248
 C -1.6827158304 3.314298891 1.0476538
 H 5.27099496 -0.92696798 -0.40086876
 H 4.23361531 -0.10240485 1.9952689
 H -3.4382752997 -4.1013315495 -0.40086876
 H -2.2054928571 -3.6152159842 1.9952689
 H -1.8327196619 5.0282995286 -0.40086876
 H -2.0281224545 3.7176208333 1.9952689
 H 3.18673083 -0.81693151 -2.16397824
 H -2.3008488563 -2.3513240997 -2.16397824
 H -0.8858819753 3.1682556088 -2.16397824

CH2_Br_Cu2+_2b

1 2
 C 0.2082059274 3.7272566095 -0.4024642054
 C -0.3123736315 3.1697740081 0.927399266
 C -0.7316467086 3.1851234501 -1.4934410807
 C 0.0456725989 1.6764321178 0.9533140964
 N 0.3157723019 1.1860056866 -0.4434794726
 C -0.6733608047 1.6389076577 -1.4602940467
 C 1.6366950197 1.7200319172 -0.8634994797
 H 0.1772972464 4.8188596817 -0.3981717393
 H -1.3953216161 3.3249556379 0.9826552826
 H 0.1372272771 3.6756496631 1.7869208335

H -0.4375193442 3.544321221 -2.4835855038
H -1.7400670789 3.5646064416 -1.3051960454
C 2.712480947 0.8454326723 -0.2543469882
C 3.9779545384 1.3009320614 0.0691056092
C 4.9115482977 0.3758156554 0.5378786576
H 4.2470508988 2.3442529903 -0.0476385952
C 3.2661150019 -1.3308450216 0.3183390667
C 4.5580067028 -0.9617807431 0.6644489238
Cl 6.4996678289 0.9017178568 0.95529746
H 2.9274851475 -2.3593564932 0.3897152477
H 5.2647863409 -1.7007023327 1.0217251642
N 2.3645113545 -0.4505188222 -0.1280429035
H 1.699140214 1.5431081184 -1.943616839
C -0.8757933677 0.7520567838 1.7278448852
C -1.8376694178 1.2034520588 2.6181859717
C -1.3022774205 -1.452317948 2.2591962918
C -2.5501328999 0.251591743 3.3484464566
H -2.0360004599 2.2580561717 2.7645226798
C -2.2840207501 -1.1006643642 3.1776549439
H -1.0563625541 -2.4921298912 2.0618607882
Cl -3.7644205658 0.767106359 4.4629968833
H -2.8227811184 -1.8566009884 3.7360947061
N -0.6157867253 -0.5505193648 1.5590489518
H 1.0143766681 1.5676698271 1.4559207937
H -0.2538371119 1.2965070099 -2.4133643134
C -1.923184097 0.7982350608 -1.3086924412
C -3.2212432319 1.2598322804 -1.4130057383
C -4.2571622807 0.3252597011 -1.3480754349
H -3.4430390993 2.3105752479 -1.5532561984
C -2.6328784747 -1.3958674246 -1.1002065589
C -3.9677550389 -1.0242033835 -1.199213304
Cl -5.8938352368 0.8593520685 -1.4596763445
H -2.3352533434 -2.4324433202 -0.9745242082
H -4.753541454 -1.7686742358 -1.1595388608
N -1.6384787548 -0.508995456 -1.1486505211
Cu 0.3460052757 -0.8728710191 -0.438128927
Br 0.4220963137 -3.1894985089 -0.6792592906
C 1.6630273865 3.2469471956 -0.6101312771
H 2.1291173917 3.7607371597 -1.4550210423
H 2.2486619074 3.4938372036 0.2828384004

CH2_Br_Cu2+_2e

1 2
C -0.3670895601 -3.0713610219 -1.9661792504
C 0.1079709333 -3.0809630106 -0.5084899462
C 0.5811441744 -2.1201591134 -2.717867965
C -0.2931202081 -1.7292379486 0.1006805709
N -0.5492483906 -0.7335569734 -0.9952582976
C 0.475285364 -0.718062247 -2.0709075424
C -1.8449042175 -1.07445952 -1.6291598718
H -0.3035130132 -4.0733480557 -2.3974501464
H 1.1939809082 -3.2230036895 -0.4878084311
H -0.3435598472 -3.8974883272 0.0634148126
H 0.320666803 -2.0598899114 -3.7787202907
H 1.5960835932 -2.5250422361 -2.6617442782
C -2.9525583147 -0.5324385341 -0.7487556044
C -4.1989849002 -1.1092508698 -0.6645424178
C -5.212357812 -0.4870503369 0.1092219474
H -4.3955910326 -2.0240656047 -1.2084236514
C -3.5774073801 1.2173378359 0.6125733516
C -4.8523616502 0.7183154812 0.755468065

H -3.2774368532 2.1425233019 1.0939652868
H -5.5572243659 1.268812735 1.3638747015
N -2.628262026 0.6173953032 -0.1215869369
H -1.8897867454 -0.4806226895 -2.5495403317
C 0.5816409622 -1.1666317524 1.2082873953
C 1.5592856377 -1.9039549289 1.8443301455
C 0.9110145363 0.6284414191 2.5929148666
C 2.2651170377 -1.335154976 2.9336388168
H 1.7709007883 -2.9140964758 1.5219139608
C 1.9051776489 -0.0194384784 3.2980643772
H 0.6262330115 1.6479375916 2.8397460418
H 2.3894135292 0.496966614 4.1163471785
N 0.24663626 0.0780266544 1.5734773288
H -1.2759833601 -1.8471973958 0.5721358889
H 0.065403959 -0.0320096447 -2.8210312181
C 1.6898589886 0.0199713003 -1.5479409966
C 2.9956553478 -0.3381435294 -1.7849811633
C 4.046456441 0.4932899388 -1.3183312353
H 3.2099074076 -1.2400113478 -2.3418652966
C 2.3220357643 1.9391616016 -0.4469290677
C 3.660224118 1.6676180111 -0.634702586
H 1.9959925327 2.8312212202 0.0790545795
H 4.3896517159 2.3694548842 -0.2533350036
N 1.341017453 1.1431865069 -0.887734507
Cu -0.6375849571 1.1617600483 -0.1700202714
Br -0.7896464957 3.4106164135 0.4983816119
C -1.830700675 -2.5745116157 -2.0107101196
H -2.2625643905 -2.7165027308 -3.005378292
H -2.4276969468 -3.1687801202 -1.3091516624
N -6.4524151032 -1.0195280019 0.2188403163
N 3.2377317707 -2.0233350867 3.5885012321
N 5.3487659837 0.1752642131 -1.5236061267
C -7.4685881831 -0.3382466127 1.0065285451
H -7.6768976494 0.6621925326 0.60982685
H -8.3929061786 -0.9138945768 0.9736362279
H -7.1633048685 -0.2466884417 2.0552155673
C 3.569457724 -3.3780519037 3.187767725
H 4.3775957802 -3.7510901749 3.816413771
H 2.7136531573 -4.0556342423 3.3008498762
H 3.9102853959 -3.4149138338 2.1454389344
H 4.4494266171 -0.505941517 4.4288422422
H 3.2092894945 -1.1667386164 5.5238065804
H 4.6438962973 -2.1208199017 5.123641248
C 5.7012057892 -1.0280907946 -2.2567514646
H 5.3105037561 -1.9252052166 -1.7613068979
H 5.3226101119 -1.0003838122 -3.2860812856
H 6.7862088964 -1.1171371627 -2.3002554682
C 6.3953433517 1.0764345345 -1.0680285308
H 7.3673121559 0.6574814137 -1.326591864
H 6.3118302374 2.0607185824 -1.5437820361
H 6.3612059646 1.2071035879 0.0198471685
C 3.9147517374 -1.4173130153 4.7224906863
C -6.7826765604 -2.2529231781 -0.474947346
H -7.8142782159 -2.5239109487 -0.2533870018
H -6.6886263249 -2.1405572969 -1.5619873016
H -6.1402229112 -3.0790743048 -0.1473161933

CH2_Br_Cu2+_2a

1 2
C 0.2099255494 3.7081625608 -0.4523616431
C -0.3139244679 3.1726560396 0.8852204264

C -0.7260523379 3.1483463941 -1.5374831366
 C 0.0466601513 1.680714674 0.9357415993
 N 0.3194495126 1.1641655623 -0.451812861
 C -0.6665465767 1.6030223495 -1.4798666122
 C 1.640953751 1.6949808056 -0.8785728189
 H 0.1783935596 4.7994043094 -0.465796404
 H -1.3970879767 3.327476981 0.9369819648
 H 0.1331876619 3.6926213315 1.7374070889
 H -0.4293903166 3.4915961226 -2.5323110723
 H -1.7358161074 3.5288542374 -1.3592888339
 C 2.7190266648 0.8349908703 -0.2547342164
 C 3.9854543034 1.2981072914 0.0595958723
 C 4.8990564227 0.3707452101 0.538199629
 H 4.2744187355 2.3345731525 -0.0645822097
 C 3.2767835748 -1.3384839466 0.3560770332
 C 4.5724601178 -0.9617433293 0.6939504045
 H 2.9356671767 -2.3646507949 0.4440732332
 H 5.2953058799 -1.6778630799 1.0639676971
 N 2.3798364839 -0.4611005733 -0.1020941506
 H 1.7059758824 1.5010335366 -1.9556717077
 C -0.8754960743 0.7724280895 1.7263649373
 C -1.8256702516 1.2410993402 2.6218463808
 C -1.3079384357 -1.4311699782 2.2930358711
 C -2.5179890262 0.2916715763 3.3597094567
 H -2.0341736699 2.292848871 2.7699294864
 C -2.2769083827 -1.0612842513 3.2221140916
 H -1.0659940421 -2.4730873996 2.1039648755
 H -2.8219535546 -1.7908715927 3.8077441352
 N -0.6316087491 -0.5362189464 1.5754460778
 H 1.0144534259 1.5820057264 1.4426001192
 H -0.2441445579 1.2452768842 -2.4261605582
 C -1.9194006507 0.769438672 -1.32246493
 C -3.2167934132 1.2318163215 -1.4460970303
 C -4.232923491 0.2879963182 -1.3776101774
 H -3.4598146048 2.2752288999 -1.6006461054
 C -2.6351673804 -1.4286973425 -1.0898578473
 C -3.971833931 -1.0566687919 -1.2105348326
 H -2.3360103379 -2.4624078379 -0.9468813969
 H -4.7730706251 -1.7839045419 -1.1725746892
 N -1.6459703906 -0.5377327719 -1.1390218885
 Cu 0.3513379724 -0.8898625122 -0.4099167344
 Br 0.422248023 -3.2031804322 -0.5974498405
 C 1.6656962962 3.2257183651 -0.6487344472
 H 2.1334494392 3.7256788737 -1.5007268733
 H 2.2502281043 3.4874547762 0.2406499563
 N -5.6366295757 0.7483454052 -1.4905972401
 O -6.4994025197 -0.1050646863 -1.4357644875
 O -5.8090744223 1.9460671246 -1.6240312378
 N 6.2618264015 0.8328706698 0.8909463806
 O 6.4893395883 2.0199566041 0.7465650961
 O 7.0374455184 -0.0090526937 1.297039046
 N -3.5473643415 0.7524494038 4.31955442
 O -4.1319457369 -0.1053272646 4.9512126037
 O -3.7268442487 1.9544394173 4.3948780998

CH2_Br_Cu+_2c

1 2
 C -0.6525697778 -3.4602629784 -0.7286528435
 C -0.0994226318 -2.876338703 0.5770190468
 C 0.2366255084 -2.9156100306 -1.861331167
 C -0.4694443604 -1.3854858826 0.5947976572

N -0.8042767655 -0.9277906793 -0.8025793297
 C 0.1795244052 -1.3682223575 -1.8269646563
 C -2.1234032038 -1.4892178386 -1.1816562882
 H -0.6010271499 -4.5511846446 -0.7118451455
 H 0.9834024321 -3.0329751958 0.6022784998
 H -0.5197913915 -3.3717527516 1.4569027213
 H -0.1043604741 -3.2757491254 -2.83621108
 H 1.2531855348 -3.294801928 -1.7228472621
 C -3.1978296423 -0.6132754155 -0.571637701
 C -4.4390016365 -1.0806204563 -0.1933954431
 C -5.3967020016 -0.1714361827 0.2850255783
 H -4.6612715741 -2.1392464803 -0.2467433927
 C -3.7686677628 1.5602806445 -0.0325299123
 C -5.0384280143 1.17900939 0.3575214185
 H -3.4506756326 2.5971340604 0.000040948
 H -5.7438646457 1.9329759843 0.6827605485
 N -2.861156368 0.6898343502 -0.4909041274
 H -2.2071122463 -1.3394804981 -2.2649465257
 C 0.4852340927 -0.4085909038 1.2635361077
 C 1.7416522888 -0.7335667743 1.737656403
 C 0.730749454 1.7896086756 1.8872105639
 C 2.5465516802 0.2846986224 2.2687365352
 H 2.1152967549 -1.7484046501 1.7026300708
 C 2.0105584075 1.5692172577 2.3721158368
 H 0.295079307 2.784349908 1.8975690889
 H 2.5929734672 2.394195262 2.7639659468
 N -0.0117920577 0.8355904241 1.324177753
 H -1.4118868607 -1.2662155256 1.1389490767
 H -0.234880455 -1.0173732431 -2.7795802301
 C 1.4264678737 -0.5299918528 -1.6323720043
 C 2.7217930861 -0.9964512818 -1.6786626222
 C 3.7796562134 -0.0943611606 -1.4748658815
 H 2.922262555 -2.0496102479 -1.8269704589
 C 2.1348168714 1.6328957041 -1.2439115986
 C 3.4647146311 1.2506702452 -1.2645718573
 H 1.8412534198 2.6660944429 -1.0867340267
 H 4.2384644371 1.9980003627 -1.1433131107
 N 1.1313467957 0.7680236518 -1.4157396015
 Cu -0.8746607817 1.1256741737 -0.8324357625
 Br -0.9573100828 3.4364138651 -1.1288562802
 C -2.1211679399 -3.0083796257 -0.8934534274
 H -2.609994876 -3.5482708849 -1.7089586195
 H -2.6690122413 -3.241636522 0.0266988031
 N 5.09439734 -0.5374296299 -1.4689171372
 N -6.6540995104 -0.6057164386 0.674009882
 N 3.8583174993 0.014151903 2.6487091715
 C 6.1558287834 0.0797930395 -0.817608593
 C 5.5707883708 -1.6895706449 -2.0868937241
 C 6.9054540568 -1.7870595982 -1.8332452619
 C 7.2739310646 -0.6707708611 -1.0191079377
 C -7.4971745217 0.0429166044 1.5702463972
 C -7.2894440547 -1.7640658476 0.2380191298
 C -8.5062710389 -1.8366990821 0.8443649189
 C -8.6332957187 -0.6961666326 1.6979250197
 C 4.6733212328 -0.9600171032 2.0874810558
 C 4.5976088075 0.714443895 3.5905767827
 C 5.9049152952 -0.8710348515 2.6657306971
 C 5.8536834387 0.1834633834 3.6275031458
 H 6.0011270596 0.9541835712 -0.2050755355
 H 4.9326112834 -2.2892775619 -2.7173913754
 H 7.5614554959 -2.5617257827 -2.2034381782

H 8.2550969228 -0.4564131731 -0.6209190831
H -7.1840704546 0.941454107 2.0788850732
H -6.8452027621 -2.3939453812 -0.5170201789
H -9.24205297 -2.6124910825 0.6892761336
H -9.4697219001 -0.4590929225 2.339288437
H 4.3230198987 -1.5824372082 1.2780068619
H 4.1416324266 1.4858540922 4.192290809
H 6.7600848701 -1.4820989667 2.4161268421
H 6.652100443 0.5012489694 4.282424399

CH2_Br_Cu2+_2f

1 2
C -0.5049314827 -2.8987414889 -2.295081895
C -0.0128957068 -3.0411271954 -0.8488773163
C 0.4366122947 -1.890278243 -2.9783220968
C -0.3922598744 -1.7454498189 -0.1165123218
N -0.6463972338 -0.6548698819 -1.1244378156
C 0.3965051422 -0.5645834215 -2.1785979393
C -1.9421319257 -0.9159919097 -1.7923441585
H -0.4570526766 -3.8594855849 -2.8134556986
H 1.0692890511 -3.2059111241 -0.8592923964
H -0.4688895646 -3.8981919694 -0.3443336831
H 0.129254726 -1.7073535071 -4.0123482534
H 1.4428257082 -2.3171382807 -3.0195504653
C -3.0454450512 -0.4096821072 -0.8862001247
C -4.3037890707 -0.96286426 -0.8489626741
C -5.3061292959 -0.3719876501 -0.0369460474
H -4.5202153542 -1.8429539211 -1.4418882676
C -3.6404874138 1.2548323805 0.5956440661
C -4.9262185518 0.7762981695 0.6964920977
H -3.3214305826 2.1360359032 1.1426524627
H -5.6322495818 1.299080421 1.3287958517
N -2.7013014041 0.6865915071 -0.1771769912
H -1.9585895893 -0.2576616742 -2.6694172042
C 0.5046534091 -1.2496181332 1.0095058359
C 1.7339298103 -1.7878914402 1.3235533486
C 0.6741134331 0.3290764255 2.6602750669
C 2.5029652377 -1.203496648 2.3589321259
H 2.1331257465 -2.6156277866 0.7537977513
C 1.9115794951 -0.1333608487 3.0618401333
H 0.222108412 1.1880330628 3.148207677
H 2.4166791696 0.3473118155 3.8902438407
N -0.0259562541 -0.1951783512 1.649331354
H -1.3683736833 -1.8879157323 0.3582490987
H 0.0523176169 0.2341022312 -2.8459555869
C 1.6312639393 -0.0003378936 -1.5067964723
C 2.9095012139 -0.4795523937 -1.6572428141
C 3.9603024984 0.1000260708 -0.9043426572
H 3.1014579547 -1.3235860794 -2.3065726105
C 2.3197386369 1.6380748002 -0.0399745312
C 3.6286407394 1.2110876051 -0.1001048608
H 2.0271397316 2.4820700935 0.5769296408
H 4.381297786 1.7380807739 0.4721926248
N 1.3231312984 1.0448202479 -0.7089806643
Cu -0.7046178911 1.1517207053 -0.1390061054
Br -0.7517020028 3.3322496053 0.7200151186
C -1.9620224117 -2.3834156377 -2.2786004433
H -2.4124250174 -2.44701334 -3.2732097298
H -2.5571739947 -3.0158697969 -1.6097538814
N 5.2113918846 -0.4065364056 -0.9404030427
N -6.5508899122 -0.8799877977 0.0287220198

N 3.7529608669 -1.6401384944 2.643208298
C 6.2882007283 0.0491882497 -0.0643492699
C 5.6279993284 -1.4949456259 -1.8227946179
C 7.1480827268 -1.5356040896 -1.6469900693
C 7.3502374576 -1.0415553237 -0.2109936924
C -7.5919733873 -0.3625882805 0.9192333294
C -7.0202425582 -1.9998807542 -0.7873098989
C -8.5356369037 -1.9897563628 -0.5726879708
C -8.6871456074 -1.4282428631 0.8442734628
C 4.4078054753 -2.7458444203 1.9540311658
C 4.6070619597 -1.0231629769 3.6562268145
C 5.6224977346 -3.0470319778 2.8340133953
C 5.9720339977 -1.6847925122 3.4414389753
H 5.9241110303 0.1461415712 0.9647276399
H 6.6652734831 1.0293189693 -0.3860099376
H 5.3350199522 -1.2918234605 -2.8583498529
H 5.1603766666 -2.4423687277 -1.5157190076
H 7.6221434441 -0.8460290111 -2.3528023034
H 7.5583853283 -2.53229573 -1.8214486356
H 8.3587347923 -0.6682770605 -0.0221682727
H 7.1515151655 -1.8538082897 0.4980343833
H -7.9489881367 0.6135080159 0.5641029059
H -7.2035437728 -0.23649852 1.9349424121
H -6.5682333966 -2.9410661758 -0.4442838433
H -6.7510259321 -1.8536336006 -1.838871473
H -8.9759343195 -2.9818434326 -0.6916073258
H -9.0085991489 -1.3194123099 -1.2978513381
H -8.4956166954 -2.2116770901 1.5850443375
H -9.6787833746 -1.0146103803 1.0380178477
H 4.7026954344 -2.4434080915 0.9366605385
H 3.7405068946 -3.6101367999 1.8716224066
H 4.2141928949 -1.2208160866 4.6625087199
H 4.6492328989 0.0637500911 3.5194808653
H 6.4462883525 -3.4907656071 2.2695165722
H 5.3399506325 -3.7508754704 3.6234388358
H 6.5697467682 -1.0968628705 2.7367353828
H 6.541059811 -1.7648659966 4.3697935295

CH2_Br_Cu2+_2d

1 2
C 0.33913123 3.7301740774 -0.4212561488
C -0.2048562833 3.2062009079 0.9128994372
C -0.6178276129 3.2113122404 -1.5085497709
C 0.0995953008 1.7015594299 0.9566156909
N 0.3528120795 1.1871731093 -0.4345769791
C -0.613904812 1.6642938666 -1.4614993333
C 1.6947973293 1.6651901452 -0.8546081442
H 0.3488019932 4.8223375718 -0.428841018
H -1.2821223442 3.3986545012 0.9641043489
H 0.2603710016 3.7055952248 1.7680664582
H -0.3104566788 3.5519909513 -2.5013598675
H -1.6129571724 3.626262233 -1.3239681806
C 2.7357393859 0.7621460013 -0.2272790883
C 4.021220908 1.1652980023 0.0949988625
C 4.9187359433 0.2172411253 0.5834549657
H 4.3243437255 2.1974297295 -0.0423901371
C 3.1970409695 -1.4279292882 0.3869199426
C 4.5024144628 -1.0985870653 0.7308605414
H 5.9318130839 0.5079349755 0.8413911911
H 2.8112607578 -2.4384956741 0.472539557
H 5.1707621188 -1.865604497 1.1039113044

N 2.3370404813 -0.5173458699 -0.0797599667
 H 1.7546511489 1.4734176408 -1.9323202216
 C -0.8525717057 0.8233835741 1.7471436806
 C -1.7751720845 1.3134039239 2.6611956722
 C -1.3670492109 -1.362862592 2.2922802136
 C -2.5147196503 0.4022981734 3.4141067307
 H -1.9147037351 2.3789645255 2.8020974688
 C -2.3094542007 -0.9585238287 3.2321446163
 H -1.1683443154 -2.4113109688 2.086973356
 H -3.2414050913 0.7586358916 4.1370723386
 H -2.8645521177 -1.6956324579 3.8007770549
 N -0.6568583979 -0.4905832802 1.5782212253
 H 1.0657346112 1.5664889169 1.4579540526
 H -0.1969534468 1.3010808229 -2.4080288123
 C -1.8955867691 0.8721651232 -1.3179096313
 C -3.1793419982 1.36821172 -1.4605588253
 C -4.2501341094 0.4750052735 -1.4108955229
 H -3.3532100736 2.4256446053 -1.622030208
 C -2.6816606092 -1.2978291216 -1.092394061
 C -4.000340107 -0.877436013 -1.2313219575
 H -5.2666548878 0.8385289368 -1.5206006032
 H -2.4154967292 -2.3397616638 -0.9432989465
 H -4.805127484 -1.6024557842 -1.1988715516
 N -1.6603181311 -0.4419542586 -1.1334919697
 Cu 0.3043701711 -0.8687561049 -0.4037249832
 Br 0.3045983944 -3.1908136805 -0.637287406
 C 1.7754799018 3.1936207165 -0.6201396787
 H 2.2614143136 3.6801666089 -1.4701146833
 H 2.3688732867 3.4291369126 0.2708401671

CH2_Cu1+_1d

1 1
 C -0.0000000002 0. 3.2366585056
 C 0.3458151803 -1.4085366686 2.7028875437
 C 1.0469209467 1.0037530657 2.7028875437
 C 0.6284014726 -1.2432733435 1.1888134048
 N -0.0000000002 0. 0.7329225445
 C -1.390907036 0.0774250325 1.1888134048
 C 0.7625055627 1.165848311 1.1888134048
 H -0.0000000002 0. 4.3289913152
 H -0.4954829516 -2.0879203957 2.884926259
 H 1.2170682449 -1.8206401968 3.2210559722
 H 2.0559335792 0.6148593749 2.884926259
 H 0.9681865388 1.9643321168 3.2210559722
 C 1.9474369842 1.3994716217 0.260717068
 C 3.1241335749 1.9898465319 0.7047335873
 C 4.1461510816 2.244232756 -0.2044490503
 H 3.2389140327 2.2560730022 1.7497403564
 C 2.75743506 1.3119621196 -1.9034182926
 C 3.9614012052 1.8980194637 -1.5359864505
 H 5.0711033498 2.7056983882 0.125591971
 H 2.5687393994 1.0241540381 -2.9324815407
 H 4.7288474549 2.0743420741 -2.2807195694
 N 1.7683430463 1.0665669268 -1.0356470209
 H 0.1018482624 2.0310692903 1.0447111126
 C 0.2382594838 -2.3862657116 0.260717068
 C 0.1611908585 -3.7005023069 0.7047335873
 C -0.242525006 -3.0439898712 -1.9034182926
 C -0.1295129624 -4.7127885428 -0.2044490503
 H 0.334359516 -3.9330183343 1.7497403564
 C -0.3369675305 -4.3796838104 -1.5359864505

H -0.3974262857 -2.7366705949 -2.9324815407
 H -0.1923481361 -5.7445535205 0.125591971
 H -0.5679907955 -5.1324730638 -2.2807195694
 N 0.0395025299 -2.0647134643 -1.0356470209
 C -2.1856964687 0.9867940899 0.260717068
 C -3.2853244341 1.7106557749 0.7047335873
 C -4.0166381199 2.4685557868 -0.2044490503
 H -3.5732735494 1.6769453321 1.7497403564
 C -2.5149100547 1.7320277517 -1.9034182926
 C -3.6244336754 2.4816643466 -1.5359864505
 H -4.8787552145 3.0388551323 0.125591971
 H -2.1713131145 1.7125165568 -2.9324815407
 H -4.1608566601 3.0581309898 -2.2807195694
 N -1.8078455769 0.9981465375 -1.0356470209
 H -1.8098817338 -0.9273314624 1.0447111126
 H 1.7080334707 -1.1037378279 1.0447111126
 Cu -0.0000000002 0. -1.3932739078
 C -1.3927361277 0.404783603 2.7028875437
 H -2.1852547844 -0.14369192 3.2210559722
 H -1.5604506284 1.4730610209 2.884926259

CH2_Cu1+_4a

1 1
 C 0.0000000005 0. 2.9690782548
 C -0.0127854947 -1.4513535519 2.4361670973
 C 1.2633017939 0.7146042123 2.4361670973
 C 0.3316620839 -1.3540594176 0.9261155669
 N 0.0000000005 0. 0.4697625335
 C -1.3384808951 0.3898019191 0.9261155669
 C 1.0068188127 0.9642574985 0.9261155669
 H 0.0000000005 0. 4.0614925284
 H -0.9982005697 -1.9003775063 2.6046403757
 H 0.7215445244 -2.0628242203 2.969201851
 H 2.1448754829 0.0857217013 2.6046403757
 H 1.4256859169 1.6562879978 2.969201851
 C 2.1517741524 0.9033728367 -0.0589330342
 N 1.9690702738 0.5223198817 -1.3173579124
 H 0.5493537228 1.9548915973 0.8074464087
 C -0.2935432498 -2.3151774971 -0.0589330342
 N -0.5816975164 -3.6262756888 0.1356316941
 N -0.5321928497 -1.9664248194 -1.3173579124
 C -1.8582309011 1.4118046605 -0.0589330342
 N -2.8495981087 2.3169026714 0.1356316941
 N -1.4368774226 1.4441049377 -1.3173579124
 H -1.9676626455 -0.5016915195 0.8074464087
 H 1.4183089242 -1.4532000778 0.8074464087
 Cu 0.0000000005 0. -1.7712536998
 C -1.2505162977 0.7367493396 2.4361670973
 H -2.1472304398 0.4065362225 2.969201851
 H -1.1466749117 1.814655805 2.6046403757
 N 3.4312956266 1.3093730174 0.1356316941
 C 3.1764737892 0.6710999344 -1.9479623568
 C 4.0921890493 1.1593810232 -1.0640789054
 C 4.0303055915 1.848049869 1.3472708551
 H 3.304741572 0.4209984758 -2.9897436232
 H 5.1363271903 1.4107446716 -1.1695176399
 H 3.3533321293 2.5622801877 1.818773028
 H 4.9462200612 2.3731008391 1.0750319668
 H 4.2752479 1.0524864119 2.0548924961
 C -3.0501479427 2.9642491617 -1.0640789054
 C -2.1694264855 2.4153570282 -1.9479623568

C -3.615610929 2.5663220923 1.3472708551
 H -3.7899043182 3.7428174927 -1.1695176399
 H -2.0169661603 2.6514909159 -2.9897436232
 H -3.895665798 1.622930717 1.818773028
 H -4.5282756422 3.0970018057 1.0750319668
 H -3.0491039191 3.1762300825 2.0548924961
 C -1.0420411051 -4.123630185 -1.0640789054
 C -0.414694661 -4.4143719613 1.3472708551
 H -1.3464228705 -5.1535621643 -1.1695176399
 H 0.5423336702 -4.1852109047 1.818773028
 H -0.4179444174 -5.4701026448 1.0750319668
 H -1.2261439794 -4.2287164944 2.0548924961
 C -1.0070473022 -3.0864569627 -1.9479623568
 H -1.2877754102 -3.0724893918 -2.9897436232

CH2_Cu1+_4b

1 1
 C 0.0000000002 0.0000000003 3.4859539972
 C 1.363629656 0.5158616128 2.9493566595
 C -1.1285640889 0.9230071174 2.9493566595
 C 1.1251814087 0.8039915327 1.4497625661
 N 0.0000000002 0.0000000003 1.0066700534
 C 0.1336863875 -1.3764314494 1.4497625661
 C -1.2588677954 0.5724399177 1.4497625661
 H 0.0000000002 0.0000000003 4.5775186049
 H 2.1400521311 -0.2431637332 3.0995217139
 H 1.6763411951 1.421014417 3.4776512866
 H -0.8594400947 1.9749213779 3.0995217139
 H -2.0688051812 0.7412468522 3.4776512866
 N -1.5743764338 1.654458218 0.5219056407
 C -1.2373267051 1.5534533407 -0.8043744955
 H -2.018553674 -0.2039547674 1.3178213221
 N 2.2199910633 0.5362208785 0.5219056407
 C 1.9639934092 0.2948296897 -0.8043744955
 N -0.6456146288 -2.1906790955 0.5219056407
 C -0.7266667034 -1.8482830294 -0.8043744955
 H 1.1859068474 -1.6461413766 1.3178213221
 H 0.8326468273 1.850096145 1.3178213221
 Cu 0.0000000002 0.0000000003 -1.2414086935
 C -0.2350655665 -1.4388687292 2.9493566595
 H 0.3924639868 -2.1622612682 3.4776512866
 H -1.2806120358 -1.7317576437 3.0995217139
 N -1.3981881798 -2.8850961525 -1.3476271496
 C -1.2326737353 -3.4175441668 0.7771745516
 C -1.7147821407 -3.8542069099 -0.4078170113
 N -1.7994724704 2.6534145599 -1.3476271496
 C -2.3433431993 2.7762988534 0.7771745516
 C -2.480450025 3.4121483515 -0.4078170113
 N 3.1976606509 0.2316815936 -1.3476271496
 C 3.5760169353 0.6412453144 0.7771745516
 H -1.25692751 -3.8684935079 1.7568029858
 H -2.2534812595 -4.7539616542 -0.6614351285
 H -2.7217498971 3.022777909 1.7568029858
 H -2.9903109313 4.3285528455 -0.6614351285
 H 3.9786774079 0.8457155998 1.7568029858
 C -1.6911588019 3.0050525832 -2.7533970084
 C 3.4480312778 -0.0379398066 -2.7533970084
 C -1.7568724752 -2.9671127756 -2.7533970084
 H -1.103291636 2.2319385178 -3.2478902704
 H -1.1895854131 3.9696977045 -2.86403432
 H -2.6840672912 3.0556155231 -3.2071138539

H 2.4845612742 -0.1604906737 -3.2478902704
 H 4.0326517641 -0.9546376638 -2.86403432
 H 3.9882743129 0.7966626988 -3.2071138539
 H -1.3812696375 -2.0714478432 -3.2478902704
 H -2.8430663503 -3.0150600397 -2.86403432
 H -1.304207021 -3.8522782209 -3.2071138539
 C 4.1952321664 0.4420585594 -0.4078170113
 H 5.2437921915 0.4254088097 -0.6614351285

CH2_Cu1+_1b

1 1
 C 0. -0.0000000002 3.1713663856
 C -1.0307969898 1.0205619347 2.6381774182
 C -0.3684340668 -1.4029773469 2.6381774182
 C -1.185522286 0.7310882953 1.1244846912
 N 0. -0.0000000002 0.6668391736
 C 1.2259021793 0.6611482686 1.1244846912
 C -0.0403798932 -1.3922365643 1.1244846912
 H 0. -0.0000000002 4.2634786085
 H -0.6677052608 2.0389791323 2.8207420925
 H -1.9888990137 0.9168158041 3.1562058113
 H -1.4319550961 -1.5977392845 2.8207420925
 H 0.2004637298 -2.1808449737 3.1562058113
 C -0.926416151 -2.2104765714 0.1941095296
 C -1.6174733425 -3.3249364589 0.6480708106
 C -2.3531669512 -4.0752634565 -0.2649027746
 H -1.5819489854 -3.6158604121 1.6913965558
 C -1.6617808768 -2.568252863 -1.9649488919
 C -2.3823462279 -3.6961074805 -1.6005027124
 Cl -3.2241059489 -5.4680019442 0.2682814884
 H -1.655476233 -2.233413505 -2.9968102879
 H -2.9463483138 -4.2565155923 -2.336133329
 N -0.9469186684 -1.8357720127 -1.1027348532
 H 0.9744666242 -1.7859489849 0.9800217373
 C -1.4511207897 1.9075382067 0.1941095296
 C -2.070742768 3.0632412338 0.6480708106
 C -1.3932817842 2.7232708861 -1.9649488919
 C -2.3526982047 4.0755340871 -0.2649027746
 H -2.3404524806 3.1779382147 1.6913965558
 C -2.0097498592 3.9112260941 -1.6005027124
 H -1.1064547158 2.5503912254 -2.9968102879
 Cl -3.1233756171 5.5261586281 0.2682814884
 H -2.2130764775 4.6798702841 -2.336133329
 N -1.1163658642 1.7379416283 -1.1027348532
 C 2.3775369407 0.3029383642 0.1941095296
 C 3.6882161106 0.2616952247 0.6480708106
 C 4.7058651559 -0.0002706311 -0.2649027746
 H 3.922401466 0.437922197 1.6913965558
 C 3.055062661 -0.1550180236 -1.9649488919
 C 4.3920960871 -0.215118614 -1.6005027124
 Cl 6.347481566 -0.0581566844 0.2682814884
 H 2.7619309489 -0.3169777209 -2.9968102879
 H 5.1594247913 -0.4233546922 -2.336133329
 N 2.0632845326 0.0978303839 -1.1027348532
 H 1.0594438786 1.7368873439 0.9800217373
 H -2.0339105027 0.0490616405 0.9800217373
 Cu 0. -0.0000000002 -1.4623856719
 C 1.3992310566 0.3824154117 2.6381774182
 H 1.7884352839 1.2640291692 3.1562058113
 H 2.0996603569 -0.4412398483 2.8207420925

CH2_Cu1+_1e

1 1

C 0.0000000001 0.0000000004 3.1144062078
C -0.7630965895 -1.2325180989 2.5805385976
C 1.4489402794 -0.0446019821 2.5805385976
C -0.4545366501 -1.3166523899 1.0644368513
N 0.0000000001 0.0000000004 0.6125295761
C -0.9129860928 1.0519664815 1.0644368513
C 1.3675227431 0.2646859095 1.0644368513
H 0.0000000001 0.0000000004 4.207281335
H -1.8367331041 -1.1073237159 2.7658581641
H -0.445069771 -2.1436765864 3.0973332293
H 1.8773370207 -1.0369956697 2.7658581641
H 2.0790132673 0.6863965656 3.0973332293
C 2.360204871 -0.4279865214 0.1374904691
C 3.585982991 -0.8610100583 0.6032696005
C 4.5272603115 -1.4347344374 -0.2831047479
H 3.818998259 -0.7425003453 1.653376129
C 2.8800879769 -1.0685321156 -2.0016037073
C 4.1263913111 -1.5290081035 -1.633477956
H 2.5648547957 -1.1388218124 -3.0380315418
H 4.7706115797 -1.9544318809 -2.391638084
N 1.9917517686 -0.5218531319 -1.1590741633
H 1.527754843 1.3405225719 0.9141492155
C -1.5507496357 -1.8300041151 0.1374904691
C -2.5386480791 -2.6750473379 0.6032696005
C -2.3654199455 -1.9599632947 -2.0016037073
H -2.552523291 -2.936099336 1.653376129
C -3.387355516 -2.8090556489 -1.633477956
H -2.268676018 -1.6518185033 -3.0380315418
H -4.0778934489 -3.1542548785 -2.391638084
N -1.4478139538 -1.463981063 -1.1590741633
C -0.8094552351 2.2579906376 0.1374904691
C -1.0473349116 3.5360573974 0.6032696005
C -1.0211136849 4.6380896585 -0.2831047479
H -1.2664749677 3.6785996824 1.653376129
C -0.5146680312 3.0284954115 -2.0016037073
C -0.7390357949 4.3380637536 -1.633477956
H -0.2961787775 2.7906403169 -3.0380315418
H -0.6927181306 5.1086867606 -2.391638084
N -0.5439378146 1.9858341961 -1.1590741633
H -1.9248040226 0.6528132194 0.9141492155
H 0.3970491799 -1.9933357901 0.9141492155
Cu 0.0000000001 0.0000000004 -1.5283759198
C -0.6858436897 1.2771200821 2.5805385976
H -1.633943496 1.457280022 3.0973332293
H -0.0406039163 2.1443193867 2.7658581641
N -1.25154829 5.9070395481 0.142908675
N -4.4898721644 -4.0373923867 0.142908675
N 5.7414204546 -1.8696471602 0.142908675
C -4.5687607418 -4.416502687 1.5420369945
H -5.4232765358 -5.076797716 1.6875364181
H -3.6682538833 -4.9532512487 1.8656523711
H -4.7064245821 -3.5402655688 2.1876377099
C -3.5061466264 -3.20335522 -0.2831047479
C -5.4570177347 -4.5612413794 -0.8065536484
H -6.1593022143 -5.2094100039 -0.283072673
H -6.0295411201 -3.7549157066 -1.2806484261
H -4.9690279804 -5.1536214928 -1.5899325293
C -1.5404231522 6.1649142104 1.5420369945
H -0.7127476279 5.8460160342 2.1876377099

H -1.6849975243 7.2350941104 1.6875364181
H -2.4555144713 5.6534266754 1.8656523711
C -1.2216420402 7.0065366775 -0.8065536484
H -1.9786531443 6.8801152102 -1.5899325293
H -1.4318302952 7.9388171898 -0.283072673
H -0.2370818312 7.0991936371 -1.2806484261
C 6.1091838942 -1.7484115222 1.5420369945
H 5.4191722102 -2.3057504642 2.1876377099
H 7.1082740603 -2.1582963932 1.6875364181
H 6.1237683548 -0.7001754256 1.8656523711
C 6.6786597751 -2.4452952969 -0.8065536484
H 6.2666229514 -3.3442779293 -1.2806484261
H 6.947681125 -1.7264937162 -1.5899325293
H 7.5911325097 -2.7294071847 -0.283072673

CH2_Cu1+_1a

1 1

C 0.0000000001 0.0000000007 3.1508721866
C -1.2966462016 -0.651112764 2.6180135968
C 1.212203296 -0.7973721674 2.6180135968
C -1.069571799 -0.8920215768 1.1053041203
N 0.0000000001 0.0000000007 0.6446929577
C -0.2377274472 1.3722871387 1.1053041203
C 1.3072992466 -0.4802655597 1.1053041203
H 0.0000000001 0.0000000007 4.2426501987
H -2.1464984561 0.0175053819 2.7993830801
H -1.5050547715 -1.5916655433 3.1360950343
H 1.0580891234 -1.8676748822 2.7993830801
H 2.1309501814 -0.5075828936 3.1360950343
C 1.802629211 -1.5780965405 0.1744751792
C 2.6389878105 -2.590670868 0.6255247912
C 3.102100812 -3.5082379219 -0.3019742584
H 2.9358968354 -2.673048056 1.6637672594
C 1.9086332513 -2.3831341531 -1.99628125
C 2.749831904 -3.4282106179 -1.6350896471
H 1.5918949504 -2.2629443015 -3.0263939615
H 3.1125201711 -4.1476401728 -2.3580810186
N 1.4449711339 -1.4799470844 -1.1244671652
H 2.0039823195 0.3567277224 0.9630629299
C -2.2679862996 -0.7720744189 0.1744751792
C -3.5630806901 -0.9900950489 0.6255247912
C -3.0181713433 -0.4613578043 -1.99628125
C -4.5892735693 -0.9323791461 -0.3019742584
H -3.7828759401 -1.2060372132 1.6637672594
C -4.3438334371 -0.6673189748 -1.6350896471
H -2.755714728 -0.2471493153 -3.0263939615
H -5.1482218413 -0.6217014503 -2.3580810186
N -2.0041573388 -0.5114081663 -1.1244671652
C 0.465357089 2.3501709615 0.1744751792
C 0.9240928801 3.5807659191 0.6255247912
C 1.4871727578 4.4406170702 -0.3019742584
H 0.8469791051 3.8790852713 1.6637672594
C 1.1095380924 2.8444919596 -1.99628125
C 1.5940015335 4.0955295949 -1.6350896471
H 1.1638197781 2.5100936189 -3.0263939615
H 2.0357016707 4.7693416253 -2.3580810186
N 0.5591862052 1.9913552529 -1.1244671652
H -1.3109264287 1.5571357372 0.9630629299
H -0.6930558904 -1.9138634574 0.9630629299
Cu 0.0000000001 0.0000000007 -1.477785096
C 0.0844429061 1.4484849336 2.6180135968

H -0.6258954095 2.0992484391 3.1360950343
H 1.0884093331 1.8501695024 2.7993830801
N 3.9920924478 -4.5993988359 0.1526510564
O 4.3826149619 -5.3782274298 -0.695207571
O 4.2602402022 -4.629692742 1.3397491153
N 1.987150011 5.756952893 0.1526510564
O 1.879311426 6.0043226133 1.3397491153
O 2.4663741014 6.4845696079 -0.695207571
N -5.9792424583 -1.1575540549 0.1526510564
O -6.8489890629 -1.1063421759 -0.695207571
O -6.1395516278 -1.3746298691 1.3397491153

CH2_Cu1+_1f

1 1
C 0.0000000002 -0.0000000005 2.9975946179
C 1.4484048741 0.0582790873 2.463679365
C -0.7746736073 1.2252158713 2.463679365
C 1.3452422226 0.3610444355 0.9475590528
N 0.0000000002 -0.0000000005 0.4959205956
C -0.3599474574 -1.3455361573 0.9475590528
C -0.9852947645 0.9844917202 0.9475590528
H 0.0000000002 -0.0000000005 4.0905436043
H 1.9459516067 -0.9012940775 2.6488796421
H 2.0252684577 0.8320286023 2.9804277911
H -0.1924322361 2.1358905637 2.6488796421
H -1.7331921352 1.3379196318 2.9804277911
C -0.968067249 2.1950968826 0.0209565381
C -1.2932921284 3.4534498548 0.4861912765
C -1.3416437821 4.5521839274 -0.4030849791
H -1.5102536491 3.5924359632 1.538080382
C -0.7234778142 2.9841441806 -2.1201410324
C -1.037350926 4.2750223502 -1.7533287573
N -1.6588549316 5.7952646296 0.0199945231
H -0.4905070759 2.7593380277 -3.1563805624
H -1.0574535016 5.0504496641 -2.5088360608
N -0.6832880115 1.9421145309 -1.2761607158
H -1.9660750161 0.5143013155 0.7973539294
C 2.3850432894 -0.2591776117 0.0209565381
C 3.63742137 -0.6067010903 0.4861912765
C 2.9460835768 -0.8655219248 -2.1201410324
C 4.6131288157 -1.1141943662 -0.4030849791
H 3.8662676309 -0.4882999559 1.538080382
C 4.2209534208 -1.2391389212 -1.7533287573
H 2.6349103683 -0.954877426 -3.1563805624
N 5.8482738574 -1.4610218034 0.0199945231
H 4.9025444612 -1.609443237 -2.5088360608
N 2.0235645274 -0.37931249 -1.2761607158
C -1.4169760397 -1.9359192725 0.0209565381
C -2.3441292409 -2.8467487661 0.4861912765
C -3.2714850329 -3.4379895628 -0.4030849791
H -2.3560139812 -3.1041360088 1.538080382
C -2.222605762 -2.1186222574 -2.1201410324
C -3.1836024942 -3.0358834306 -1.7533287573
N -4.1894189252 -4.3342428277 0.0199945231
H -2.1444032918 -1.8044606032 -3.1563805624
H -3.845090959 -3.4410064287 -2.5088360608
N -1.3402765153 -1.5628020425 -1.2761607158
H 0.5376395035 -1.9598215684 0.7973539294
H 1.4284355132 1.4455202514 0.7973539294
Cu 0.0000000002 -0.0000000005 -1.6447447049
C -0.6737312662 -1.2834949602 2.463679365

H -0.2920763218 -2.1699482356 2.9804277911
H -1.75351937 -1.2345964878 2.6488796421
C 6.8544346853 -2.0804792318 -0.8409276633
C 6.329648905 -1.2508570138 1.3834068569
C 7.9313337015 -2.5411362008 0.1438015611
C 7.8336078166 -1.5148380005 1.2766457312
C -5.2289652086 -4.8958749508 -0.8409276633
C -4.2480984022 -4.8562082424 1.3834068569
C -6.1663553543 -5.5981683716 0.1438015611
C -5.2286920985 -6.0266843728 1.2766457312
C -1.6254694761 6.976354181 -0.8409276633
C -2.0815505021 6.1070652547 1.3834068569
C -1.7649783465 8.1393045708 0.1438015611
C -2.6049157174 7.5415223717 1.2766457312
H 7.2488879192 -1.3505741837 -1.5616448919
H 6.4230135731 -2.9152726527 -1.4035168891
H 5.8435189274 -1.9507057845 2.0781058268
H 6.112380884 -0.2313079504 1.7204819955
H 8.9213972156 -2.5816346454 -0.3149680809
H 7.6896091932 -3.5416341752 0.5178975782
H 8.3532694884 -0.5924971113 0.9964800447
H 8.2592386527 -1.8705054866 2.2173096009
H -4.7940755116 -5.6024339959 -1.5616448919
H -5.736206962 -4.1048565974 -1.4035168891
H -4.6111202276 -4.0852829469 2.0781058268
H -3.2565090024 -5.1778231486 1.7204819955
H -6.6964597933 -6.4353393039 -0.3149680809
H -6.9119497625 -4.8885798195 0.5178975782
H -4.6897522935 -6.9378950265 0.9964800447
H -5.7495245949 -6.2174577464 2.2173096009
H -2.4548124069 6.9530081781 -1.5616448919
H -0.6868066105 7.0201292486 -1.4035168891
H -1.2323986991 6.0359887299 2.0781058268
H -2.855871881 5.4091310974 1.7204819955
H -2.2249374217 9.0169739477 -0.3149680809
H -0.7776594301 8.4302139931 0.5178975782
H -3.6635171942 7.5303921363 0.9964800447
H -2.5097140571 8.0879632315 2.2173096009

CH2_Cu1+_1c

1 1
C 0.0255216333 -0.037055633 2.9860285706
C 1.4706689592 0.0169075773 2.4415063545
C -0.745640085 1.1984745554 2.4698666448
C 1.3555514462 0.3393582738 0.9306066095
N 0.0058716316 -0.014060286 0.4825863125
C -0.3537897603 -1.3627019299 0.9286855836
C -0.9730813909 0.9687815755 0.9547718996
H 0.0343968018 -0.0469045307 4.0783041669
H 1.9627789517 -0.9478486085 2.613083361
H 2.056588764 0.780940694 2.961593121
H -0.1553758155 2.103260942 2.6578170992
H -1.6982693414 1.3135261717 2.9960514515
C -0.9641827288 2.1840669222 0.0359518485
C -1.2811308252 3.4462105771 0.5075861958
C -1.3306237274 4.5278846795 -0.3801574068
H -1.4689861332 3.5984898614 1.5634160263
C -0.725057389 2.9890070548 -2.1067428915
C -1.0427185782 4.2796693893 -1.724406009
N -1.6518090731 5.8046125332 0.0675213871
H -0.5010130331 2.7684834023 -3.1452158298

H -1.0923296334 5.0653661205 -2.468021696
 N -0.6860412945 1.948604614 -1.2644487362
 H -1.957491746 0.5035265464 0.812096079
 C 2.3851528704 -0.269579693 -0.0128726181
 C 3.646139526 -0.6279816644 0.4314904025
 C 2.9198431005 -0.8663665839 -2.170201713
 C 4.5898181123 -1.1202278694 -0.4782451293
 H 3.8929000282 -0.5475546399 1.4831251867
 C 4.2039959226 -1.2379734316 -1.8157434746
 H 2.596047906 -0.9444263861 -3.2028360476
 N 5.8650706569 -1.4821279036 -0.0582545854
 H 4.8943853179 -1.5828316908 -2.5754596557
 N 2.0161410681 -0.385374042 -1.3068020153
 C -1.4173518168 -1.941000494 0.0040183335
 C -2.3375746863 -2.8691940221 0.4595992585
 C -3.2540478672 -3.4357158591 -0.4344643127
 H -2.3204109282 -3.1832523725 1.4962530483
 C -2.2326431798 -2.1086367117 -2.1412248927
 C -3.1920726698 -3.0334351049 -1.7709606552
 N -4.1919148482 -4.3665676194 -0.0016015084
 H -2.1665681525 -1.7758793563 -3.1718387384
 H -3.8938282087 -3.4054061687 -2.5070632611
 N -1.3560427988 -1.5601506011 -1.2902225118
 H 0.5400632255 -1.9800977731 0.7688609601
 H 1.4418929835 1.4255164506 0.7939221151
 Cu -0.0123396954 0.0042020665 -1.6511738482
 C -0.6601617802 -1.3121540135 2.4462023045
 H -0.2808170909 -2.2050365837 2.9525401994
 H -1.7386277607 -1.259041134 2.638118824
 C 6.6882987324 -2.4152832611 -0.6743069149
 C 6.5318300076 -0.9744981751 1.0491350237
 C 7.8483391283 -2.4965389231 0.0365488753
 C 7.753236573 -1.5748335932 1.1241850361
 C -4.7899479272 -5.3422897656 -0.7880151045
 C -4.6894554142 -4.480986579 1.2899230264
 C -5.6429308128 -6.0595930876 -0.003559855
 C -5.5868560211 -5.5065269062 1.3126705251
 C -1.2608123304 6.9961631644 -0.528558002
 C -2.4158696842 6.1061301697 1.1873128776
 C -1.7651710187 8.0270412703 0.2066829096
 C -2.5066707534 7.4622647742 1.2895756187
 H 6.3474591154 -2.9787352293 -1.5292271086
 H 6.1005309336 -0.1844575916 1.6444658669
 H 8.678506848 -3.1513907768 -0.1854063537
 H 8.5106402562 -1.3715744477 1.8674295463
 H -4.5078785376 -5.4737466478 -1.8212706351
 H -4.4047303634 -3.7809030601 2.0601243625
 H -6.2398743243 -6.9000093401 -0.3269934914
 H -6.1568474166 -5.8262560923 2.173060744
 H -0.6098831968 6.9998587915 -1.389282603
 H -2.8792326713 5.3258359017 1.7712783706
 H -1.6157064211 9.0776317853 0.0036958136
 H -3.0555615691 8.0016103188 2.0480056648

CH2_Cu1+_4c

-2 1

C -0.0000000003 -0.0000000001 3.1125723881
 C 0.3933033954 -1.3965084707 2.575974958
 C 1.0127601132 1.0388649659 2.575974958
 C 0.6476703153 -1.2381883545 1.0518938592
 N -0.0000000003 -0.0000000001 0.61265702

C -1.3961377268 0.0581952292 1.0518938592
 C 0.7484674107 1.1799931223 1.0518938592
 H -0.0000000003 -0.0000000001 4.2117343949
 H -0.4173689818 -2.1143324188 2.7617930797
 H 1.2898749287 -1.7692093275 3.0902259117
 H 2.0397500764 0.6957140671 2.7617930797
 H 0.8872427566 2.0016691184 3.0902259117
 C 1.9457247482 1.3588740854 0.1556800223
 N 1.808543855 1.0708725127 -1.1735886688
 H 0.0587751358 2.0208073876 0.8968864377
 C 0.2039571048 -2.3644841051 0.1556800223
 N 0.0231308732 -2.1016811804 -1.1735886688
 C -2.1496818538 1.0056100167 0.1556800223
 N -1.831674729 1.0308086647 -1.1735886688
 H -1.779458103 -0.9595029343 0.8968864377
 H 1.7206829664 -1.0613044562 0.8968864377
 Cu -0.0000000003 -0.0000000001 -1.5767671143
 C -1.4060635095 0.3576435018 2.575974958
 H -2.1771176861 -0.2324597939 3.0902259117
 H -1.6223810953 1.4186183487 2.7617930797
 C -2.6819207394 1.9243202823 -1.741938311
 C -3.1994625211 1.876248624 0.4354365559
 C -3.551320055 2.4723833539 -0.8021937143
 C 3.0074706196 1.3604513484 -1.741938311
 C 3.2246102332 1.832691508 0.4354365559
 C 3.9168068204 1.8393417059 -0.8021937143
 C -0.325549881 -3.2847716337 -1.741938311
 C -0.0251477129 -3.708940135 0.4354365559
 C -0.3654867661 -4.3117250629 -0.8021937143
 H -2.6162790498 2.1378360309 -2.80527986
 H -3.6583767166 2.0463045651 1.4057502697
 H -4.3244747101 3.2154986023 -0.9812114692
 H 3.1595598372 1.1968461033 -2.80527986
 H 3.6013400961 2.1450948889 1.4057502697
 H 4.9469408309 2.1373556541 -0.9812114692
 H -0.5432807882 -3.3346821372 -2.80527986
 H 0.0570366198 -4.1913994571 1.4057502697
 H -0.6224661217 -5.3528542593 -0.9812114692

CH2_Cu2+_1d

2 2

C 0.0000000005 0. 3.2192276102
 C 1.4152909298 -0.3073880352 2.687870528
 C -0.4414396169 1.3793719161 2.687870528
 C 1.4163450128 0.0257698908 1.177523425
 N 0.0000000005 0. 0.7092084178
 C -0.6858551256 -1.2394757066 1.177523425
 C -0.7304898858 1.2137058158 1.177523425
 H 0.0000000005 0. 4.3103916085
 H 1.6621680228 -1.3603122008 2.8617579381
 H 2.1680200793 0.2959683847 3.2017098919
 H 0.3469809123 2.1196358331 2.8617579381
 H -1.3403261788 1.7295762718 3.2017098919
 C -0.4027485761 2.3722899565 0.2550279574
 C -0.4573598718 3.6962387789 0.6586809492
 C -0.2172146387 4.6987924258 -0.2794938102
 H -0.6927850855 3.9478854459 1.6869132967
 C 0.1221151763 3.0007954887 -1.9225484662
 C 0.0779363268 4.3467953618 -1.5911370183
 H -0.2594868075 5.7421673174 0.0148332
 H 0.3557793648 2.6781551478 -2.9317159529

H 0.273965411 5.0965710308 -2.348555213
 N -0.1184827811 2.0347574723 -1.0234257684
 H -1.7945767589 0.9887378536 1.0354709949
 C 2.2558376562 -0.8373544796 0.2550279574
 C 3.4297166176 -1.4520341214 0.6586809492
 C 2.5377075373 -1.6061525888 -1.9225484662
 C 4.1778809279 -2.1612828173 -0.2794938102
 H 3.7653616308 -1.3739732391 1.6869132967
 C 3.7254670457 -2.2408925194 -1.5911370183
 H 2.1414607116 -1.6471915415 -2.9317159529
 H 5.1026061741 -2.646361491 0.0148332
 H 4.2767772801 -2.7855465206 -2.348555213
 N 1.8213930528 -0.9147696374 -1.0234257684
 C -1.8530890787 -1.5349354769 0.2550279574
 C -2.9723567444 -2.2442046576 0.6586809492
 C -3.9606662878 -2.5375096085 -0.2794938102
 H -3.0725765439 -2.5739122068 1.6869132967
 C -2.6598227122 -1.3946428999 -1.9225484662
 C -3.8034033711 -2.1059028424 -1.5911370183
 H -4.8431193652 -3.0958058263 0.0148332
 H -2.497240075 -1.0309636063 -2.9317159529
 H -4.5507426896 -2.3110245102 -2.348555213
 N -1.7029102703 -1.1199878349 -1.0234257684
 H 0.0410162813 -2.0485179895 1.0354709949
 H 1.753560479 1.0597801359 1.0354709949
 Cu 0.0000000005 0. -1.2208339933
 C -0.9738513115 -1.071983881 2.687870528
 H -0.8276938991 -2.0255446565 3.2017098919
 H -2.0091489337 -0.7593236323 2.8617579381

CH2_Cu2+_4a

2 2
 C 0.0241769927 -0.1275594819 3.3342741988
 C 1.4301394338 -0.4893969667 2.8102405261
 C -0.3538920488 1.2761470343 2.8158423475
 C 1.458763364 -0.1088086488 1.3111169786
 N 0.0446134652 -0.0991169333 0.818259382
 C -0.6716506503 -1.3306643812 1.2801004246
 C -0.665065117 1.1253567846 1.308092429
 H 0.0154315996 -0.1399260169 4.425333845
 H 1.6281371522 -1.5554992918 2.9613664116
 H 2.1994639402 0.0674419017 3.3510412773
 H 0.4665137643 1.9794000316 2.9920336944
 H -1.2326088492 1.6586598155 3.3411659016
 C -0.306221786 2.2283145065 0.347385773
 N -0.3689479871 3.5627881207 0.5142911356
 N 0.0447953434 1.9342438457 -0.9037420301
 H -1.7330637305 0.9136544366 1.1793793825
 C 2.2360384478 -0.9485823578 0.3318814259
 N 3.4221309457 -1.5667705703 0.4866586551
 N 1.8083972005 -1.0755981646 -0.9234846581
 C -1.7849291586 -1.5617796632 0.2923384954
 N -2.9122597994 -2.2853638023 0.4273596695
 N -1.6788767639 -1.0977952931 -0.9521033406
 H 0.0485311484 -2.1484381928 1.1590247093
 H 1.8101687487 0.9245556354 1.207381162
 Cu 0.0604927727 -0.0766265162 -1.1635221195
 C -0.990619189 -1.1515782636 2.7832125875
 H -0.8936167414 -2.1088712339 3.3014693824
 H -2.0135938916 -0.7946436184 2.9406480469
 C -2.787732661 -1.5266854207 -1.636782837

C -3.3922553273 -2.9959700449 1.6119116846
 H -2.9563734867 -1.2809603654 -2.6737036331
 H -3.8954466357 -2.3096467023 2.2957371758
 H -2.5596702151 -3.4878409094 2.1159450291
 H -4.0985328413 -3.7611107578 1.2908301691
 C 0.2292480169 3.1250038174 -1.5600045519
 C -0.0267369437 4.1415904632 -0.6891584886
 C -0.7448084159 4.305339584 1.7167960073
 H 0.5282613521 3.1729129903 -2.5955219948
 H 0.002960853 5.2132678828 -0.8138051547
 H -1.5900534908 3.8208619075 2.2067535714
 H -1.0497167989 5.3083926031 1.4197866989
 H 0.099734214 4.3776539895 2.4048450444
 C 3.7541183092 -2.1243873799 -0.7297012507
 C 2.7476551503 -1.8162780637 -1.5954220134
 C 4.2513197579 -1.6413482946 1.6889453666
 H 4.6670901238 -2.6836912558 -0.8659048061
 H 2.6413420191 -2.0744013459 -2.6375799668
 H 4.2521450963 -0.6796206903 2.2030278863
 H 5.2732490474 -1.8700250883 1.3877844454
 H 3.8915930454 -2.4261657113 2.3571813231
 C -3.5583921122 -2.2662813218 -0.7902248888
 H -4.4978666633 -2.7757626017 -0.9407805093

CH2_Cu2+_4b

2 2
 C 0.0156003847 -3.0279569111 1.5662194481
 C 1.4224410599 -2.7028864473 1.0113042123
 C -0.3863030689 -1.926569434 2.5753752526
 C 1.4151329481 -1.2006705838 0.6712388899
 N 0.008374382 -0.7766786757 0.4404910146
 C -0.6786125322 -1.7614671622 -0.4371295108
 C -0.7074216401 -0.6728755977 1.7400963444
 H 0.0186964135 -4.0033276486 2.0539090386
 H 1.6345127217 -3.311655316 0.1258967075
 H 2.1969951504 -2.9133719859 1.7528211531
 H 0.4298462776 -1.7379943321 3.2809584162
 H -1.264211361 -2.2237376641 3.154222976
 N -0.3376580878 0.6135558415 2.3064573319
 C -0.0774376399 1.6696173447 1.4858349223
 H -1.7724424705 -0.6416511453 1.495539333
 N 2.1633125052 -0.7830802111 -0.5027838063
 C 1.8005152511 0.3443994365 -1.1761050638
 N -1.8044972353 -1.0604135362 -1.0314306458
 C -1.7137400364 0.2730718121 -1.2959066421
 H 0.0304329905 -2.0005667308 -1.2340572208
 H 1.7696141345 -0.6161512094 1.5243164599
 Cu 0.002435401 1.0243404867 -0.4599650436
 C -0.9940116051 -3.0191267048 0.3942796472
 H -0.8861114754 -3.9124737744 -0.2256920654
 H -2.020985449 -2.9992444543 0.7743322844
 N 0.101488952 2.7046326854 2.3180607201
 C -0.3440169339 0.9959010929 3.6363810922
 C -0.0612857781 2.3197872371 3.6388112625
 H -0.5487873063 0.317616994 4.4499561699
 H 0.0406016544 3.0148134194 4.4582241178
 N -2.851512104 0.5650339901 -1.9409502327
 C -3.6403855298 -0.5622683551 -2.1010232466
 C -2.9789970619 -1.5961899661 -1.5298528136
 N 2.7542209169 0.5019463115 -2.104203982
 C 3.3459152928 -1.307314219 -0.9940119655

C 3.7138944926 -0.4926018639 -2.0106780439
 H -4.5967737491 -0.5301180059 -2.6001998857
 H -3.2399841213 -2.6396591515 -1.4462359789
 H 3.8201468086 -2.1879522735 -0.5896692222
 H 4.5658200947 -0.53524183 -2.6719449414
 C 0.4317920966 4.0653469353 1.903454604
 C -3.2292973884 1.8942440133 -2.4132293786
 H 0.5226385557 4.0850110163 0.8178003928
 H 1.3791209696 4.3688813436 2.3526667709
 H -0.3601600204 4.7487849215 2.2152777207
 H -2.4413739395 2.5961360675 -2.1415133387
 H -4.1661165746 2.2006377548 -1.94428524
 H -3.3469770715 1.8807864128 -3.4983461613
 C 2.7885706434 1.5728361642 -3.0965008961
 H 1.9089985174 2.2012742241 -2.9595948825
 H 2.7773168803 1.1463729951 -4.1011929145
 H 3.6900146853 2.1731666895 -2.9605431599

CH2_Cu2+_1b

2 2
 C 0.0000000002 -0.0000000002 -3.177056478
 C -1.3668031126 -0.479410251 -2.6461919156
 C 0.2682201006 1.4233913428 -2.6461919156
 C -1.408395352 -0.1499129682 -1.135684779
 N 0.0000000002 -0.0000000002 -0.6661187632
 C 0.8340261149 -1.1447496699 -1.135684779
 C 0.5743692377 1.2946626373 -1.135684779
 H 0.0000000002 -0.0000000002 -4.2681640619
 H -1.4822623927 -1.5545209007 -2.8212497781
 H -2.1880325438 0.0274134677 -3.1593625666
 H -0.6051233939 2.0609373373 -2.8212497781
 H 1.1177570318 1.8811850332 -3.1593625666
 C 0.1051691479 2.402845311 -0.2120404592
 C -0.0043929573 3.7168902098 -0.6264939806
 C -0.3673869014 4.6876787223 0.3115508797
 H 0.1956760352 3.998644908 -1.6540893632
 C -0.4904026686 2.9705709004 1.9592627466
 C -0.6158671238 4.3084978221 1.629362788
 Cl -0.5075849847 6.3255358331 -0.1633203208
 H -0.6821753576 2.6325244602 2.9720752834
 H -0.9025890172 5.0359225087 2.3795216889
 N -0.1330256961 2.0333468787 1.0671492339
 H 1.6580635146 1.2052651337 -0.9918467365
 C -2.1335096546 -1.1103435022 -0.2120404592
 C -3.216724866 -1.862249518 -0.6264939806
 C -2.3273885291 -1.9099866198 1.9592627466
 C -3.8759554075 -2.6620057513 0.3115508797
 H -3.5607660886 -1.8298620371 -1.6540893632
 C -3.4233350041 -2.6876054862 1.629362788
 H -1.9387453797 -1.9070434201 2.9720752834
 Cl -5.2242822316 -3.6023494084 -0.1633203208
 H -3.9099423153 -3.299626273 2.3795216889
 N -1.6944172035 -1.131877072 1.0671492339
 C 2.0283405072 -1.2925018095 -0.2120404592
 C 3.2211178239 -1.8546406925 -0.6264939806
 C 4.2433423095 -2.0256729717 0.3115508797
 H 3.365090054 -2.1687828716 -1.6540893632
 C 2.8177911983 -1.0605842813 1.9592627466
 C 4.0392021285 -1.6208923366 1.629362788
 Cl 5.7318672169 -2.7231864255 -0.1633203208
 H 2.6209207379 -0.7254810408 2.9720752834

H 4.8125313331 -1.7362962364 2.3795216889
 N 1.8274429002 -0.9014698073 1.0671492339
 H 0.2147584673 -2.0385576918 -0.9918467365
 H -1.8728219813 0.8332925574 -0.9918467365
 Cu 0.0000000002 -0.0000000002 1.26549701
 C 1.0985830126 -0.9439810925 -2.6461919156
 H 1.0702755125 -1.9085985016 -3.1593625666
 H 2.0873857872 -0.5064164373 -2.8212497781

CH2_Cu2+_1e

2 2
 C -0.0000000005 -0.0000000004 3.1345807619
 C 1.1857326068 0.8299547624 2.6024359483
 C -1.3116282128 0.6118971782 2.6024359483
 C 0.9492759674 1.0502670913 1.0910073008
 N -0.0000000005 -0.0000000004 0.624937948
 C 0.4349199978 -1.3472306497 1.0910073008
 C -1.3841959666 0.2969635571 1.0910073008
 H -0.0000000005 -0.0000000004 4.2261159546
 H 2.1257403096 0.2963629547 2.7802474829
 H 1.2515629792 1.7934688377 3.1148454594
 H -1.3195280034 1.6927636324 2.7802474829
 H -2.1789710651 0.1871509154 3.1148454594
 C -2.0018853264 1.3340963027 0.1698076347
 C -2.9834229948 2.194592412 0.5964189373
 C -3.5939859746 3.094353763 -0.3224838481
 H -3.2951719839 2.1666949805 1.6322293032
 C -2.118552235 2.1507342571 -1.98635243
 C -3.1092706507 3.0399700548 -1.6566728478
 H -1.7418703898 2.1106901375 -3.003369126
 H -3.501299807 3.6874617118 -2.4291602364
 N -1.559043516 1.2929526396 -1.1102652738
 H -1.9463819136 -0.6323982488 0.9397401476
 C 2.1563039521 1.0666353957 0.1698076347
 C 3.3922842768 1.4864238966 0.5964189373
 C 2.9218666205 0.7593529251 -1.98635243
 C 4.476781954 1.5653062723 -0.3224838481
 H 3.5239988869 1.7703551566 1.6322293032
 C 4.1873266192 1.1727223422 -1.6566728478
 H 2.6988464731 0.4531589378 -3.003369126
 H 4.944085421 1.1884837221 -2.4291602364
 N 1.8992515894 0.7036949697 -1.1102652738
 C -0.1544186272 -2.4007316997 0.1698076347
 C -0.4088612835 -3.6810163099 0.5964189373
 C -0.8827959809 -4.6596600366 -0.3224838481
 H -0.2288269045 -3.9370501383 1.6322293032
 C -0.803314387 -2.9100871835 -1.98635243
 C -1.07805597 -4.2126923984 -1.6566728478
 H -0.9569760848 -2.5638490766 -3.003369126
 H -1.4427856155 -4.8759454352 -2.4291602364
 N -0.3402080748 -1.9966476105 -1.1102652738
 H 1.5208639045 -1.3694170585 0.9397401476
 H 0.4255180076 2.001815306 0.9397401476
 Cu -0.0000000005 -0.0000000004 -1.3081245198
 C 0.1258956045 -1.4418519419 2.6024359483
 H 0.9274080843 -1.9806197544 3.1148454594
 H -0.8062123076 -1.9891265883 2.7802474829
 N 5.697880358 1.9813968083 0.0520526353
 N -4.564880151 3.9438107334 0.0520526353
 N -1.1330002084 -5.9252075429 0.0520526353
 C -1.6125323235 -6.8985431529 -0.9255176849

H -2.5767607111 -6.5932026191 -1.3455986665
H -0.8894049977 -7.0307867667 -1.7372796627
H -1.7479882985 -7.8606639735 -0.4346031486
C -0.9170582492 -6.3420097685 1.4327585586
H -1.5475180003 -5.7692199977 2.1219870674
H -1.1799313914 -7.3934701215 1.53440077
H 0.1335848684 -6.2270599921 1.7218570957
C -5.0338124463 3.9652006238 1.4327585586
H -5.812967252 4.7185856194 1.53440077
H -5.4595845786 2.9978421054 1.7218570957
H -4.2225320783 4.2247998989 2.1219870674
C -5.1680474581 4.845765532 -0.9255176849
H -4.4215006052 5.5281415438 -1.3455986665
H -5.6441374501 4.2856407045 -1.7372796627
H -5.9335405427 5.4441342577 -0.4346031486
C 5.9508706941 2.3768091434 1.4327585586
H 5.3259997087 3.2292178854 1.7218570957
H 5.7700500771 1.5444200976 2.1219870674
H 6.9928986419 2.6748845009 1.53440077
C 6.7805797801 2.0527776197 -0.9255176849
H 7.6815288398 2.4165297145 -0.4346031486
H 6.9982613149 1.065061074 -1.3455986665
H 6.5335424462 2.7451460609 -1.7372796627

CH2_Cu2+_1a

2 2
C 0.0000000003 -0.0000000007 3.1608763914
C 0.2501854229 1.4271046617 2.6304881634
C -1.3610016024 -0.4968854003 2.6304881634
C -0.0847555726 1.4139031837 1.1199726341
N 0.0000000003 -0.0000000007 0.6491763965
C 1.2668538629 -0.6335511136 1.1199726341
C -1.1820982893 -0.7803520721 1.1199726341
H 0.0000000003 -0.0000000007 4.2518730003
H 1.2919901982 1.7172230963 2.8045715815
H -0.3830822637 2.1552122255 3.1435548062
H -2.1331539245 0.2602847836 2.8045715815
H -1.6749274061 -1.4093650861 3.1435548062
C -2.3522566407 -0.5027183062 0.1969477165
C -3.6692423305 -0.6120849832 0.6100734283
C -4.657227383 -0.4133533287 -0.3420968209
H -3.9433078463 -0.8507566209 1.6314892664
C -3.0087367608 -0.0116181912 -1.9846869354
C -4.3540859138 -0.1109109478 -1.6560420239
H -2.7015250837 0.2317301613 -2.9959537216
H -5.1354130801 0.0443506193 -2.3907926451
N -2.0341243781 -0.2073341959 -1.0844656672
H -0.9157174861 -1.8350892169 0.9789470097
C 0.7407614973 2.2884731594 0.1969477165
C 1.3045400216 3.4836995618 0.6100734283
C 1.4943067328 2.611451563 -1.9846869354
C 1.9706392092 4.2399538885 -0.3420968209
H 1.2348770781 3.8403830796 1.6314892664
C 2.0809912596 3.8262044847 -1.6560420239
H 1.5514467494 2.22372427 -2.9959537216
H 2.6061153041 4.4252228759 -2.3907926451
N 0.8375055094 1.8652704831 -1.0844656672
C 1.6114951443 -1.7857548553 0.1969477165
C 2.3647023099 -2.8716145806 0.6100734283
C 2.6865881748 -3.8266005619 -0.3420968209
H 2.7084307692 -2.9896264607 1.6314892664

C 1.514430029 -2.5998333739 -1.9846869354
C 2.2730946551 -3.715293539 -1.6560420239
H 1.1500783352 -2.4554544334 -2.9959537216
H 2.5292977769 -4.4695734973 -2.3907926451
N 1.1966188697 -1.6579362892 -1.0844656672
H 2.047092623 0.1245100014 0.9789470097
H -1.1313751359 1.7105792134 0.9789470097
Cu 0.0000000003 -0.0000000007 -1.2822723841
C 1.1108161805 -0.9302192634 2.6304881634
H 2.0580096707 -0.7458471414 3.1435548062
H 0.8411637273 -1.977507882 2.8045715815
N 3.494316075 -5.0027051486 0.0729780855
O 3.7630027798 -5.8038261775 -0.7964112033
O 3.8068968345 -5.0493623439 1.2463327214
N 2.5853117088 5.5275190628 0.0729780855
O 3.1447595189 6.1607690892 -0.7964112033
O 2.4694276454 5.821550539 1.2463327214
N -6.0796277828 -0.5248139162 0.0729780855
O -6.9077622977 -0.3569429138 -0.7964112033
O -6.2763244789 -0.7721881971 1.2463327214

CH2_Cu2+_1f

2 2
C -0.0000000001 -0.0000000004 3.0407249278
C 0.8398971757 1.1785726525 2.5083916884
C -1.4406224456 0.138085964 2.5083916884
C 0.5438292714 1.3069583616 0.9968873174
N -0.0000000001 -0.0000000004 0.5311025183
C 0.8599445074 -1.1244491458 0.9968873174
C -1.403773779 -0.1825092169 0.9968873174
H -0.0000000001 -0.0000000004 4.1323223447
H 1.9041076565 0.9898375903 2.6865593801
H 0.5797426185 2.1087039196 3.0207042098
H -1.8092783275 1.1540868064 2.6865593801
H -2.1160624731 -0.552280125 3.0207042098
C -2.3321928791 0.5895275977 0.0762053335
C -3.5425562466 1.07618368 0.5026970522
C -4.4138067041 1.7247449055 -0.4182203144
H -3.8301924625 0.9616800964 1.5402772945
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C -3.9385715743 1.8383267094 -1.7524902965
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N -1.9000427429 0.6987701155 -1.2045748876
H -1.6229154535 -1.2461320673 0.8448023371
C 1.6766423156 1.7249744804 0.0762053335
C 2.7032805296 2.5298518633 0.5026970522
C 2.5036861138 1.6843798657 -2.0813570648
C 3.7005762555 2.9600962798 -0.4182203144
H 2.7479356253 2.8362039251 1.5402772945
C 3.5613234181 2.4917396826 -1.7524902965
H 2.391597295 1.3224616884 -3.0984142235
N 4.7083565319 3.7536346928 -0.0463427121
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H 1.0822568371 -3.7978840226 1.5402772945
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 H -0.2677242998 2.028552044 0.8448023371
 Cu -0.0000000001 -0.0000000004 -1.4016974634
 C 0.6007252697 -1.3166586176 2.5083916884
 H 1.5363198544 -1.5564237957 3.0207042098
 H -0.0948293292 -2.1439243978 2.6865593801
 C -6.5020812826 2.9499716335 -0.9386519607
 C -6.1797325841 2.0250185406 1.293846399
 C -7.5653179066 3.5075197097 0.0091139711
 C -7.6377174539 2.4547189726 1.1187165505
 C 1.3361487923 -6.3643146773 1.293846399
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 C 0.74505778 -8.3055173502 0.0091139711
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 C 4.8435837916 4.3392961355 1.293846399
 C 5.8057910166 4.1559817508 -0.9386519607
 C 5.9447077166 5.3870978551 1.1187165505
 C 6.8202601264 4.7979976393 0.0091139711
 H -6.9361168865 2.2737735262 -1.686003451
 H -5.952393733 3.7392935499 -1.4601389204
 H -5.6520042453 2.6623526792 2.0154950348
 H -6.0894147399 0.9830988788 1.6170799712
 H -8.5206311096 3.6639078904 -0.4946973282
 H -7.2356951248 4.4688097144 0.4161087608
 H -8.2408800462 1.6007093431 0.7945917885
 H -8.0660166116 2.8384691639 2.0463009797
 H 0.5203370682 -6.2259555988 2.0154950348
 H 2.1933187661 -5.7651372988 1.6170799712
 H 1.4989128067 -7.1437401909 -1.686003451
 H -0.2621263403 -7.0245709616 -1.4601389204
 H 1.0872782441 -9.2110369429 -0.4946973282
 H -0.2522551754 -8.5007006498 0.4161087608
 H 2.7341850675 -7.9371661416 0.7945917885
 H 1.5748219016 -8.4046098755 2.0463009797
 H 5.1316671769 3.5636029185 2.0154950348
 H 3.8960959736 4.7820384189 1.6170799712
 H 5.4372040796 4.8699666636 -1.686003451
 H 6.2145200731 3.2852774106 -1.4601389204
 H 6.4911947099 5.5661407104 2.0463009797
 H 5.5066949785 6.3364567974 0.7945917885
 H 7.4879503 4.0318909343 0.4161087608
 H 7.4333528653 5.5471290514 -0.4946973282

CH2_Cu2+_1c

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 C -1.4316801352 0.2152628433 2.5219242507
 C 0.6086583145 1.2785839338 1.0109634038
 N 0.0000000002 -0.0000000002 0.543171751
 C 0.8029570107 -1.1664055296 1.0109634038
 C -1.4116153247 -0.1121784047 1.0109634038
 H 0.0000000002 -0.0000000002 4.1447879394
 H 1.9548899976 0.8861470744 2.6988361363
 H 0.6931559642 2.0744997356 3.0350740315
 H -1.7448708766 1.2499108619 2.6988361363

H -2.1431474532 -0.4369591944 3.0350740315
 C -2.3008913324 0.7008334364 0.0881812749
 C -3.491954338 1.2472484076 0.5097946897
 C -4.3115631558 1.9332660095 -0.410231257
 H -3.7826856538 1.1641403815 1.5491772652
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 H -2.2636971523 1.5350435689 -3.0841364011
 H -4.4277976231 2.5228091601 -2.5030709124
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 H -1.6851471377 -1.1639367849 0.8635929987
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 C 2.5887952581 1.5495502412 -2.0674944927
 C 3.8300390547 2.7672902181 -0.410231257
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 C 3.68414679 2.3130664157 -1.733360828
 H 2.4612353031 1.1928974558 -3.0841364011
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 H 4.3987156335 2.5731806443 -2.5030709124
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 C 0.5435061066 -2.3430470638 0.0881812749
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 C 0.4815241015 -4.700556228 -0.410231257
 H 0.8831676831 -3.8579720618 1.5491772652
 C 0.0475522446 -3.0167375794 -2.0674944927
 C 0.161100882 -4.3470979194 -1.733360828
 N 0.6035291291 -6.0107445288 -0.0246955184
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 H 0.0290819901 -5.0959898048 -2.5030709124
 N 0.2393675855 -2.0160439419 -1.1896923806
 H 1.850572393 -0.8774118383 0.8635929987
 H -0.1654252549 2.0413486227 0.8635929987
 Cu 0.0000000002 -0.0000000002 -1.3892849738
 C 0.5294169769 -1.3475027892 2.5219242507
 H 1.4499914894 -1.6375405417 3.0350740315
 H -0.2100191204 -2.1360579368 2.6988361363
 C -6.2231716158 3.4637244971 -0.72063523
 C -6.2268956243 2.163559948 1.1328412249
 C -7.3463267131 3.7497675214 -0.0159911149
 C -7.3548169081 2.9170347099 1.1526935245
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 H 6.3034681976 3.0991872608 -1.6229740618
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CH2_Cu2+_4c

-1 2

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N 0.0000000008 0. 0.5951520281
C -0.8406694841 -1.1410520841 1.0496076852
C -0.5678453486 1.2985671722 1.0496076852
H 0.0000000008 0. 4.194142131
H 1.5007068974 -1.5440440239 2.7360065565
H 2.1869168901 0.051816902 3.0745630354
H 0.5868279017 2.0716723081 2.7360065565
H -1.1383331973 1.8680171311 3.0745630354
C -0.0286988023 2.3624797256 0.1414573429
N 0.1494793005 2.019984114 -1.173564613
H -1.6490808568 1.1911314146 0.8984186509
C 2.0603168606 -1.1563859703 0.1414573429
N 1.6746179089 -1.1394449279 -1.173564613
C -2.031618056 -1.2060937553 0.1414573429
N -1.824097207 -0.8805391861 -1.173564613
H -0.2070096347 -2.0237116228 0.8984186509
H 1.8560904939 0.8325802082 0.8984186509
Cu 0.0000000008 0. -1.366404182
C -1.0912639072 -0.9520854379 2.5627462182
H -1.0485836904 -1.9198340331 3.0745630354
H -2.0875347968 -0.5276282842 2.7360065565
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C 3.2457099186 -2.7396773555 -0.9046977407
C 3.0245901308 -2.1265960932 0.355096952
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H 0.2801871861 4.2233337403 1.2935630731
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H -3.1232780392 -0.7959336613 -2.855767959
H 0.8723402504 3.1028049563 -2.855767959

CH2_1b

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H 0.6793278081 -2.1321981555 2.5019849503
H 2.0234271033 -1.0415248171 2.8077285909
H 1.5424222111 1.4991993179 2.6200299775

H -0.0758875447 2.1025439013 2.9554665422
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C 1.0559190788 2.083537372 -1.3243762457
C 1.9616408905 2.7953357439 -2.0888236662
H 0.257574038 1.4912644701 -1.7592446592
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C 2.9659880938 3.53691435 -1.472816749
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H 3.6892849663 4.0995547442 -2.0511562819
N 2.1408858425 2.8475743792 0.6799819331
H -0.7808653094 1.8722697816 0.7492656707
C 1.2958653675 -2.0503948573 -0.0588123854
C 0.7331145357 -2.0872092808 -1.3373394877
C 2.1916734173 -4.1380902999 -0.3039256299
C 0.9324322042 -3.2304831119 -2.0949758865
H 0.1510059451 -1.2470629326 -1.699229788
C 1.6772250671 -4.2872612059 -1.5868125387
H 2.7805637798 -4.9386307877 0.1383259405
Cl 0.2429423431 -3.343515771 -3.6929359707
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H -1.1738618133 -1.6311249608 0.6193031597
H 2.0583401961 -0.2188998489 0.6363906747
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CH2_1e

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C 2.0741341716 3.7689582693 -1.1398173181
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H 2.6776326275 4.536375233 -1.6092837286
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 C 3.1069829998 -3.7567719746 -0.420911985
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 H 3.980588696 -4.3043932314 -0.0696522584
 H 2.9919032102 -4.8932672999 -2.2262010228
 N 2.658218548 -2.7990829775 0.3908911316
 C -2.49302456 -0.9521334605 0.0733749143
 C -3.5160186413 -0.1185824964 0.5019830334
 C -4.6066508931 0.1688431241 -0.3441528437
 H -3.4660473085 0.31932158 1.4892754293
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 H -0.977580498 -2.2687024635 0.6526685153
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 H -1.5686039189 -2.1303517656 2.8834234302
 H -2.2119241167 -0.4979222582 2.7726199846
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 H -0.8181680128 -3.3515045457 -4.5594781503
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 H -7.3860173053 2.0070334048 -0.4031090895
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CH2_1a

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 C 1.1737046971 -0.8226573994 0.8447443267
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 C -1.2082429641 -0.5655797608 0.8589853685
 C 0.200367361 1.3689143903 0.9409425025

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 H 0.6748486038 -2.1443884307 2.5258413092
 H 2.0238182391 -1.0640842461 2.8480055691
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 C 1.0012373475 2.1243268684 -1.3002556219
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 H 3.6567170458 4.0914397766 -2.0837195809
 N 2.1877130948 2.7958301407 0.6757062592
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 C 1.71800044 -4.2931581825 -1.5610090803
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 H -1.1533331795 -1.6407985484 0.643020026
 H 2.080161172 -0.2247912231 0.6824551094
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 H -1.7569703021 -1.2859044054 2.861323954
 H -2.0125012159 0.44852365 2.6440028958
 N -6.1004703779 0.2087593561 0.2144356079
 O -6.2728006151 -0.2408327478 1.3349897945
 O -6.9820654677 0.5984270186 -0.5315159045
 N 1.7333059342 2.8770664035 -3.5278563924
 O 0.7578240222 2.3174087122 -3.9979871986
 O 2.5837435135 3.469092963 -4.1720286828
 N 0.3403257523 -3.3590690214 -3.383087249
 O -0.3783177829 -2.4468888534 -3.7522415207
 O 0.5923050234 -4.3630557209 -4.029179116

CH2_1c

O 1
 C 1.2208474817 -1.0713146186 3.6583652234
 C -0.2684484156 -0.7280720856 3.8224638339
 C 1.3513909694 -2.2610932419 2.6919124208
 C -0.8749759604 -0.6538484808 2.3957563557
 N 0.1925791924 -0.4933733017 1.3948507114
 C 1.107429093 0.5900973431 1.8117601992
 C 0.9408227118 -1.7526487028 1.2839789585
 H 1.6648421325 -1.3173246929 4.6276752933
 H -0.3904343815 0.2260468073 4.3478247853
 H -0.7872249067 -1.4851485551 4.4166424028
 H 0.7064788689 -3.087787242 3.0077507007

H 2.3743767371 -2.6493167717 2.6756240201
 C 0.1896309704 -2.7685663097 0.4430007951
 C -0.7825435393 -2.351610511 -0.4624742015
 C -1.4211809964 -3.3042151413 -1.251507374
 H -1.0408747972 -1.3012034352 -0.5106711171
 C -0.0774206678 -4.9483234905 -0.1627654129
 C -1.0510459043 -4.641767359 -1.1030641569
 N -2.4124409407 -2.9216856837 -2.1709163369
 H 0.2295152266 -5.9827560485 -0.0238582811
 H -1.4889617422 -5.4222023139 -1.7144939794
 N 0.5404175194 -4.0482488306 0.6037932137
 H 1.850098184 -1.5188814516 0.7153491665
 C -1.9625882292 0.390150008 2.2430708276
 C -2.0233393374 1.2060484529 1.1187943536
 C -3.8561681115 1.3158635806 3.1096880427
 C -3.049286985 2.1433075554 1.0247084058
 H -1.2654393373 1.1183564317 0.3497357846
 C -3.9980437219 2.196733635 2.044220796
 H -4.5791269275 1.3348338723 3.9225960018
 N -3.0997436999 3.0189005499 -0.0734179396
 H -4.8023639823 2.9234442267 2.0334178391
 N -2.863026429 0.4356856223 3.2327754644
 C 1.8522123954 1.0988841725 0.5865730775
 C 3.1833840877 0.8044435108 0.3158687543
 C 3.7637938608 1.272717177 -0.8651108235
 H 3.7668919317 0.1908393535 0.9907937462
 C 1.6568856234 2.2514856897 -1.3844513125
 C 2.9795628645 2.0181156076 -1.7399852381
 N 5.1073247821 0.9902003304 -1.1588402415
 H 1.0145514355 2.8334587128 -2.0425083305
 H 3.3885752693 2.4318666268 -2.6543736025
 N 1.0969316277 1.8197146405 -0.2579780108
 H 0.4635373243 1.4215430512 2.1132680883
 H -1.3526223954 -1.615806438 2.1732864772
 C 1.940044167 0.1403849626 3.0395958002
 H 2.0195248673 0.9618297843 3.7596966906
 H 2.9628719672 -0.1507038917 2.7765639744
 C -1.9992705376 3.4634565857 -0.7804588464
 C -4.2356735338 3.5864041327 -0.6143103336
 C -3.8596144981 4.382142134 -1.6616091056
 C -2.4390172407 4.3096012009 -1.7618366788
 C -2.5109377466 -1.6867855152 -2.7826351563
 C -3.4624830183 -3.7096515524 -2.6014650914
 C -3.6094704887 -1.6959432634 -3.5963400202
 C -4.2181236974 -2.9794867305 -3.4764424029
 C 6.1218937042 0.8398673026 -0.2327698809
 C 5.6358939254 0.815553722 -2.4233309495
 C 6.9719084827 0.5533404563 -2.2976715166
 C 7.2821994649 0.5765941901 -0.9065670714
 H -1.0041217595 3.1565731862 -0.4875772261
 H -5.2141705878 3.3336181228 -0.2347922971
 H -4.5280864701 4.9482305703 -2.29495723
 H -1.812581349 4.8329439449 -2.4708086667
 H -1.766896005 -0.9237447474 -2.6128893458
 H -3.605866842 -4.7036780083 -2.2062355758
 H -3.9400924722 -0.8747772157 -4.2162716477
 H -5.11711857 -3.3208923356 -3.9698726242
 H 5.9339357292 0.988048578 0.8198856092
 H 4.9992848398 0.8415666394 -3.2947626158
 H 7.6543456083 0.3537330497 -3.111525181
 H 8.2528231798 0.4268024457 -0.4555719915

CH2_1f

O 1

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 C 1.0796881922 -1.3666617187 2.0287129536
 C -0.0951808635 0.8071024905 2.4461558843
 C 0.9904967079 -0.8851088685 0.5581773157
 N -0.3545113195 -0.3562116596 0.2765487689
 C -1.3772803418 -1.3077118211 0.7559911222
 C -0.505593403 0.9378983378 0.9533810547
 H 0.0373080973 -0.8383753812 3.8657515321
 H 1.0005820746 -2.4582907699 2.0881551919
 H 2.0477521896 -1.0954233856 2.4590692331
 H 0.8899883097 1.2543891562 2.6156989115
 H -0.79960042 1.3473529813 3.087185037
 C 0.2246812693 2.0303142346 0.189827323
 C 0.5297306464 1.8379452745 -1.1494388119
 C 1.2211132198 2.8328641372 -1.8580513043
 H 0.239444468 0.9052468347 -1.6138734707
 C 1.1410856171 4.1063057015 0.1762739703
 C 1.5206815097 4.0151059143 -1.1537163264
 N 1.5801451499 2.6402744245 -3.1598051395
 H 1.3695681498 5.0154908538 0.7307603041
 H 2.0529068812 4.8364139989 -1.6205223703
 N 0.5157144893 3.1487115607 0.8671398412
 H -1.5711240896 1.1917457254 0.89909848
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 C 0.7481839731 -2.035119339 -1.6694163171
 C 2.9808122363 -3.4449438209 -1.0957271338
 C 1.2082745899 -2.9466859728 -2.6364426093
 H -0.1561004684 -1.4584694054 -1.8174915321
 C 2.3797541045 -3.6625957231 -2.3262843812
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 N 0.5375428646 -3.1138228631 -3.8112446895
 H 2.8021607156 -4.3876549678 -3.0130278643
 N 2.5421449873 -2.5957058573 -0.1645474638
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 C -3.7139297775 -0.2881719835 0.5692090678
 C -4.869423208 -0.0098917895 -0.1887008589
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 C -3.8370034322 -1.2975603211 -1.9273992455
 C -4.9165751338 -0.5507488737 -1.4857062729
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 H -5.7640529266 -0.3860111793 -2.1407879418
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 H 1.6735717545 -0.0358712677 0.437657237
 C -1.3993709197 -1.3208865989 2.3069737537
 H -1.5016084437 -2.3492526897 2.6710952938
 H -2.2387603164 -0.7535234189 2.7242618141
 C -0.7584824675 -2.5011442929 -4.0798207261
 C 0.9748411793 -4.0073781614 -4.8698376584
 C 0.0058849567 -3.7001062295 -6.0153004771
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 C 1.4416351555 1.3582208896 -3.8410265251
 C 2.2759603252 3.6346158777 -3.9591927597
 C 2.3282190504 1.514653326 -5.0795395407
 C 2.2799758283 3.0202770847 -5.3614833325
 C -5.8033706701 1.4613452817 1.5832122282
 C -7.1238886268 1.0053647385 -0.4005539629

C -8.0051803976 1.6861873992 0.6492198633
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 H -1.4134052813 -2.572158576 -3.2044968557
 H 0.9046844997 -5.0607453611 -4.5558013094
 H 2.0186079202 -3.8131110616 -5.14590357
 H -0.1297829669 -4.5514142695 -6.687186057
 H 0.3851545425 -2.8585660003 -6.6061953702
 H -1.8125809082 -4.1830275577 -4.9388722444
 H -1.9599411316 -2.7064481943 -5.9059292463
 H 0.3922271528 1.1703303455 -4.114926443
 H 1.7660772033 0.530681731 -3.1990784493
 H 3.3004122627 3.7979427053 -3.5890044103
 H 1.754231177 4.5986766225 -3.9297536095
 H 1.9821965481 0.9067558227 -5.9194130846
 H 3.3533688632 1.2101276387 -4.8417064502
 H 1.3497139396 3.2765319358 -5.8807922677
 H 3.1164350679 3.3736942845 -5.9697082753
 H -4.8472203442 1.9900453288 1.6740820555
 H -5.8860018122 0.7689490118 2.4340717806
 H -7.565584941 0.0727481542 -0.7704287707
 H -6.9498908372 1.6613604317 -1.2674672874
 H -8.5312504322 0.928265547 1.2400280563
 H -8.752214002 2.3463040518 0.2018287085
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 H -6.6854950562 3.3604145041 1.0398807037

CH2_1d

O 1
 C -0.1333050306 0.1726346178 2.8787968432
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 C 1.3278155606 0.0279035039 0.8782061432
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 C -0.7901072967 -1.0910512353 0.8353648293
 C -0.701095772 1.3048478237 0.7439632923
 H -0.1807776735 0.2181917697 3.9712059409
 H 1.5555810539 -1.195466192 2.6855631004
 H 2.0280578134 0.4835818915 2.902787059
 H 0.2166974284 2.2860681217 2.4667497693
 H -1.4800863646 1.8844619165 2.7027706883
 C -0.2239589364 2.4455270129 -0.1391889756
 C -0.1948623727 2.2488882251 -1.524918184
 C 0.2254298244 3.2911596158 -2.3352928582
 H -0.5015452541 1.2859278666 -1.921207435
 C 0.5348167374 4.5916771457 -0.3591877187
 C 0.6030588281 4.4947020686 -1.7418536307
 H 0.2606577798 3.171664802 -3.4145089114
 H 0.8191412366 5.5134711057 0.1443899472
 H 0.9418738741 5.3373478045 -2.3357478824
 N 0.1319818202 3.594309312 0.4355776044
 H -1.763271072 1.1624667398 0.5084353834
 C 2.1935871321 -0.9770586233 0.1412344363
 C 1.8548331842 -1.4202643589 -1.1403190179
 C 4.1153432734 -2.2199096038 0.1379405683
 C 2.7063229005 -2.3092829635 -1.7828723321
 H 0.9321433809 -1.0733338963 -1.5934493899
 C 3.8672065695 -2.7198849399 -1.1354443045
 H 5.010656664 -2.5164311474 0.68126187
 H 2.4666752613 -2.6774036672 -2.7765337269
 H 4.5620694946 -3.4120050192 -1.5998129573

N 3.3037633185 -1.3725404538 0.7727117872
 C -2.0129597467 -1.3853128535 -0.0219070452
 C -3.0524784766 -2.1732688049 0.4828864765
 C -4.1332823217 -2.4766149136 -0.3332630837
 H -3.0097655022 -2.5467310478 1.5008855786
 C -3.0758622071 -1.2052113988 -2.0452113114
 C -4.1534519575 -1.9785353362 -1.6314033414
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 H -3.0491213509 -0.7946535572 -3.0527246986
 H -4.9784691348 -2.1818628849 -2.3058235422
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 H -0.1304774667 -1.960964121 0.7174708196
 H 1.7564649894 1.0147832459 0.6600457355
 C -1.0903846698 -0.9111706168 2.3526963873
 H -0.9468899102 -1.8542985081 2.8923040769
 H -2.1285867095 -0.5945279193 2.5153121756

CH2_Cu1+_2b

I 1
 C 0.5476564265 3.1026700485 0.8632737758
 C -0.0343797019 2.0940911525 1.8644932567
 C -0.4299319616 3.1325960993 -0.3320904546
 C 0.1874764194 0.7026701338 1.2411894537
 N 0.4555315984 0.8346570446 -0.2114654374
 C -0.4739063221 1.7074491175 -0.9450252586
 C 1.8115606953 1.3565899802 -0.4086582222
 H 0.6050442654 4.0959780035 1.3143072519
 H -1.0981290588 2.3120491282 2.0105395562
 H 0.4529060306 2.160206792 2.8420981659
 H -0.105562104 3.851921688 -1.0897101173
 H -1.40499636 3.4746281648 0.0281737774
 C 2.802332678 0.2079193495 -0.2812859246
 C 4.0789982699 0.3836947666 0.2270016863
 C 4.9567513811 -0.69842608 0.225200908
 H 4.3969829312 1.3461506085 0.6105371619
 C 3.244472065 -2.0050893758 -0.7779825257
 C 4.5399015395 -1.9189425176 -0.2879145162
 Cl 6.5524678009 -0.5134525024 0.8568657222
 H 2.8780790507 -2.9390479477 -1.1901802923
 H 5.198125799 -2.7789481649 -0.3085342207
 N 2.3837396128 -0.9798805536 -0.7803381298
 H 1.8702678796 1.6479225754 -1.4642070383
 C -0.841869386 -0.3777967137 1.5463853724
 C -1.7723246672 -0.2451871095 2.5675592932
 C -1.5419718548 -2.5334307412 1.115093075
 C -2.6183117089 -1.3168229084 2.8433784687
 H -1.8451318417 0.6633390568 3.1520919353
 C -2.508217734 -2.4903604864 2.110719709
 H -1.4138540126 -3.4289162427 0.5148640448
 Cl -3.7979738953 -1.1775951204 4.0980644797
 H -3.1477123701 -3.342626856 2.3059320206
 N -0.7292303145 -1.5129945019 0.8317108776
 H 1.1216693882 0.2955649253 1.6501516404
 H -0.0550204404 1.7640564235 -1.9561172858
 C -1.7729381799 0.9484296864 -1.160801692
 C -3.0333853038 1.4613731567 -0.912064685
 C -4.1440423761 0.6696861473 -1.2038129753
 H -3.1675111457 2.455071468 -0.5028762187
 C -2.6621876297 -1.0191032158 -1.9734629221
 C -3.9661023232 -0.5912558518 -1.7530352164
 Cl -5.7322474284 1.2685102143 -0.8822933863

H -2.4741994457 -1.9978489635 -2.4034879767
H -4.8093068796 -1.2230507113 -2.0046515714
N -1.5852757415 -0.2873104613 -1.680223923
Cu 0.3269475544 -1.1266059916 -1.0154944658
C 1.9703451699 2.6350349302 0.454542565
H 2.4956781148 3.4152653169 -0.1031576754
H 2.5485855168 2.4440670391 1.3665779342

CH2_Cu1+_2e

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C 0.013692562 1.9207649249 1.7692727325
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C 0.2742178443 0.5168287388 1.192148135
N 0.553243913 0.6233935651 -0.2633006625
C -0.4100251529 1.4341825177 -1.0177701466
C 1.892516567 1.1726815926 -0.4781643746
H 0.6112909059 3.9229208781 1.1655694947
H -1.053145651 2.128116394 1.9042623565
H 0.491677201 2.0255483092 2.7482556687
H -0.0396276887 3.5741284196 -1.2490913657
H -1.3578413709 3.2438361626 -0.1374327246
C 2.9115685102 0.0482886903 -0.3385199859
C 4.1683514071 0.2637511887 0.1831214809
C 5.1200966103 -0.7849103198 0.2168690167
H 4.4189973175 1.2496763129 0.5522815364
C 3.416943574 -2.1391730697 -0.8185082879
C 4.6953953289 -2.0211985632 -0.3161409357
H 3.0867927832 -3.0875210752 -1.229992311
H 5.3462157017 -2.8849891264 -0.3435440602
N 2.5152132089 -1.1464266338 -0.8439491545
H 1.9343251055 1.4496828495 -1.5388021304
C -0.7302379721 -0.601037782 1.4615244372
C -1.9621733051 -0.4039224064 2.0480320651
C -1.1195988182 -2.8464744731 1.2419386363
C -2.8622934509 -1.4876528264 2.1843275037
H -2.254484664 0.5879687886 2.3615107032
C -2.379464842 -2.7545496229 1.801324856
H -0.7431871644 -3.8134172451 0.9180630157
H -2.9757875046 -3.6511815629 1.9092034066
N -0.306056051 -1.8071646271 1.0332454272
H 1.2120538041 0.1413247454 1.6164214677
H -0.0231525645 1.4481173177 -2.0437842269
C -1.699723463 0.6334846569 -1.1212671838
C -2.9467653138 1.1560829656 -0.8627927869
C -4.0869534171 0.3205475145 -0.8902788552
H -3.0373727691 2.1981781651 -0.5893380697
C -2.5829511976 -1.4372359082 -1.5550313091
C -3.866155527 -1.0205526862 -1.2600662344
H -2.4076753366 -2.4656796095 -1.8547148789
H -4.6759884322 -1.7345801212 -1.3323783193
N -1.4970095386 -0.657265753 -1.4850726074
Cu 0.4761995554 -1.3552027211 -1.0505759513
C 2.0193190495 2.4689176434 0.3615451524
H 2.5365063041 3.2500540839 -0.2035348038
H 2.5895670528 2.3030602158 1.2836053319
N -4.1314713067 -1.3067882198 2.6438430409
N 6.3632713082 -0.6066652171 0.7292985166
N -5.3199398581 0.7869775858 -0.5509825046
C -5.5272942849 2.2049829161 -0.3167074168
H -6.5912954822 2.3932864588 -0.1746397561

H -4.9990445396 2.554641457 0.58073205
H -5.1925410243 2.8023558311 -1.1724684768
C -6.4385745039 -0.1335303985 -0.4600189424
H -6.2059278208 -0.9599655911 0.2231284177
H -7.3074989323 0.3936660405 -0.0660246102
H -6.7076209572 -0.5519762649 -1.4379781091
C -4.6132139833 0.0273151595 2.9473149059
H -5.6564596125 -0.0299883032 3.2583797007
H -4.045370571 0.4877668675 3.7648232035
H -4.5563931826 0.6795042616 2.0657669335
H 6.9348317244 -2.5558963713 1.3191107077
H 7.5273892014 -2.0536659273 -0.2854204072
H 8.2460416458 -1.3770720591 1.182372489
C 7.3107049327 -1.7090126171 0.7328093683
C 6.756309984 0.6879914323 1.2576155184
H 6.7250632258 1.464936924 0.4838603491
H 6.1103186586 0.9929432848 2.0898971465
H 7.7778639577 0.6275955669 1.6316476171
C -5.0295138652 -2.4425995509 2.7425413269
H -5.9959180439 -2.1068821993 3.1188651436
H -5.1877271371 -2.9169264112 1.7646821911
H -4.6444337212 -3.1993202768 3.436042988

CH2_Cu1+_2a

1 1
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C -0.023188014 2.0455505625 1.9131321896
C -0.4175978402 3.1483962923 -0.2523884028
C 0.1918250607 0.6728419178 1.2480467162
N 0.459821787 0.8421971549 -0.2016772893
C -0.4632222121 1.74375018 -0.9100893843
C 1.8187704486 1.3657464911 -0.3821355807
H 0.623162134 4.0591123932 1.4194505174
H -1.0852396592 2.263776091 2.0700873763
H 0.467189055 2.0799562277 2.8905817724
H -0.0943778944 3.890881692 -0.9875041729
H -1.3921347949 3.4787899482 0.1195512496
C 2.8051455638 0.2115768625 -0.2839430293
C 4.0844721071 0.3680584469 0.2270096405
C 4.935659782 -0.7243451706 0.1859710433
H 4.4268688594 1.3083930676 0.6410119753
C 3.2363236609 -1.9985523353 -0.841205846
C 4.5356266785 -1.9311973886 -0.3515688458
H 2.8611223862 -2.917240649 -1.2779492571
H 5.2052884228 -2.7810880587 -0.3869995263
N 2.3864188554 -0.9650903025 -0.8105112354
H 1.8811205296 1.6853718481 -1.4292971592
C -0.8425601273 -0.4089380848 1.5251423497
C -1.7647086569 -0.3046178535 2.5585697099
C -1.5587938057 -2.555330469 1.0291526645
C -2.5980374806 -1.3865097716 2.7908017106
H -1.8459014666 0.5761587477 3.1821111533
C -2.5164133032 -2.540315689 2.0368746301
H -1.4363168242 -3.4294932876 0.398090484
H -3.1663641688 -3.3849892348 2.2267026977
N -0.7482918188 -1.5247873401 0.7766930364
H 1.1236820841 0.2488702253 1.6455157032
H -0.040343078 1.8307817596 -1.9174934129
C -1.7656086737 1.0017792092 -1.1559809943
C -3.0259256362 1.5220816674 -0.9155781195
C -4.1197831215 0.7384242638 -1.2528324318

H -3.1796812468 2.502777669 -0.4843112714
 C -2.6631831612 -0.9432003636 -2.0363333258
 C -3.9686277537 -0.5057219707 -1.829332616
 H -2.4731944428 -1.9113194948 -2.4878910229
 H -4.8266955519 -1.1056731554 -2.1049008896
 N -1.5895058457 -0.2248302362 -1.7019253175
 Cu 0.3242334916 -1.0956975072 -1.0439260954
 C 1.9823217096 2.6189467199 0.5166786793
 H 2.5094000449 3.4121332991 -0.0202123892
 H 2.562009395 2.4016731314 1.4217327894
 N -3.5992592187 -1.2969609116 3.8773647307
 O -3.6307299869 -0.2576897214 4.5103865042
 O -4.311570974 -2.2672957074 4.0478785564
 N 6.3040034645 -0.5876742274 0.732219348
 O 7.0214253719 -1.5667522927 0.6654248421
 O 6.5991070243 0.4939458088 1.2063875805
 N -5.4796136534 1.2564784613 -0.9858749764
 O -5.557752522 2.3538067768 -0.4640047204
 O -6.4113339698 0.5428312711 -1.3033107888

CH2_Cu1+_2c

1 1
 C -0.6416289946 -3.3045632865 -0.7401390915
 C 0.126569452 -2.6545884935 0.4197732919
 C 0.010655672 -2.8239992405 -2.048977095
 C -0.2326191598 -1.1534406565 0.398573402
 N -0.8135214442 -0.7794757368 -0.9196092797
 C -0.0254250886 -1.2715814487 -2.083092717
 C -2.165249504 -1.3518832203 -1.0424263553
 H -0.5817013 -4.3932906644 -0.669042724
 H 1.1993846379 -2.8217369326 0.2784669814
 H -0.146978275 -3.098395213 1.3822256704
 H -0.5282263495 -3.2240142017 -2.9136568363
 H 1.031115805 -3.2133847346 -2.1161074671
 C -3.2191183676 -0.4889238827 -0.3569064652
 C -4.4143161323 -1.0436749184 0.0666321146
 C -5.4272671841 -0.2226530772 0.577873432
 H -4.556150087 -2.1159206738 0.0155340815
 C -3.952513495 1.6251239579 0.2201738352
 C -5.1771997464 1.1522746977 0.6448189641
 H -3.7315803237 2.6856967211 0.2641850884
 H -5.9282687584 1.8488631976 0.995105738
 N -2.9819034298 0.8405955833 -0.277522125
 H -2.4133360242 -1.2743028215 -2.1077617701
 C 0.8575558737 -0.1745695938 0.8330205633
 C 1.9586157213 -0.581640368 1.564740278
 C 1.5688003936 2.0219882355 0.9020777737
 C 2.927293663 0.3540021467 1.9465610783
 H 2.0681014438 -1.6199335914 1.8492110646
 C 2.7194183728 1.6902610621 1.5888893424
 H 1.3724313607 3.0511329728 0.6226619943
 H 3.4451989697 2.4586853275 1.8231721836
 N 0.6473789195 1.1240717638 0.5275329572
 H -1.0508048922 -0.9970386129 1.1155183754
 H -0.589859007 -0.9378034978 -2.9566318544
 C 1.2726775311 -0.4902232518 -2.1647900494
 C 2.4850224712 -0.9584412715 -1.6845836371
 C 3.5750570173 -0.0856310627 -1.6277456151
 H 2.5760722689 -1.9580418568 -1.277857085
 C 2.1680946876 1.5592223687 -2.6345094648
 C 3.4146598728 1.2018599359 -2.1368062985

H 2.0151894995 2.5514505835 -3.0510521796
 H 4.24141981 1.9018077222 -2.165650349
 N 1.106903414 0.7540063628 -2.636142781
 Cu -1.0716716454 1.3425391649 -0.4311882291
 C -2.1176480301 -2.8558198985 -0.6670325993
 H -2.7383745476 -3.4439076295 -1.3495747675
 H -2.4944122935 -3.0289479403 0.348351578
 N 4.7742755773 -0.4887991781 -1.0348300245
 N -6.6347347448 -0.7577379992 1.001351514
 N 4.0555318491 -0.0368789433 2.6519872626
 C 5.6506262329 0.3387607623 -0.3520940512
 C 5.266914754 -1.7828320526 -0.988901734
 C 6.4428229554 -1.7668414955 -0.2938239449
 C 6.6800871147 -0.4226317523 0.1200398113
 C -7.4974120337 -0.183753275 1.9286543464
 C -7.1891814746 -1.959903277 0.5757275978
 C -8.3768395065 -2.133162297 1.2191185247
 C -8.5671002876 -1.0116619362 2.0854758074
 C 4.6075877074 -1.3107263681 2.6618477021
 C 4.8299146745 0.7818129984 3.4647915681
 C 5.7065075465 -1.2935688626 3.4658822813
 C 5.8417344825 0.0313413218 3.9839642991
 H 5.4295416345 1.386987384 -0.2195421182
 H 4.7751270384 -2.5814544272 -1.5238838657
 H 7.0783898085 -2.621358365 -0.1106881187
 H 7.5045875761 -0.0652162356 0.7192087034
 H -7.2402963732 0.7332940838 2.4357464568
 H -6.7189269854 -2.548619908 -0.1965651608
 H -9.0527360313 -2.9646033127 1.0807209842
 H -9.3988729868 -0.8458212991 2.7546987983
 H 4.2296934476 -2.0850398851 2.0126206626
 H 4.5452798868 1.8043720326 3.6590084639
 H 6.3636426514 -2.1308369069 3.6511754257
 H 6.5946427086 0.3823451671 4.6749558558

CH2_Cu1+_2f

1 1
 C 0.549442592 3.0738316474 0.6071702335
 C -0.2260188836 2.088390018 1.4944287992
 C -0.2157189409 3.1946254618 -0.7235164535
 C -0.0307133579 0.6900278401 0.8701621702
 N 0.4346854514 0.8161058978 -0.5354105352
 C -0.3542246988 1.7794030207 -1.3489537713
 C 1.8324843891 1.2757301362 -0.5537620514
 H 0.6126652524 4.0507860531 1.0936474531
 H -1.2814170143 2.3791199646 1.5209525441
 H 0.1429477079 2.1016648209 2.5254337467
 H 0.3235144439 3.8520861693 -1.4133345968
 H -1.1889529276 3.6634098574 -0.5484508192
 C 2.8177556869 0.1281608607 -0.3551252403
 C 4.0802677946 0.3727188367 0.1433131765
 C 5.0441955874 -0.662136442 0.2006276163
 H 4.3304363213 1.3699521182 0.4826893941
 C 3.3468267093 -2.0828040747 -0.7424690974
 C 4.6293579319 -1.9281847353 -0.2724955609
 N 6.2863834012 -0.4494550582 0.6760723627
 H 3.0158577478 -3.0502748651 -1.1045798608
 H 5.3015728161 -2.776662621 -0.2834629047
 N 2.434289609 -1.0942373553 -0.798756787
 H 2.0117009772 1.6015958662 -1.5851760589
 C -1.1844160167 -0.3039970572 1.0135559649

C -2.1551924465 -0.1524881672 1.9839358295
 C -2.1231041141 -2.2878906965 0.3121294449
 C -3.1706536725 -1.1232704623 2.1367006972
 H -2.1417581747 0.7253485433 2.6165435579
 C -3.1420565911 -2.208271158 1.233928622
 H -2.0736077539 -3.1262695765 -0.3742591299
 N -4.1196609556 -1.024738893 3.0979851385
 H -3.8876208872 -2.9923806446 1.2640801797
 N -1.1406813081 -1.3814234339 0.1990075629
 H 0.8088761024 0.2097701813 1.3924214339
 H 0.123444098 1.7644831946 -2.3311716525
 C -1.72963191 1.189978348 -1.5940446926
 C -2.8427368955 1.5333187915 -0.8516355792
 C -4.0214861724 0.7692840147 -0.9729224546
 H -2.787896288 2.3306944438 -0.1221362328
 C -2.8612380118 -0.4590362241 -2.681109015
 C -4.0152976108 -0.2476396102 -1.945982208
 N -5.0913200542 0.9944195897 -0.1677787289
 H -2.848969066 -1.2298430415 -3.4484474102
 H -4.8939390513 -0.8527679955 -2.1351209437
 N -1.7199492688 0.211753283 -2.5127893736
 Cu 0.4786154829 -1.3432913436 -0.933706631
 C 1.9694304071 2.512755189 0.3712009278
 H 2.6158892689 3.2683190535 -0.0858445127
 H 2.4148679153 2.2430425056 1.3367778259
 C -5.1231407783 -2.0642642814 3.3305557593
 C -4.0891788902 -0.0323630266 4.1722799615
 C -5.957951004 -1.5135950374 4.4884200899
 C -4.958526134 -0.6544074323 5.2683044208
 C 7.2861035632 -1.5067385071 0.8354262096
 C 6.7929325726 0.8634791296 1.0755206895
 C 8.3860668433 -0.835896032 1.6607367653
 C 8.2974635094 0.6331640649 1.2364001637
 C -6.2258016943 0.0835303211 -0.0718120699
 C -5.1370782133 2.0585873705 0.8246289392
 C -6.9119638938 0.5044852725 1.2305012976
 C -6.571888746 1.9925730531 1.3492214018
 H -4.6367095502 -3.012519641 3.5994145539
 H -5.7239718866 -2.2361581619 2.4300825337
 H -4.4983287908 0.9265536115 3.8238250438
 H -3.0637722807 0.1405588421 4.5151849818
 H -6.3990786698 -2.3103586522 5.0906622732
 H -6.7750023346 -0.8927489805 4.1056079434
 H -4.3408810538 -1.2873920297 5.9138274142
 H -5.4382208461 0.1000973004 5.8952593926
 H 7.6570749231 -1.8352250676 -0.1450548999
 H 6.8543094293 -2.373758597 1.3460457389
 H 6.3279859492 1.1844978374 2.0181030816
 H 6.5694687398 1.6149576863 0.3106937791
 H 9.3674643826 -1.2775144232 1.4766140458
 H 8.1636953152 -0.9360365489 2.7283234698
 H 8.800276091 0.7800596611 0.274841399
 H 8.7448822493 1.3175147533 1.9600654186
 H -5.880627487 -0.957609331 -0.0398594574
 H -6.8931884855 0.1921565508 -0.9377241897
 H -4.9044061647 3.0287507693 0.3720344401
 H -4.4043480998 1.8754271107 1.6273658417
 H -6.4634376222 -0.0385710363 2.0676620976
 H -7.9852978626 0.3029104021 1.2243714092
 H -6.6608070974 2.37458137 2.369179907
 H -7.2303716042 2.5864194276 0.7070077745

CH2_Cu1+_2d

1 1

C 0.4302376682 3.0759377433 1.159351065
 C -0.1367195244 1.9624849869 2.051990864
 C -0.546038225 3.2079374182 -0.0306448993
 C 0.1089562506 0.6444322654 1.292733195
 N 0.3820474285 0.9274098246 -0.136906802
 C -0.5529978547 1.8546321541 -0.7906980406
 C 1.7323156358 1.4827429937 -0.2694845679
 H 0.4687739378 4.0204024176 1.7074265368
 H -1.204453955 2.145550193 2.216225742
 H 0.348386591 1.9383540238 3.0328525673
 H -0.2398439249 4.0125172898 -0.7058250928
 H -1.5301531893 3.4828758499 0.3615660833
 C 2.738661765 0.3408756651 -0.2409584973
 C 4.0126241373 0.4726680726 0.2914568356
 C 4.9060626611 -0.5913326418 0.1978002797
 H 4.3091563987 1.4012090832 0.7668097795
 C 3.2061725779 -1.8140065097 -0.9445868655
 C 4.4968673892 -1.756886976 -0.4336358752
 H 5.9061158576 -0.5053153453 0.6099240046
 H 2.8462807865 -2.7048019971 -1.4483936407
 H 5.1572135142 -2.6103169317 -0.5345601319
 N 2.3382931722 -0.7985232638 -0.8558300886
 H 1.7958586192 1.8757654854 -1.2912230504
 C -0.9020549455 -0.4773785684 1.4885024619
 C -1.8228463795 -0.482909641 2.5293862823
 C -1.568179357 -2.5894299726 0.8289184408
 C -2.6449471516 -1.5927041441 2.7046849224
 H -1.8964690954 0.3597260658 3.2066735413
 C -2.5184201095 -2.6699594597 1.8393486647
 H -1.4280069431 -3.4065682081 0.1276503251
 H -3.3701715442 -1.6126103292 3.5117320841
 H -3.1345911578 -3.5559759257 1.9402784341
 N -0.7787741193 -1.5268387811 0.6546524521
 H 1.0498772922 0.215759887 1.6626054339
 H -0.1143580082 2.0280058861 -1.7800755474
 C -1.8356285236 1.108157013 -1.1193474925
 C -3.1148862041 1.5888820992 -0.893587657
 C -4.2088025837 0.8329002498 -1.3124174743
 H -3.2658428054 2.5442405935 -0.4046158457
 C -2.6701528016 -0.7843485488 -2.1506445973
 C -3.9852734333 -0.3734779316 -1.9578789225
 H -5.2186572966 1.1913865515 -1.14140885
 H -2.4475783595 -1.7201203287 -2.6539948719
 H -4.8045702511 -0.9886367101 -2.3117774865
 N -1.6165192262 -0.0747205553 -1.7406782249
 Cu 0.2864738062 -0.9434304031 -1.1320158345
 C 1.8627469302 2.6757202196 0.7137542162
 H 2.3748761069 3.516099669 0.2367422028
 H 2.4417308331 2.408689562 1.6060734021

CH2_Cu2+_2b

2 2

C -0.2855153544 -3.4714370071 -1.2862743801
 C 0.2321365218 -3.1683896862 0.127197161
 C 0.6660612429 -2.7350543792 -2.2548375173
 C -0.1574782311 -1.7126669234 0.4225210086
 N -0.4333190824 -1.0045668938 -0.8819544904
 C 0.5463085356 -1.216371073 -1.9749068367

C -1.7629185338 -1.4337728068 -1.3679496136
 H -0.2438809977 -4.5440133246 -1.4839201318
 H 1.3167376065 -3.3139257762 0.1566644301
 H -0.2113485062 -3.8287093541 0.8776493656
 H 0.4119330093 -2.9370683438 -3.2982523875
 H 1.6826710596 -3.1060398392 -2.0946846225
 C -2.7934655848 -0.6557018972 -0.5717382624
 C -4.0805219215 -1.1012550408 -0.3523281304
 C -4.9822112152 -0.2629899184 0.3123060482
 H -4.3939366183 -2.0797522652 -0.6990839644
 C -3.2514695727 1.3658493802 0.4964914511
 C -4.5603338614 0.9946402223 0.7420304913
 Cl -6.5849498121 -0.7839574663 0.5939271788
 H -2.880370691 2.3301542061 0.8268413888
 H -5.2335884451 1.6672642322 1.2600334227
 N -2.3810504315 0.5718002754 -0.1505209129
 H -1.8504606732 -1.062100034 -2.3952780495
 C 0.7140276012 -0.9185348088 1.3893020655
 C 1.6045345255 -1.5428511158 2.2449505578
 C 1.0886383495 1.1324582074 2.3998967167
 C 2.2555934143 -0.7739471146 3.2143947172
 H 1.7903148027 -2.6086482377 2.1910024597
 C 1.9902970249 0.5890755081 3.301358548
 H 0.8559481974 2.1921129718 2.4273555423
 Cl 3.3670936179 -1.5164139107 4.287413878
 H 2.4705164266 1.2107576938 4.0477370983
 N 0.4614284708 0.404607961 1.468292457
 H -1.1376629515 -1.7259744955 0.9141910993
 H 0.0780266944 -0.7551337338 -2.8526570026
 C 1.734018947 -0.315959263 -1.7101561974
 C 3.0360380754 -0.6095956158 -2.0561502565
 C 4.0165926885 0.3742073211 -1.8842049676
 H 3.2991755485 -1.575501709 -2.4713325753
 C 2.3323172216 1.8339060742 -1.0414061837
 C 3.6577278501 1.621259906 -1.3757852608
 Cl 5.6407563876 0.042148888 -2.3023107862
 H 2.0127315678 2.7851705035 -0.6286781853
 H 4.3919982654 2.4065419014 -1.2409322686
 N 1.3854187952 0.8977818822 -1.2060892187
 Cu -0.4411977043 0.904101508 -0.3915270276
 C -1.7583839813 -2.9862053271 -1.401999327
 H -2.2150964605 -3.3405898636 -2.328892719
 H -2.3376518177 -3.408271418 -0.5732658103

CH2_Cu2+_2e

2 2
 C -0.3116231461 3.1095073845 2.0058916657
 C 0.2007420821 3.0919922949 0.5581217177
 C 0.643894155 2.1941029004 2.8039727931
 C -0.1883250376 1.7225371584 -0.0160021526
 N -0.463321849 0.7774282495 1.1226478443
 C 0.5155129456 0.7620469651 2.2304346905
 C -1.7916564407 1.0975467567 1.6778636594
 H -0.2684946474 4.1217554341 2.4129930419
 H 1.2858002862 3.2393695527 0.55426534
 H -0.2451916732 3.8887883904 -0.044159189
 H 0.3974205988 2.1904827287 3.8689695224
 H 1.6606789839 2.5878806163 2.7101101703
 C -2.8187289009 0.4953576098 0.7342955697
 C -4.0872584549 0.9929832077 0.5976065143
 C -5.0382924944 0.3267787487 -0.2296380139

H -4.3571443013 1.887004647 1.1449675498
 C -3.2802876124 -1.2594916805 -0.7113236269
 C -4.5707584294 -0.8396700693 -0.8953472833
 H -2.91774079 -2.1429118194 -1.2266133098
 H -5.2105910351 -1.4117068928 -1.5532414495
 N -2.3945109869 -0.6347458124 0.0942596199
 H -1.8815850067 0.5248798984 2.6078643226
 C 0.6753516612 1.1275341984 -1.1243886331
 C 1.5594364128 1.904093861 -1.8363261942
 C 1.0376278534 -0.6761962989 -2.5127079121
 C 2.231730747 1.3683950886 -2.9701078478
 H 1.7167420584 2.9336685217 -1.5465303832
 C 1.9323776296 0.0200446613 -3.2890668463
 H 0.8048751276 -1.7096787597 -2.7502970259
 H 2.3858063679 -0.4786562024 -4.1350174383
 N 0.3999020301 -0.1552582724 -1.4516146077
 H -1.1699513576 1.8317930384 -0.4923816172
 H 0.0413078925 0.1412194087 2.9997281908
 C 1.697281165 -0.0804057959 1.7950387737
 C 2.9881834485 0.1407739144 2.1939107108
 C 4.0135906659 -0.7897450178 1.8551610331
 H 3.2092366237 1.012388601 2.7952157566
 C 2.2912994654 -2.0456003313 0.719515928
 C 3.6056756296 -1.9113227553 1.0834137744
 H 1.976498497 -2.8954118058 0.122258333
 H 4.3082122988 -2.6731307766 0.7743924963
 N 1.3252974735 -1.1725265392 1.0678906892
 Cu -0.4679791877 -1.0059710682 0.2468751231
 C -1.7850049539 2.6100903004 2.0273779737
 H -2.2369737523 2.7730857611 3.0088348635
 H -2.3656463592 3.1912415065 1.3020042786
 N -6.2932081418 0.7757616475 -0.3717368874
 N 3.0954557946 2.102850895 -3.6967735499
 N 5.2855334377 -0.6166781554 2.2462660181
 C -7.2400791726 0.0560212797 -1.2211218269
 H -7.3882584693 -0.9680562037 -0.8632204415
 H -8.2016716051 0.5652878006 -1.194722604
 H -6.8963875886 0.031990183 -2.2604814191
 C 3.3600197304 3.4917433563 -3.3447197376
 H 4.0943069276 3.9027170139 -4.0356093295
 H 2.4519426432 4.1016688395 -3.4146021901
 H 3.7703239528 3.5719745298 -2.3317270992
 H 4.3513344007 0.6594071094 -4.6027933362
 H 2.9945295714 1.2197458707 -5.6189848131
 H 4.3863687614 2.269973491 -5.3292555664
 C 5.6608190543 0.5432804419 3.0482032228
 H 5.4458815818 1.4762282651 2.516018461
 H 5.1377631057 0.5457237187 4.0108510683
 H 6.7306135012 0.5098693634 3.2464843716
 C 6.2998092947 -1.6122768956 1.9081038704
 H 7.2562548175 -1.304465033 2.3268471369
 H 6.0450660407 -2.5913754447 2.3271079812
 H 6.4168759722 -1.7018334179 0.8229912986
 C 3.7366430109 1.5248486898 -4.8731599602
 C -6.7320919961 1.9776437714 0.3309278358
 H -7.7732931652 2.1760464356 0.0834446687
 H -6.6609608543 1.8484569747 1.4163235005
 H -6.1413462889 2.8489939661 0.0283209117

CH2_Cu2+_2a

2 2

C -0.3302077372 -3.1232807162 -1.9402686481
 C 0.1822622497 -3.084843224 -0.493690514
 C 0.6245959135 -2.2237228027 -2.7553687579
 C -0.2079303311 -1.7070231455 0.0621398053
 N -0.4784629744 -0.7690965073 -1.0918660733
 C 0.504564366 -0.7806830818 -2.2045014362
 C -1.8068676949 -1.1030705741 -1.6557814298
 H -0.2882505472 -4.1416007634 -2.3304337499
 H 1.2664632234 -3.2353671979 -0.4858031937
 H -0.2647454188 -3.86985118 0.1224691536
 H 0.3740647188 -2.2309431601 -3.8188416904
 H 1.6411940765 -2.6170093299 -2.6631772949
 C -2.8427605746 -0.483039424 -0.7393200249
 C -4.1350225533 -0.9576156829 -0.6115574792
 C -5.0108686263 -0.235929876 0.185941516
 H -4.47287773 -1.8556355795 -1.1169135279
 C -3.305207838 1.3235203203 0.6741878085
 C -4.6216627604 0.9176567928 0.8402605238
 H -2.9311275499 2.2118525905 1.171422636
 H -5.3159316447 1.473600621 1.4594209578
 N -2.439157253 0.6476508255 -0.0975510841
 H -1.8893489271 -0.5515392 -2.5993877683
 C 0.664111508 -1.1095795239 1.1593389799
 C 1.5486050954 -1.8862768251 1.8909548889
 C 1.0422182887 0.7264714574 2.5343353567
 C 2.1786428087 -1.2926641363 2.9750427588
 H 1.7508453541 -2.9256193448 1.6624623089
 C 1.9372034116 0.0194179081 3.3297026423
 H 0.8117154333 1.764334539 2.7507592296
 H 2.4272228891 0.4697498549 4.1849553777
 N 0.4240594927 0.1782180966 1.4829285681
 H -1.1897523278 -1.8086255899 0.5402047552
 H 0.0392211904 -0.1671727387 -2.9854540743
 C 1.693147279 0.0531732813 -1.7801356325
 C 2.9981963512 -0.1714967568 -2.1746867018
 C 3.9485261082 0.7752901161 -1.8191367456
 H 3.2904521274 -1.0400088958 -2.7535459211
 C 2.2884575443 2.0567133745 -0.733331715
 C 3.6183783652 1.9109273178 -1.1045785248
 H 1.9630861986 2.9166187703 -0.1574674923
 H 4.3687840115 2.6481006016 -0.8440358539
 N 1.3519557279 1.1566617606 -1.0633071837
 Cu -0.4901283529 1.0148711764 -0.2699703292
 C -1.8024302916 -2.6241183773 -1.9705303396
 H -2.2566984083 -2.8021607468 -2.947764598
 H -2.3858776281 -3.1888235424 -1.2349908178
 N 5.3618441606 0.5532969907 -2.2229337823
 O 6.1535540292 1.4125035247 -1.8990160272
 O 5.5877828111 -0.471740177 -2.8344872265
 N -6.405485471 -0.7274247755 0.340582717
 O -6.6756785118 -1.7579320205 -0.2430247553
 O -7.1367306034 -0.0551020351 1.0354554087
 N 3.1381469677 -2.1006388598 3.7704622771
 O 3.6580483838 -1.5440607877 4.7140854576
 O 3.3160516706 -3.2436733413 3.396997266

CH2_Cu2+_2c

2 2

C -0.5803667259 -1.0811046911 3.0637519598
 C -0.1197100992 0.2914535529 2.5514682778
 C 0.435923217 -2.1036028344 2.5086978185

C -0.4797020194 0.3340052033 1.0595033898
 N -0.6758434007 -1.0761606725 0.5648673191
 C 0.3492632739 -2.0672079457 0.9629874374
 C -1.9924130428 -1.553629196 1.0334821994
 H -0.5602562458 -1.1059353908 4.1549323937
 H 0.9580876288 0.3950268043 2.7136299975
 H -0.6153269716 1.1131760177 3.0761143114
 H 0.2227426253 -3.1142169891 2.866153945
 H 1.4319686483 -1.8370086529 2.8746785599
 C -3.0340988996 -0.9393805248 0.1158922196
 C -4.3300860884 -0.701500572 0.5022958212
 C -5.2663018215 -0.2036548157 -0.430924576
 H -4.6162325931 -0.8846474696 1.5302089397
 C -3.4829198269 -0.210363553 -2.0429055994
 C -4.7991161966 0.0406433478 -1.7369951236
 H -3.1093607503 -0.0236463289 -3.0440799844
 H -5.4579871726 0.3976545908 -2.5171094913
 N -2.5978222684 -0.7024355524 -1.1542563464
 H -2.0206479052 -2.6293663606 0.825565727
 C 0.3670850362 1.2030903626 0.1351253615
 C 1.220724024 2.1664690476 0.6287460966
 C 0.7516158601 1.8890750535 -2.0350181061
 C 1.8730314864 3.0453461609 -0.2592660386
 H 1.3989230178 2.2420955599 1.6927570561
 C 1.6114560812 2.8879669464 -1.6290463163
 H 0.5348524552 1.7519343262 -3.0896752167
 H 2.0425386381 3.5506849577 -2.3681124146
 N 0.1284627129 1.0595212158 -1.1864527509
 H -1.4812313576 0.7723699371 0.9737319561
 H -0.0604644118 -3.0291201627 0.6325744868
 C 1.5475499696 -1.8762667987 0.0566693928
 C 2.8515374636 -2.0703099682 0.4382997357
 C 3.8854291195 -1.9841675998 -0.5202056891
 H 3.077749785 -2.2774621499 1.4757638673
 C 2.1810967459 -1.5011449826 -2.1434853172
 C 3.509764191 -1.6946002127 -1.8454412481
 H 1.875894949 -1.2725113814 -3.159356832
 H 4.2384418385 -1.6495312806 -2.6437352567
 N 1.1992311952 -1.5955404581 -1.2293907202
 Cu -0.6502093725 -0.8872176925 -1.4054334387
 C -2.0316333741 -1.3458024448 2.5713943228
 H -2.4541250831 -2.2274227307 3.05919137
 H -2.6596344776 -0.490621828 2.8453666314
 N 5.1951715149 -2.1744809424 -0.1701046122
 N -6.5652216049 0.034485161 -0.0756532758
 N 2.7302076081 4.0156907204 0.2041171982
 C 6.3119488326 -1.8126710771 -0.934685102
 C 5.657671158 -2.7661394558 1.012982816
 C 7.0129977506 -2.7754069292 0.9815074892
 C 7.4278471112 -2.1603309415 -0.247947593
 C -7.4890681629 0.8032392807 -0.7969213778
 C -7.2098501125 -0.4471804185 1.0723042561
 C -8.4885845478 0.0019618081 1.0607549483
 C -8.6620486508 0.8041739027 -0.1181647498
 C 2.7886783507 4.5102564495 1.5103646385
 C 3.6991085515 4.6806599052 -0.55249903
 C 3.7602629585 5.4572154049 1.5636276835
 C 4.3453773433 5.5568451695 0.2585146043
 H 6.20787132 -1.29221818 -1.8731404348
 H 4.978321343 -3.1885682565 1.7358596917
 H 7.6580666154 -3.1889165676 1.7431610964

H 8.4447049689 -1.9946251824 -0.5730196557
H -7.207600075 1.3243754471 -1.6978078759
H -6.7173709577 -1.1203044174 1.7555728212
H -9.2412773967 -0.2206693009 1.8031180965
H -9.5604951658 1.3257448081 -0.4145219224
H 2.0849910691 4.194385234 2.2641947129
H 3.8757189518 4.428137655 -1.5860490557
H 4.0266670346 6.038461115 2.4344843307
H 5.1591143342 6.204157764 -0.034639826

CH2_Cu2+_2f

2 2
C -0.4182531954 3.569454083 0.6440778454
C 0.1535202073 2.9161144789 -0.6229444907
C 0.4755170587 3.086989278 1.8088089567
C -0.2518207148 1.4368952342 -0.56054976
N -0.6024277352 1.0881562788 0.8604538497
C 0.328727966 1.5494068996 1.9112333444
C -1.9423665404 1.6292737688 1.1522833295
H -0.361935317 4.657459862 0.5701844202
H 1.2415959527 3.0381485297 -0.6353737079
H -0.242758461 3.3730266129 -1.534396011
H 0.1843331071 3.5513051804 2.7547067814
H 1.5066014913 3.3915882035 1.6043960138
C -2.9461539009 0.6839819848 0.5148862489
C -4.1899189782 1.0825835689 0.1059535399
C -5.1201876349 0.1281366207 -0.4014747524
H -4.4590108766 2.1292036637 0.1785633885
C -3.3947561929 -1.5238535556 -0.0489958357
C -4.6599014173 -1.2162522619 -0.47056377
H -3.0363039336 -2.5466038944 -0.1036955724
H -5.2964250389 -2.0095311467 -0.8398511574
N -2.5286143252 -0.6168221023 0.4553156179
H -2.0879257128 1.5214191662 2.2330918877
C 0.6391582725 0.4095839497 -1.252566334
C 1.5786437123 0.787583973 -2.1819416574
C 1.0081171128 -1.8258895213 -1.6883427303
C 2.2817912066 -0.1991699099 -2.9282200319
H 1.773421331 1.8370985613 -2.3577653589
C 1.9595795219 -1.5493303323 -2.6392094759
H 0.7508121606 -2.8562244759 -1.4623253133
H 2.4325239904 -2.3673571089 -3.166993055
N 0.3373149941 -0.8853945447 -1.0012475234
H -1.2089725771 1.3351624972 -1.0859144516
H -0.1949485943 1.3308398899 2.8493688806
C 1.5021017881 0.5917569405 1.9458592744
C 2.7820638362 0.9542393322 2.2655746623
C 3.7921148628 -0.0415239999 2.4113528982
H 3.0160366069 1.9993441776 2.4224633323
C 2.0830783467 -1.6526993529 1.8569693672
C 3.3861880513 -1.384616526 2.1819230689
H 1.7654889968 -2.6749426803 1.6773851404
H 4.0832725123 -2.2066222628 2.2779956313
N 1.1273750049 -0.7063011467 1.7515211261
Cu -0.6228087023 -0.8997185897 0.8505468794
C -1.9055419163 3.1423055314 0.8069313064
H -2.3930424715 3.7219727887 1.5946514011
H -2.4377385851 3.3527870441 -0.1276810602
N 5.0446555865 0.2716814796 2.7474078153
N -6.3457690605 0.4780045426 -0.7903403601
N 3.1915386722 0.1329639955 -3.8527834824

C 6.1338632097 -0.711388935 2.8523181179
C 5.4903194343 1.6273309983 3.0998625819
C 6.8692803284 1.4018094655 3.7231551897
C 7.3856460269 0.1548139556 2.9998693809
C -7.3134534199 -0.4547073481 -1.3902441071
C -6.9003754581 1.832687122 -0.6512995371
C -8.3931032968 1.6393274409 -0.9247427165
C -8.4240830832 0.4627224048 -1.904189929
C 3.477832514 1.5110363618 -4.2680307443
C 3.9902919746 -0.8477430658 -4.5996939415
C 4.3108020748 1.337716712 -5.5400820788
C 5.0390562881 0.0107074433 -5.3085890399
H 6.1653719375 -1.3443666808 1.9604453733
H 5.9749673779 -1.3510154785 3.7295561512
H 4.7890887419 2.091884312 3.7998383379
H 5.5480137376 2.2491045382 2.197064967
H 6.7652408478 1.2047090462 4.7947440569
H 7.5206854203 2.2688730473 3.6010222582
H 8.1765402289 -0.3601705791 3.5476883821
H 7.7754948051 0.4203291906 2.0118965909
H -7.6804013998 -1.1512448295 -0.6261375559
H -6.8422945443 -1.0310488664 -2.1918480404
H -6.4356535832 2.5034204919 -1.3853508424
H -6.7080247898 2.224189508 0.3522896895
H -8.8557447507 2.5427414176 -1.3256945035
H -8.9104996689 1.3767090798 0.0033602758
H -8.1887197548 0.8029694146 -2.9176629864
H -9.3903718415 -0.0434440551 -1.9336919235
H 4.039200725 2.034098021 -3.4822482156
H 2.5484374388 2.0591700671 -4.4534448533
H 3.3540293641 -1.3858465236 -5.3141408454
H 4.4389643337 -1.5770232694 -3.9180549951
H 4.9893675404 2.1766550065 -5.7044374605
H 3.6499541895 1.2615920961 -6.4093717953
H 5.9043351616 0.159729965 -4.6544939697
H 5.3903414223 -0.4512321799 -6.2328313878

CH2_Cu2+_2d

2 2
C 0.1679426253 3.7947873721 -0.3555248885
C -0.3377867208 3.2265141667 0.9783287462
C -0.812250026 3.2834752819 -1.4342291444
C 0.0249534016 1.7345249526 0.9727689135
N 0.2677241356 1.295415916 -0.4515702228
C -0.7192216996 1.7378310461 -1.4659634217
C 1.6011190328 1.7857554728 -0.8632732332
H 0.1472605852 4.8859146655 -0.3358787794
H -1.4187208224 3.381828423 1.0554073253
H 0.129461722 3.7167093939 1.8370211422
H -0.5693731825 3.6866274887 -2.4204804274
H -1.8190128611 3.6309586893 -1.184118705
C 2.6243711741 0.847412419 -0.2521032282
C 3.930360752 1.2044589794 0.0295784191
C 4.8145434289 0.234164324 0.5002355361
H 4.2593730141 2.2261938946 -0.1263115723
C 3.0397354306 -1.3589302368 0.3938053715
C 4.3637634817 -1.0679346984 0.6826253924
H 5.8439291819 0.4960420841 0.7214527515
H 2.639746927 -2.3575242242 0.5346036826
H 5.0201142656 -1.8494093987 1.0468148607
N 2.1886371902 -0.4293197918 -0.0699811878

H 1.668273307 1.6243768152 -1.9452344977
 C -0.8482023022 0.7828669424 1.7829969318
 C -1.7019877229 1.2330349301 2.7786483636
 C -1.253272229 -1.4277117657 2.3652693261
 C -2.3465865152 0.3002931734 3.590802469
 H -1.8559031689 2.2932719731 2.941191703
 C -2.1162788277 -1.0534069879 3.3867266246
 H -1.0457054021 -2.4735755797 2.1625587951
 H -3.0148594829 0.634111528 4.3776684155
 H -2.5910628523 -1.8089958888 4.0016844013
 N -0.6320737449 -0.5342938389 1.5872101302
 H 1.0133821478 1.6345036736 1.4370985294
 H -0.2666508675 1.456006998 -2.4242391352
 C -1.9232319348 0.8251736459 -1.374653571
 C -3.2255843869 1.1926785079 -1.6561326081
 C -4.2169905574 0.2112515329 -1.6788797172
 H -3.4678325603 2.2266569131 -1.87385271
 C -2.5523993293 -1.4092899994 -1.1325183268
 C -3.8756490436 -1.1106413807 -1.4206830754
 H -5.2439165448 0.4802382405 -1.9030991627
 H -2.2401233035 -2.4242074463 -0.908817243
 H -4.6162586389 -1.9014167268 -1.4383291041
 N -1.5971195862 -0.468764769 -1.1167660693
 Cu 0.2377075278 -0.6697083771 -0.3456575729
 C 1.6285955968 3.3144794069 -0.589966098
 H 2.0806211235 3.8369741854 -1.4361470914
 H 2.2277282623 3.5533880741 0.2957229626

CH2_2b

O 1
 C -0.7132578089 -2.3709628418 1.4912443318
 C -0.5734178713 -0.9929714835 2.1502432139
 C 0.5306421497 -2.5974426118 0.6184124302
 C -0.4571356629 0.0740795208 1.0229673361
 N -0.5498223291 -0.5568739504 -0.3120556962
 C 0.4896805207 -1.5701487043 -0.5503898462
 C -1.8530629945 -1.2488413675 -0.44465567
 H -0.7773694012 -3.150514507 2.2567671083
 H 0.2921397792 -0.9866855133 2.8208096039
 H -1.4469858074 -0.781903851 2.7787504144
 H 0.5603490494 -3.623228947 0.2344526126
 H 1.4208117909 -2.4657063066 1.2449945192
 C -2.9958464336 -0.2499164935 -0.5038040103
 C -3.7170450109 0.1757349729 0.6130379538
 C -4.7224037442 1.1224224062 0.4625471195
 H -3.4983796176 -0.2185505111 1.5999433914
 C -4.224647302 1.1190306617 -1.8814693399
 C -4.9756695065 1.6023085631 -0.8131270393
 H -5.2942060503 1.4781410754 1.3129151399
 H -4.4147004031 1.474173177 -2.8912455257
 Cl -6.2228027786 2.7862253998 -1.0893391075
 N -3.262064778 0.2165700837 -1.7300100974
 H -1.8396023637 -1.6906586006 -1.4438960464
 C 0.7351506174 1.0134862321 1.098333226
 C 1.9784350285 0.6313021261 1.602936912
 C 1.5259570151 3.0920045938 0.5617288821
 C 3.0262266777 1.5361203388 1.527052246
 H 2.148624056 -0.3575333364 2.0102442162
 C 2.8164971089 2.7979614889 0.991344959
 H 1.3035026217 4.0770327381 0.1574620075
 Cl 4.6079134409 1.0761578578 2.0973604581

H 3.6168160923 3.5251375921 0.921673131
 N 0.5084455702 2.2367081151 0.6090602994
 H -1.311035937 0.7510022928 1.0736654328
 H 0.1550420801 -2.1023104713 -1.4496653246
 C 1.837371244 -0.9780302954 -0.9537848503
 C 3.0277554987 -1.6503953936 -0.6667498305
 C 4.2229570416 -1.0643447662 -1.0585593857
 H 3.0363436998 -2.599485675 -0.1448361098
 C 2.9716111689 0.7089465046 -1.9974340203
 C 4.2174730223 0.1510814619 -1.7246040861
 Cl 5.733246442 -1.8589701595 -0.6991098234
 H 2.9093435812 1.6510661169 -2.5377595068
 H 5.1368270212 0.6383795579 -2.0262475702
 N 1.8113722617 0.1674611972 -1.6392624463
 C -1.9788475666 -2.3799992381 0.6211264667
 H -2.0895495508 -3.35013673 0.1240345878
 H -2.8627216618 -2.2562323198 1.2556473334

CH2_2e

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 C -1.0457592815 -1.1896940009 1.8581058985
 C 0.3236163849 -2.5744291252 0.3195998306
 C -0.7847363782 0.0115902293 0.9018518047
 N -0.6831798142 -0.4532686365 -0.5006374944
 C 0.408199021 -1.4163023349 -0.7180995363
 C -1.9352789502 -1.138936542 -0.8997126393
 H -1.1818113972 -3.3491395795 1.6760560042
 H -0.2985546482 -1.2522189295 2.6562317348
 H -2.0157343096 -1.0713519526 2.3578505392
 H 0.4416837572 -3.5475101462 -0.1717025804
 H 1.114252484 -2.5010685448 1.0760801273
 C -3.1039750788 -0.1703097452 -0.9950643621
 C -3.9247242695 0.1210672716 0.0887657483
 C -4.9643032145 1.0598759625 -0.0385440241
 H -3.7462218437 -0.3711257518 1.0358566665
 C -4.2592795046 1.2641217874 -2.3259798494
 C -5.1178223003 1.6460704524 -1.3073159809
 H -4.3796406645 1.7061815758 -3.3136825932
 H -5.8836656151 2.3847641381 -1.5086950059
 N -3.268597215 0.3813274547 -2.2043719839
 H -1.7719433719 -1.446486653 -1.9351841068
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 C 2.9386670792 -1.4552762165 -0.5215573156
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 H 2.8592624761 -2.4539259882 -0.1128052777
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 H 2.9912942819 2.0030762759 -2.0462587421
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 N 1.803110931 0.4415860394 -1.4494320509

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 C -5.4291333377 0.9138707228 2.347529987
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 H 6.8073826238 -0.7877167023 -1.6352050671
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 H 4.9400690519 -0.7365519068 3.3734131864
 C 5.0671145296 1.5475506135 2.2201028497
 H 5.1612351467 1.7750451648 1.1483461761
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 H 5.931581892 0.9528186205 2.5211634809

CH2_2a

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 H -1.4480028309 -0.8141664548 2.7749030604
 H 0.507142145 -3.6399241592 0.1704207138
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CH2_2f

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Cu1+

1 1
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MMA•

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C -0.29162154 -0.34890785 0.
O -0.62463911 -1.52330802 0.
O -1.19471888 0.65991696 0.
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O_Br_Cu2+_4a

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N 0.0847901459 -0.1749532252 0.6467900533
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C 0.8444280392 0.9603593166 1.187073186
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N -3.2971098816 1.3206395685 0.7143191388
N -1.7543144925 1.0255259765 -0.8256267032
H -1.6649937913 -1.1878286144 1.1245956892
H 1.8609330445 -1.2294633387 0.7775089773
Cu -0.0426860901 0.0090815555 -1.5094190351
C -1.0948029666 0.1206637165 2.7684463811
H -1.793151813 -0.4639767475 3.3733996262
H -1.249996648 1.1776327448 3.005258688
C -2.7452670157 1.8015722612 -1.3622587765
C -4.0408450985 1.2376990228 1.9626247764
H -2.6920895223 2.1484243961 -2.3829180283
H -3.6415193431 1.933441394 2.7045715189
H -4.0047718864 0.2194262098 2.3546369497
H -5.0824236927 1.4904030584 1.763724015
C 2.9034759087 1.3831145818 -1.7143468558
C 3.7406724129 1.97913537 -0.8146824907
C 3.6621863118 2.4386606299 1.6596396113
H 3.0070033345 1.2538740832 -2.7809063556
H 4.7027598569 2.4540642805 -0.9311246555
H 3.0574694335 2.0912038946 2.4954050784
H 3.6387248359 3.5297180616 1.6125346196

H 4.6916096099 2.1022212189 1.796247174
 C -0.0437464966 -4.2958781777 -1.131751682
 C -0.3633392593 -3.2120162901 -1.8960077448
 C 0.8809026667 -4.622797494 1.1883992545
 H -0.0896593866 -5.3557271001 -1.3293692103
 H -0.7344944751 -3.1609476382 -2.9081811679
 H 1.7820200484 -4.1825259468 1.6189486352
 H 1.1323123529 -5.6127767039 0.8075668685
 H 0.1139160106 -4.7236581147 1.9602108204
 C -3.7098092997 1.9956438759 -0.4173398851
 H -4.6401565248 2.5419344619 -0.4390388283
 Br -0.1784801308 0.1949181069 -3.8206854773

O_Br_Cu2+_4b

1 2
 C -3.8561332391 -0.1053942407 0.0339658989
 O -3.2459264407 -1.3392397316 0.4689625611
 C -3.3981173541 1.0427012988 0.9550579642
 C -1.8956890654 -1.1128921246 0.7700249728
 N -1.3980633332 0.0257847992 0.0084452857
 C -1.8717456347 -0.0973756736 -1.3821699777
 C -1.9077655022 1.2647702014 0.6201551363
 H -4.9302533235 -0.2690386486 0.0970651561
 H -3.541473415 0.7536245607 2.0007503385
 H -3.9877621616 1.9434876569 0.7665248277
 N -1.0292129944 1.557721207 1.737380551
 C 0.2810849551 1.1766268883 1.7001644298
 H -1.7931754969 2.0539681763 -0.1278271221
 N -1.0744745233 -2.2473711209 0.4180788256
 C 0.2470944448 -2.0497648883 0.1409463455
 N -1.0211421317 0.7684821063 -2.1753296528
 C 0.2902103588 0.9169551126 -1.8287513999
 H -1.6841794721 -1.1311966353 -1.6784317721
 H -1.7686978235 -0.8954340212 1.8366077022
 Cu 0.8027408064 -0.0001775914 0.017232483
 Br 3.2008144213 -0.0380055932 0.0154310717
 C -3.3885858776 0.1739021726 -1.4092824823
 H -3.8846279428 -0.4919102015 -2.1181613214
 H -3.6203756042 1.2078112865 -1.687620921
 N 0.7258962181 -3.2963626691 -0.0011133705
 C -0.2620316076 -4.2502812063 0.1943308327
 C -1.4093231999 -3.5883655022 0.4694548744
 C 2.108078277 -3.6192735336 -0.339725725
 N 0.8034268163 1.6501782367 -2.8312021906
 C -0.1501021862 1.940500732 -3.7927908862
 C -1.310187442 1.3761115059 -3.3845407167
 N 0.7996029205 1.7120644814 2.8185989758
 C -0.1487133821 2.4246900877 3.5328633922
 C -1.3113025405 2.3352831587 2.847233891
 C 2.1839407889 1.5491743986 3.2515066365
 C 2.188058265 2.1064561923 -2.898381943
 H -0.0622424734 -5.3075170281 0.1139922031
 H -2.4081889234 -3.9353204018 0.6785746158
 H 2.6794521744 -2.6916586028 -0.3711151931
 H 2.1428201335 -4.1125159468 -1.313791189
 H 2.5245113706 -4.2806709248 0.4228948989
 H 0.078119008 2.5216741474 -4.6727563527
 H -2.2856189484 1.3529748495 -3.8443560084
 H 0.0845271256 2.9234797714 4.4607545837
 H -2.2860042072 2.7502404136 3.0504970033
 H 2.7263444294 1.0124583952 2.4733784337

H 2.2130654537 0.9832933672 4.1854194091
 H 2.6360173876 2.5317846058 3.4016311069
 H 2.7340253793 1.6689824205 -2.0626009119
 H 2.2203016886 3.1966598286 -2.8368444437
 H 2.6342738241 1.7772042272 -3.8390508272

O_Br_Cu2+_1b

1 2
 C -3.5759571104 0.6747945799 0.0479415288
 O -3.1782975404 -0.3065345149 1.0204771896
 C -2.8328282841 1.99034892 0.3187354674
 C -1.7841279075 -0.294822528 1.1896483625
 N -1.1304169349 0.2590649235 -0.0085926631
 C -1.744786473 -0.3679359324 -1.2097566963
 C -1.3497226986 1.7311524138 -0.0304578818
 H -4.6524490594 0.7893863014 0.1653523609
 H -2.9590937068 2.2644050715 1.3709638384
 H -3.2483934667 2.7972672219 -0.290534922
 C -0.308496836 2.4016670709 0.8436393412
 C -0.515156665 3.6410904593 1.4274869843
 C 0.53221094 4.2071256333 2.153337759
 H -1.4575975865 4.1659294363 1.3212943587
 C 1.8538980113 2.2910098492 1.6580514951
 C 1.7392712393 3.5281470818 2.2749418865
 H 2.7689085998 1.709109849 1.7102868148
 H 2.5676201977 3.9466778823 2.8334524413
 N 0.8546519998 1.7411702636 0.9603512598
 H -1.1492690689 2.0501460762 -1.0602280733
 C -1.237208698 -1.6792934147 1.4638427666
 C -2.0007697407 -2.6855178661 2.0248013694
 C 0.6635691794 -2.9859305378 1.432811225
 H -3.0512194627 -2.5304408307 2.2389350331
 C -0.0127163689 -4.0538421422 2.0063342743
 H 1.7156868837 -3.0469109291 1.1725584395
 H 0.5013812932 -4.9845596782 2.2135036387
 N 0.0623757323 -1.8229334692 1.163271016
 C -0.8055122535 -0.187390559 -2.383252906
 C -1.2386475757 -0.1124851232 -3.6963919059
 C -0.2737460484 -0.0299053084 -4.7005882358
 H -2.2931053697 -0.128917538 -3.9466481774
 C 1.4154442617 -0.1018997037 -3.0252513943
 C 1.0760045829 -0.0251297121 -4.3688245972
 H 2.4503123237 -0.1078448622 -2.6971247444
 H 1.8434141684 0.0361596231 -5.1308044671
 N 0.497966468 -0.1790523601 -2.0571445167
 H -1.7729447101 -1.4428650727 -0.9981012687
 H -1.5051091723 0.3551984487 2.0330307976
 Cu 0.8817870651 -0.1866711413 0.0508373565
 Br 3.155607708 -0.6976239018 0.1017652875
 C -3.1954381357 0.143487876 -1.3430890754
 H -3.8600484225 -0.6684941802 -1.6456176126
 H -3.2835330187 0.9471247836 -2.0829176688
 C -1.3642684734 -3.896554363 2.2969224837
 Cl -2.2595121317 -5.1956023963 2.994124527
 Cl 0.3207297777 5.7488867391 2.8971596801
 Cl -0.7657975116 0.0658375609 -6.3510821764

O_Br_Cu2+_1e

1 2
 C -3.3760822273 0.5431404045 0.0537467276
 O -2.9382363207 -0.3721876518 1.0682408012

C -2.6606278303 1.8885601712 0.2380767392
 C -1.5338299311 -0.3323378636 1.1960481098
 N -0.9275088666 0.184963627 -0.0386939436
 C -1.5440091075 -0.5113968496 -1.1968707098
 C -1.1772530033 1.6476616916 -0.1221441379
 H -4.4532556105 0.6403003302 0.1865920395
 H -2.7735909118 2.2141929975 1.2769953501
 H -3.1079158287 2.6516743676 -0.4049839106
 C -0.1359052193 2.3778598556 0.704842045
 C -0.3716550663 3.6263263016 1.2401029739
 C 0.6621704486 4.2964846093 1.9407110077
 H -1.3425400928 4.0862957244 1.1076917927
 C 2.0301461671 2.3634187093 1.4728279481
 C 1.8952646064 3.6102926507 2.0406237727
 H 2.9661418941 1.8163359446 1.5318781421
 H 2.7441988302 4.0401458194 2.5551580978
 N 1.0421431897 1.7406213507 0.8130602063
 H -0.9993484287 1.9206219763 -1.1689675488
 C -0.9466228833 -1.6921991161 1.5091790552
 C -1.6768413557 -2.6856393675 2.1158954285
 C 0.9714840212 -2.947125486 1.4977950092
 C -1.035333831 -3.9059432604 2.4478203835
 H -2.7233802018 -2.5079312474 2.3236092055
 C 0.3379056476 -4.0022360581 2.1175195972
 H 2.0214165734 -3.0001940378 1.2263892186
 H 0.911839129 -4.8929080895 2.3359162137
 N 0.3535922383 -1.7985973854 1.1866116837
 C -0.6334218918 -0.3533839687 -2.3973402349
 C -1.1030426292 -0.3428038449 -3.6928653707
 C -0.1839192249 -0.2793515421 -4.7706441842
 H -2.1686993601 -0.4020976614 -3.8729470222
 C 1.5534957071 -0.2394776702 -3.0947477203
 C 1.1858885552 -0.2262788129 -4.4220547598
 H 2.5979888173 -0.206194567 -2.7998676481
 H 1.9614467804 -0.1781000068 -5.174663132
 N 0.673362136 -0.3000175742 -2.0854968564
 H -1.5331026889 -1.5753894516 -0.9353476558
 H -1.2479857862 0.358970377 2.0027728874
 Cu 1.1049046541 -0.209175873 -0.0050758717
 Br 3.4094025444 -0.6633142634 0.0161597515
 C -3.0122795306 -0.0493605522 -1.3167340599
 H -3.6612744315 -0.8936422126 -1.5602243791
 H -3.1402704426 0.7127167308 -2.0939611973
 N -1.7039441032 -4.9200709865 3.0475161857
 N -0.5982677249 -0.2701355405 -6.0610815709
 N 0.4762669237 5.5240486724 2.4837246
 C -0.8067345487 6.1930335581 2.354994031
 H -1.611306014 5.6071804698 2.8160110654
 H -0.7617250419 7.1561465753 2.8621617539
 H -1.0605598596 6.376648906 1.3037027124
 C 1.567485936 6.1805129246 3.1872550308
 H 2.4268170358 6.3445324622 2.5266859761
 H 1.2286816582 7.151368585 3.5472140593
 H 1.8941637685 5.5930028516 4.0531237451
 C -1.0080614788 -6.1521138183 3.3834620534
 H -1.7079772924 -6.8423506444 3.8532152782
 H -0.603072534 -6.6377104756 2.4879679964
 H -0.1876272842 -5.9687935081 4.0873054939
 C 0.3790853102 -0.2215743855 -7.1375645941
 H -0.1416299129 -0.2240712384 -8.0945375666
 H 0.9851573719 0.6902147281 -7.0840681406

H 1.0460250236 -1.091282041 -7.1114306115
 C -3.1103791319 -4.7685386296 3.3817942739
 H -3.4664016155 -5.6825986087 3.8558006649
 H -3.2688176322 -3.9395276275 4.0819536035
 H -3.7174772408 -4.5936998285 2.4855861543
 C -2.0149440984 -0.3415277306 -6.3739490052
 H -2.4626257715 -1.2719662213 -6.0034146391
 H -2.5617901314 0.5081769789 -5.947354121
 H -2.1456908489 -0.3136146524 -7.4551582738

O_Br_Cu2+_1a

1 2

C -3.5662169481 0.6730240196 0.0553531556
 O -3.162911801 -0.3137949806 1.0219378175
 C -2.8218159495 1.9869684916 0.3296835678
 C -1.771575863 -0.2982799986 1.1902565649
 N -1.1180654483 0.2560816351 -0.0098457439
 C -1.7399761436 -0.3680583143 -1.2098195735
 C -1.3403094021 1.7287959438 -0.0280162371
 H -4.6420386215 0.7862583387 0.1778754609
 H -2.944264243 2.2572132756 1.3833458283
 H -3.2394763666 2.7968133783 -0.2739331958
 C -0.296781802 2.3997708717 0.8417457772
 C -0.5015163515 3.6383665058 1.4304805459
 C 0.5557286277 4.1815755982 2.1434165235
 H -1.4362582157 4.1791025119 1.3450959373
 C 1.8775749951 2.2871118796 1.6466304554
 C 1.7653475796 3.5256837232 2.2686180257
 H 2.7912369101 1.7028157864 1.6902487876
 H 2.5842393552 3.9599771073 2.8281393389
 N 0.871030488 1.7452760336 0.9550433016
 H -1.1455642306 2.0511173571 -1.0579550272
 C -1.2248978009 -1.6823447281 1.4661357195
 C -1.9867031046 -2.6895397336 2.0317272073
 C 0.6840568822 -2.9906862404 1.4306703226
 H -3.037616095 -2.5566965394 2.2563462905
 C 0.0095687852 -4.060568517 2.0101233133
 H 1.7349472401 -3.0471633272 1.1655540052
 H 0.5073989306 -4.9978159142 2.224623006
 N 0.0738273457 -1.8327996594 1.1638873945
 C -0.8066246147 -0.1885301688 -2.3873646566
 C -1.2443890912 -0.107886207 -3.6996494733
 C -0.2719937148 -0.0278441502 -4.6852216931
 H -2.2936941958 -0.1146882457 -3.9682512386
 C 1.4204774694 -0.1108575543 -3.037810414
 C 1.075988763 -0.0298352777 -4.3833530338
 H 2.4549795909 -0.1220476914 -2.7094503366
 H 1.8254730137 0.0306486789 -5.1624176109
 N 0.5006658805 -0.1855789585 -2.0731205089
 H -1.7698944024 -1.4434982236 -1.0003505152
 H -1.4912397288 0.352024891 2.033389031
 Cu 0.8905834747 -0.1893799757 0.0420799228
 Br 3.1571592195 -0.6999961985 0.0848921254
 C -3.1901137838 0.1464346415 -1.3384716791
 H -3.8563106683 -0.6635167914 -1.6424467744
 H -3.2796385547 0.9522833427 -2.0755920506
 C -1.3321337012 -3.8835780686 2.2942678704
 N -0.7010624805 0.0651939919 -6.1000862197
 O -1.9007357928 0.0817224525 -6.3065368986
 O 0.1779752335 0.1199791715 -6.9365404969
 N 0.373277617 5.5031636627 2.7879598353

O -0.7147435621 6.0316429054 2.6505941708
O 1.3226764493 5.9494338906 3.4001764064
N -2.0997942142 -4.9999853116 2.8943591094
O -3.279856559 -4.7965433986 3.1096826762
O -1.4887203994 -6.0259559118 3.1196838831

O_Br_Cu2+_1c

1 2
C 0.479222928 -0.3669069297 2.8139683646
C -1.0229881955 -0.2401010889 2.5253857421
C 1.0315695523 -1.6268506879 2.1289721088
C -1.1900631433 -0.4240459766 0.9998628281
N 0.1313586897 -0.1657867734 0.3674814488
C 0.7144736158 1.0450459628 0.9669960673
C 1.0528503304 -1.3050475493 0.6190133707
H 0.6850944163 -0.355982617 3.8834800465
H -1.368466084 0.7452158339 2.853954926
H -1.5846082993 -0.9961641224 3.0806306394
H 0.3882592801 -2.4836008018 2.3594224397
H 2.0384770062 -1.8540930977 2.4857432976
C 0.7324190319 -2.4125086684 -0.3625149018
C 0.9388353717 -3.749545941 -0.0845543612
C 0.6870377199 -4.6997733419 -1.0864175241
H 1.2721237727 -4.0606018286 0.8980636547
C 0.0381426132 -2.8837221583 -2.5101858951
C 0.2273560107 -4.241016829 -2.3256901279
N 0.8867426434 -6.0518321393 -0.8468512074
H -0.3066005949 -2.4814691138 -3.457787711
H 0.0487171352 -4.9226677212 -3.147673916
N 0.2845483904 -1.981223063 -1.5540115583
H 2.0510266949 -0.9371545798 0.3558178173
C -2.2444593591 0.4214377521 0.3126808888
C -3.4134736756 0.8019147606 0.9438554564
C -2.8924688968 1.4244273481 -1.659712328
C -4.3740469486 1.5255363219 0.2215280482
H -3.5744767411 0.5643171945 1.9884685657
C -4.0935464922 1.8360625213 -1.1139140536
H -2.6358649837 1.6346109015 -2.6933501974
N -5.5616785502 1.9214841699 0.8194142992
H -4.8092002236 2.3634537316 -1.7319021154
N -1.9816605923 0.7286559458 -0.9680352438
C 1.8260391831 1.5572460108 0.0764504582
C 2.953969981 2.1711004582 0.5758702333
C 3.8993172106 2.6718012801 -0.3331366355
H 3.1022036874 2.2264402301 1.6467699064
C 2.4895028032 1.8648362444 -2.10283271
C 3.6414255887 2.5164440109 -1.7010871654
N 5.053078135 3.2969864342 0.1156703333
H 2.254836074 1.7164330903 -3.152256063
H 4.3149192828 2.9154922907 -2.4489460478
N 1.5904578541 1.3876127765 -1.2341461813
H -0.0825859688 1.8035360881 0.9899565416
H -1.4296440758 -1.4703694117 0.775976374
Cu -0.0713463399 0.1210035214 -1.6683382193
O 1.1656019807 0.7724316688 2.2716114323
C 0.2521838571 -7.0973273766 -1.5079668392
C 1.7528574027 -6.5938658674 0.0963922575
C 0.7061958458 -8.2702402463 -0.9856396453
C 1.6662851036 -7.9511460331 0.0245453258
C 5.2213417714 3.9048532415 1.3552822127
C 6.2413662092 3.4216686277 -0.5959129614

C 7.136978402 4.0885845538 0.1831266677
C 6.4865099519 4.4043600719 1.4169133704
C -6.1694260298 1.3103002545 1.9105894559
C -6.3469836968 3.0009863969 0.4308572691
C -7.3145914858 1.9896243548 2.1967140903
C -7.4214197068 3.0687145432 1.2648110918
H -0.5079397088 -6.9074852076 -2.2498784887
H 2.4025598052 -5.9637376276 0.6839676736
H 0.3843231672 -9.2579001021 -1.2824946997
H 2.2368302653 -8.6510859446 0.617765959
H 4.403923248 3.9795415154 2.0554473096
H 6.3578908166 2.9733012469 -1.5702806458
H 8.1561195762 4.3224818916 -0.0886488463
H 6.9078815935 4.9511338957 2.2480523248
H -5.7656081267 0.4064173994 2.339860075
H -6.0363841084 3.6568787837 -0.3676270544
H -8.0162473181 1.740218968 2.9795228989
H -8.2021604839 3.8144558594 1.2262625476
Br -0.2914341689 0.4291146932 -3.9750824744

O_Br_Cu2+_1f

1 2
C -3.2185886588 0.4791861408 -0.1138767001
O -2.7944266118 -0.3947914779 0.9416923865
C -2.5030341054 1.8300409908 0.0245422225
C -1.3909199393 -0.3532352375 1.0830268113
N -0.7701595525 0.1144872704 -0.1639358136
C -1.3740880717 -0.6261734476 -1.3008028331
C -1.0159077438 1.5728914136 -0.3079945059
H -4.2971173034 0.5831245726 0.002403837
H -2.6275571937 2.1972588191 1.0481434863
H -2.9412590658 2.5673714173 -0.6539101509
C 0.0164524859 2.3339035509 0.5019369949
C -0.2238187357 3.6011913976 0.987332493
C 0.8041951823 4.2924492665 1.6755580641
H -1.1946217122 4.0591858371 0.8418756051
C 2.1740698338 2.343414836 1.3000151477
C 2.0349549794 3.6099971881 1.8195749062
H 3.1082129167 1.7970146983 1.3880734081
H 2.8777944883 4.0694688191 2.3199674591
N 1.1923817567 1.6991029358 0.6496483676
H -0.8249719958 1.8037729412 -1.3626099739
C -0.8109660998 -1.7012186809 1.4545376943
C -1.5509963537 -2.6716564375 2.0850316302
C 1.1060210315 -2.9610700342 1.5083505945
C -0.9136034134 -3.8798297723 2.4649889024
H -2.6039319601 -2.4978703181 2.2656830137
C 0.4630158577 -3.9931108809 2.1552231449
H 2.1596120774 -3.0227227583 1.2533430998
H 1.0276404621 -4.8767007665 2.4245691707
N 0.4935666894 -1.8218185823 1.1516445734
C -0.4502196413 -0.5155145514 -2.4961533243
C -0.9045546298 -0.5504219096 -3.7961255574
C 0.0296660823 -0.525624834 -4.8622844147
H -1.9680325747 -0.600937086 -3.9953304413
C 1.7470929721 -0.4255107315 -3.1715845481
C 1.3958583626 -0.4587739479 -4.502344558
H 2.7876701741 -0.3846354089 -2.8640029789
H 2.175594659 -0.4494556872 -5.2532001778
N 0.853715042 -0.4513547097 -2.1713176835
H -1.3672174936 -1.6790990995 -0.997708742

H -1.1121773655 0.3682527157 1.8653936375
 Cu 1.2609888475 -0.2805697511 -0.091477192
 Br 3.5661563869 -0.736692708 -0.0257410781
 C -2.8403748065 -0.1681696706 -1.4552480151
 H -3.4876791876 -1.021057903 -1.6718121021
 H -2.9588329564 0.5622032077 -2.2637624086
 N 0.6156430168 5.5330804352 2.1667695032
 C 1.6113889504 6.2486830955 2.966538235
 C -0.6005955415 6.3172594123 1.9563348476
 N -1.5875324785 -4.8661728472 3.0877901177
 C -1.0008462424 -6.1643503742 3.4226429282
 C -2.980156985 -4.7529676972 3.5208105214
 N -0.3671582674 -0.5629069112 -6.1498787327
 C 0.5504972154 -0.4498396609 -7.2847484428
 C -0.3841953639 -0.2579851839 -8.4806560267
 C -1.6431197918 -1.0275698707 -8.0699468269
 C -2.2093357518 -7.0049390643 3.839788524
 C -3.171838004 -5.9694646411 4.4294110875
 C 0.8317563334 7.4425184432 3.5211844251
 C -0.2109376816 7.7183880954 2.4335191199
 C -1.7560787794 -0.7430522602 -6.5701810234
 H 2.4518422254 6.5691600675 2.3359819645
 H 2.0050899215 5.6052837299 3.7600549385
 H -1.4317309583 5.904781688 2.5456157345
 H -0.8917808245 6.3063755858 0.9002942207
 H -0.276896533 -6.0586581005 4.2421692897
 H -0.4786365949 -6.5876913148 2.5583025845
 H -3.6560559718 -4.7823582996 2.654863026
 H -3.1459585355 -3.8090863484 4.050805124
 H 1.1542764304 -1.3623003719 -7.3828994759
 H 1.2308701994 0.3971891429 -7.1492239777
 H 0.0564267593 -0.6211643462 -9.4112493655
 H -0.6142120592 0.8052785581 -8.6065127005
 H -1.5004235894 -2.1007673269 -8.2340270389
 H -2.5352248678 -0.7171901614 -8.6177786846
 H -1.9401238735 -7.7923021166 4.5466921115
 H -2.6554850877 -7.4781794675 2.9587039836
 H -2.8760119738 -5.718312374 5.4533885101
 H -4.2091622415 -6.3098373665 4.4508181775
 H 1.4777148312 8.2991933379 3.7234241099
 H 0.3375404848 7.1618658495 4.4572158515
 H 0.2419783632 8.278667721 1.6089003406
 H -1.0708538042 8.2853864854 2.7959473626
 H -2.3396313952 0.1673771579 -6.3731391397
 H -2.222546495 -1.5720643266 -6.0266086553

O_Br_Cu2+_1d

1 2
 C 3.6352009107 -0.1131505656 0.076470058
 O 3.0267454849 -1.1484852042 0.8651474921
 C 3.1813448734 -0.2508284508 -1.3833394317
 C 1.6616641823 -1.2701028401 0.5499175418
 N 1.1587524747 -0.0102327251 -0.0235127944
 C 1.6439431807 1.1164499525 0.8178939895
 C 1.6816153456 0.1226029727 -1.4105354611
 H 4.7102503395 -0.2551587655 0.1782681391
 H 3.3472083935 -1.2804898006 -1.7157349928
 H 3.7663056598 0.4089117651 -2.0296936978
 C 0.7951560951 -0.6641591513 -2.3552498888
 C 1.2414422681 -1.1579833072 -3.5725111091
 C 0.3320160654 -1.8074757685 -4.4038337137

H 2.2762066816 -1.0336160749 -3.8730463264
 C -1.3565067778 -1.4220166138 -2.7587553824
 C -0.98778914 -1.9426849471 -3.9925608794
 H 0.6549159709 -2.2018539595 -5.3617362314
 H -2.3713327949 -1.4894133167 -2.379189826
 H -1.7246561043 -2.4417836989 -4.6108106198
 N -0.482273434 -0.7984829948 -1.9623775262
 H 1.5674382691 1.1808621803 -1.6739140181
 C 0.8336375004 -1.6379932425 1.7618653677
 C 1.3494001961 -2.3119911018 2.8551239162
 C -1.302354367 -1.6392814975 2.6423247454
 C 0.4727947972 -2.6611816101 3.8806196775
 H 2.405609184 -2.5506495592 2.8957883965
 C -0.871728936 -2.3265944992 3.7711756269
 H -2.3364051579 -1.3410113533 2.5006391326
 H 0.8388115739 -3.1906372742 4.7541908487
 H -1.5821519678 -2.5855701302 4.5475687849
 N -0.4614768651 -1.3008502226 1.6601590694
 C 0.7852311887 2.3324314228 0.5429522539
 C 1.2358196061 3.6374586683 0.6714267501
 C 0.331197295 4.6783232038 0.4706909777
 H 2.2679434131 3.8429329632 0.9338365338
 C -1.3600558192 3.0473424578 0.0378687356
 C -0.9866992788 4.3813340464 0.1491556733
 H 0.6567301955 5.7089070984 0.5673163534
 H -2.3745695673 2.7458493933 -0.2040928841
 H -1.7191735318 5.1632789905 -0.01321573
 N -0.4913425175 2.0507547846 0.2300993165
 H 1.4411964119 0.8170620893 1.8524081093
 H 1.5147514772 -2.0469923546 -0.2158031331
 Cu -0.9002563714 -0.0383078106 -0.0137898501
 Br -3.2345045564 -0.0539850117 0.00605957
 C 3.1720366592 1.2416151678 0.6345550099
 H 3.6551377703 1.4548497037 1.5905023627
 H 3.4387737234 2.0412369918 -0.0657409358

O_Br_Cu2+_4c

-2 2
 C 3.6428457934 0.0939606676 0.0062964753
 O 3.0818953385 1.3718664626 0.3002733306
 C 3.1759759481 -0.9430496204 1.0425698539
 C 1.6768836119 1.2359472474 0.5865640439
 N 1.1791897712 -0.0121025041 -0.0024012015
 C 1.6408198862 -0.1114558884 -1.4109198344
 C 1.665897517 -1.1669875693 0.7950209464
 H 4.7293995799 0.2298397927 0.0439830826
 H 3.3507403727 -0.557644256 2.053440287
 H 3.7427318619 -1.8752771825 0.9284953306
 C 0.788987092 -1.2851293901 2.0027904294
 N -0.5157999272 -0.9268839011 1.8459001854
 H 1.5294625935 -2.0353662005 0.1387518298
 C 0.848317673 2.3622204321 0.0611177094
 N -0.4673207943 2.0699593293 -0.1470860002
 C 0.7874359799 -1.1361893992 -2.0890223369
 N -0.5201776378 -1.1695876408 -1.7084265664
 H 1.4452993932 0.8807837086 -1.8319758249
 H 1.5593137096 1.1258612242 1.6739014726
 Cu -0.9394226441 0.0103658114 0.0029120703
 Br -3.4044582518 0.0495986997 0.008174599
 C 3.1697339273 -0.3399897926 -1.3925951332
 H 3.6578911639 0.2622605217 -2.1662009514

H 3.4150467296 -1.3949411588 -1.5710435349
 C -1.0538574403 3.2202460819 -0.5599177155
 C -0.1230542182 4.2538147644 -0.615914082
 C 1.1170297854 3.6950671305 -0.2111952201
 C -1.1164368432 -2.1283711059 -2.4597308204
 C -0.2012218764 -2.7129231062 -3.3292816279
 C 1.0416386383 -2.070660885 -3.0845432055
 C -1.1234427393 -1.1474186609 3.0380669272
 C -0.2183775618 -1.6528496272 3.9656943003
 C 1.0296136614 -1.7373843108 3.2940312354
 H -0.3097065495 5.2789187368 -0.9231311988
 H 2.0792142804 4.1887772033 -0.1319414321
 H -0.3982373407 -3.509376909 -4.0411149238
 H 1.9909605527 -2.2528656798 -3.5799205871
 H -0.4253954192 -1.9150770567 4.9992054681
 H 1.9745355138 -2.0943540356 3.6933482977
 H -2.1116754968 3.2290614983 -0.7964577226
 H -2.1697078454 -2.3435193044 -2.320028891
 H -2.1770177888 -0.9203541271 3.1539309355

O_Br_Cu2+_2b

1 2
 C 0.4587529446 3.6189755105 -0.4374683137
 C -0.0790821017 3.1554235678 0.9163782481
 C -0.5551719312 3.1843142568 -1.510070748
 C 0.136765339 1.6365072055 0.9337514482
 N 0.3467268596 1.1405367109 -0.4730425092
 C -0.6323889849 1.6405443177 -1.4756618456
 C 1.6557998433 1.6430430959 -0.9114716576
 H 0.6326761774 4.6931968792 -0.4721902954
 H -1.1359123411 3.4296698563 0.9971235094
 H 0.4565773688 3.6218070336 1.7462086192
 H -0.2383971634 3.5208806791 -2.4997120897
 H -1.5122122891 3.6675029058 -1.293544566
 C 2.7277083256 0.7917611013 -0.2667976183
 C 3.9594777017 1.2765849735 0.1219500958
 C 4.8851936258 0.3564513072 0.6174434727
 H 4.1882660878 2.3324618049 0.0389996908
 C 3.2810122442 -1.3804909336 0.2906169793
 C 4.5504652735 -0.9911983656 0.696355003
 H 2.9564950615 -2.4150660928 0.3374304707
 H 5.2556426185 -1.7235482445 1.0702641518
 N 2.3835212163 -0.5071076066 -0.1770260863
 H 1.7216363406 1.4735962114 -1.9963843385
 C -0.8430195646 0.7730576485 1.701191101
 C -1.7936055 1.2735718256 2.5751463394
 C -1.3804346268 -1.4074003525 2.2282917156
 C -2.5616653923 0.3580428882 3.2968028209
 H -1.9422320688 2.3372178738 2.716146884
 C -2.3563548127 -1.0056420189 3.1329023053
 H -1.1816965362 -2.4583080762 2.0370137546
 H -2.937420146 -1.7335709758 3.6861452079
 N -0.6433935369 -0.5413069939 1.5349201507
 H 1.1006943942 1.4479007316 1.4185165245
 H -0.2488022363 1.2680569072 -2.4323084567
 C -1.9196677346 0.8697574404 -1.2941560023
 C -3.1943070364 1.3970465312 -1.3475673436
 C -4.2712252962 0.5113254119 -1.2550588943
 H -3.3668469386 2.4598043133 -1.4687108677
 C -2.7218130195 -1.2888225131 -1.0817726478
 C -4.0405979999 -0.8520763273 -1.1305899165

H -2.4713762911 -2.3401106455 -0.9748524259
 H -4.8596445457 -1.5584657933 -1.0708773578
 N -1.688307687 -0.4508261792 -1.155926143
 Cu 0.325825649 -0.9094784195 -0.4538532375
 Br 0.326721914 -3.2159212482 -0.6661160147
 O 1.7555558672 3.0176421207 -0.6410572246
 Cl -3.766771206 0.9331814887 4.3905703699
 Cl -5.8831460997 1.1230717929 -1.3016221387
 Cl 6.4406682338 0.897096395 1.1258898769

O_Br_Cu2+_2e

1 2
 C 0.6568309053 3.3044691993 -0.7740626432
 C 0.0856524195 2.9936522409 0.610310081
 C -0.3378859524 2.7659036129 -1.8187839656
 C 0.2709100509 1.4819536739 0.7960182856
 N 0.5143597028 0.8476541424 -0.5512143428
 C -0.4541297172 1.2381052429 -1.6060154857
 C 1.8346136455 1.2796244297 -1.0137265965
 H 0.8396331128 4.3685344337 -0.9198125217
 H -0.9637580589 3.3027912244 0.6411032771
 H 0.6173474453 3.5344822677 1.3964246662
 H 0.0167919096 2.9787518122 -2.8300390384
 C 2.8748236314 0.4751933132 -0.265886703
 C 4.0928095845 0.9806593959 0.1086421953
 C 5.0374682609 0.1179111874 0.7248542096
 H 4.2994279437 2.025559766 -0.0818946567
 C 3.3799525274 -1.6313535166 0.4992297893
 C 4.6337933899 -1.2279584073 0.9016994646
 H 3.0449700585 -2.6545286958 0.6359395106
 N 2.493546676 -0.8057316501 -0.0775391081
 H 1.9120913653 1.0013986534 -2.0754006334
 C -0.752038345 0.6805248277 1.5826428566
 C -1.9814842505 1.1547483271 1.9847612971
 C -1.1539553109 -1.3896261716 2.4695325053
 C -2.8822316365 0.2788757458 2.6395923311
 H -2.2701004013 2.1723673327 1.7621251734
 C -2.4080817029 -1.0209379777 2.9153518107
 H -0.7919933705 -2.4027360038 2.6199724915
 H -3.0146566957 -1.7505435827 3.4353948628
 N -0.3338933187 -0.5764614374 1.7980082782
 H 1.2134398784 1.3220801822 1.3261641081
 H -0.092231907 0.7393935378 -2.512580478
 C -1.7545796603 0.5388685844 -1.2803485079
 C -3.001784848 1.1098840279 -1.3480281545
 C -4.1356118817 0.3500157037 -0.9647436419
 H -3.1023834855 2.140694779 -1.6606355058
 C -2.6080952966 -1.4822981297 -0.5948107634
 C -3.8974460398 -0.9914333147 -0.5953074713
 H -2.3963319046 -2.5099689013 -0.3158519701
 H -4.7042656222 -1.6551853192 -0.3147165594
 N -1.5404255758 -0.7427573366 -0.915359538
 Cu 0.4693712226 -1.1883142422 -0.3163024145
 Br 0.4036139819 -3.5161618551 -0.3322164034
 O 1.950085567 2.6781676998 -0.8879097973
 N -4.1468110515 0.6674886507 2.9583913968
 H -1.2891427475 3.2905557123 -1.6902586966
 H 5.2885223967 -1.9599926828 1.3550490294
 N 6.2534444468 0.5614949729 1.1164181948
 N -5.378102413 0.8968570515 -0.9349525285
 C -6.501336672 0.1126167826 -0.4495313544

H -6.308328395 -0.2556779093 0.5654097881
H -7.3907578585 0.7413046032 -0.4160959727
H -6.7125296038 -0.7440376874 -1.1007568135
C -5.0564211981 -0.2800452289 3.5786080286
H -4.6673794609 -0.6335345847 4.5398503597
H -6.0123365956 0.2085837819 3.766928058
H -5.234589089 -1.1512137759 2.9338825766
C -5.5978366544 2.2447952923 -1.4310136576
H -6.6634317329 2.4696636454 -1.3992518747
H -5.0767286989 2.9930628433 -0.8193018369
H -5.264259053 2.3469350198 -2.4701061866
C 6.6287491946 1.9498707336 0.8997618757
H 6.6229442945 2.2038727261 -0.1667645471
H 5.9544351849 2.6325211304 1.4299884939
H 7.6370638298 2.1112973658 1.2790484879
C 7.1990953717 -0.3559978769 1.734238607
H 6.793173509 -0.7809361192 2.6593963546
H 7.4633217726 -1.1742073173 1.0542830551
H 8.111541482 0.1843908765 1.9834456875
C -4.6339856556 1.9699166572 2.5450782056
H -5.6700938528 2.0835170255 2.8638987293
H -4.0550459637 2.7808154212 3.0025540675
H -4.5986930833 2.0820740877 1.4525721791

O_Br_Cu2+_2a

1 2
C 0.4578797031 3.5970472535 -0.4920862671
C -0.0901839454 3.1575095251 0.8657054588
C -0.5447215874 3.1416444785 -1.5658469678
C 0.1335873474 1.6404724331 0.9125142111
N 0.3501169261 1.1152859589 -0.4833623337
C -0.6237865791 1.5989613963 -1.5012263697
C 1.6608012982 1.6159727047 -0.9260776322
H 0.6324106835 4.6701814931 -0.544924834
H -1.1489360957 3.4279158635 0.9336183211
H 0.4361248699 3.6416133656 1.6912301614
H -0.2177374159 3.4576189162 -2.5588372739
H -1.5038968402 3.6292068202 -1.3699896307
C 2.735940218 0.7801167872 -0.266770087
C 3.9689663153 1.2743929599 0.1126287066
C 4.8756276715 0.3519016322 0.6156155238
H 4.2161922395 2.3249897701 0.0216048527
C 3.2944687627 -1.3893561498 0.328081438
C 4.5676262549 -0.9910076893 0.7250400072
H 2.9679927659 -2.4221831036 0.3916345324
H 5.2889456072 -1.69974794 1.1121141009
N 2.4011797771 -0.5192563569 -0.1502967024
H 1.7299633094 1.4299068634 -2.0083145214
C -0.8444289954 0.7915936004 1.6963085931
C -1.7834448292 1.3072302785 2.5755249126
C -1.3812452551 -1.3886927889 2.2623613108
C -2.527434139 0.3918639699 3.3072320125
H -1.9460685322 2.3682061538 2.7167116886
C -2.3438613615 -0.9707185158 3.1783869805
H -1.1839740584 -2.4412109556 2.0806004593
H -2.9274056912 -1.672885331 3.7605074162
N -0.6578920987 -0.5278983255 1.5494829737
H 1.0967293221 1.4667237034 1.4049526693
H -0.2371372533 1.2062894639 -2.448683929
C -1.9157650115 0.8392218424 -1.3125026806
C -3.1891567555 1.3701838844 -1.3864547511

C -4.2485612742 0.4767527825 -1.2882682407
H -3.381098853 2.4269300822 -1.5239902094
C -2.7279771371 -1.3208926462 -1.0695756739
C -4.0484726896 -0.8807051918 -1.140888983
H -2.4777486195 -2.3698078426 -0.9426398464
H -4.8837179194 -1.5670734667 -1.0800813831
N -1.6978124088 -0.4810548139 -1.1466254673
Cu 0.3313078803 -0.9298999428 -0.4253098153
Br 0.3284760694 -3.2323900739 -0.5854650484
O 1.7573588854 2.9911477464 -0.6723447173
N -5.6306568143 1.0070048342 -1.3455583131
O -6.5322062469 0.1967218515 -1.2678951737
O -5.7471068849 2.2133739195 -1.460177357
N -3.5494716786 0.902153885 4.2501479911
O -4.1766122896 0.0741294748 4.880270714
O -3.6801404756 2.1110651868 4.3126390442
N 6.2113188741 0.8271466339 1.047108985
O 6.4216862877 2.0213610871 0.9496354385
O 6.982628668 -0.0138174679 1.4645557059

O_Br_Cu2+_2c

1 2
C -0.8048137732 -3.3374273475 -0.5643341068
C -0.2892912387 -2.7438472623 0.7461778024
C 0.1860077808 -2.9459475739 -1.6762035912
C -0.5432406688 -1.2337109437 0.638415288
N -0.8022902191 -0.8740994598 -0.804475487
C 0.2015837765 -1.4018026413 -1.7637094382
C -2.0896917444 -1.4629280528 -1.1851741847
H -0.9273731142 -4.4182695327 -0.5117072549
H -0.1227223873 -3.3722987262 -2.6333590766
H 1.1629828658 -3.3723553435 -1.4307145157
C -3.1864374805 -0.6048643875 -0.5939036079
C -4.376352781 -1.1070649913 -0.1230678153
C -5.3527119809 -0.2028263427 0.3300590904
H -4.5219051547 -2.1793899014 -0.0861746286
C -3.8209842989 1.5735107875 -0.1992888368
C -5.0551331498 1.1649561404 0.2718935501
H -3.5498665047 2.6228489944 -0.252310713
H -5.7811182994 1.9114635748 0.5675359508
N -2.8915698431 0.7100116923 -0.6260918234
H -2.1711713869 -1.3815087482 -2.2795912943
C 0.4456924131 -0.2596904078 1.2515262957
C 1.6791309883 -0.6025087506 1.7682548544
C 0.7742089569 1.966171742 1.7130509167
C 2.519745994 0.4184240932 2.236566661
H 2.0083269671 -1.632603195 1.8121468941
C 2.0356555365 1.7279322393 2.236869172
H 0.3808789568 2.9760753826 1.6429048458
H 2.6463121476 2.5546105339 2.5790128068
N 0.0008198719 1.0048382261 1.2074451952
H -1.4936380884 -1.0153794232 1.1327807473
H -0.1822480665 -1.1154678316 -2.7498279159
C 1.4523121737 -0.5680999554 -1.5979299973
C 2.7411275567 -1.0500653569 -1.5602123646
C 3.8016424532 -0.1413117195 -1.399230923
H 2.9299258519 -2.1150911079 -1.6090410411
C 2.1663902585 1.6131200695 -1.3790270249
C 3.4925231082 1.2199117579 -1.3255867375
H 1.8802314921 2.6587762638 -1.3201726848
H 4.2691689845 1.9699741582 -1.2480367697

N 1.1589348541 0.7451695011 -1.5025712952
 Cu -0.8834576594 1.1656819346 -0.9628295293
 Br -0.965457285 3.4448299019 -1.380766841
 O -2.1275998359 -2.8173399905 -0.8110190683
 N 5.1098152622 -0.5901145217 -1.3000379572
 N -6.5664494683 -0.6560941367 0.8180410893
 N 3.8130942919 0.1230577144 2.6560373823
 C 6.1549395858 0.0880338947 -0.6833556483
 C 5.5933502302 -1.8106434628 -1.7619054207
 C 6.9163945219 -1.889765188 -1.4482148222
 C 7.269692435 -0.689908733 -0.7552551811
 C -7.4148188632 0.0431622825 1.6715012613
 C -7.1482937517 -1.889840139 0.5401428804
 C -8.3361684226 -1.9588984662 1.2004963145
 C -8.500162746 -0.7370924364 1.9266551744
 C 4.591256439 -0.9280670484 2.1878489319
 C 4.5681489003 0.8590660322 3.5577667769
 C 5.8149124844 -0.851103989 2.783501445
 C 5.7965954259 0.2754264751 3.6613353537
 H 5.9895556325 1.0273040387 -0.1793538164
 H 4.9726026328 -2.4732210361 -2.345012037
 H 7.5753863616 -2.7075531721 -1.7021243255
 H 8.2379908153 -0.4400509105 -0.3465515553
 H -7.1393467097 1.0092796168 2.064531442
 H -6.6917571925 -2.579350503 -0.1526393576
 H -9.0292941616 -2.7868708242 1.1645800869
 H -9.3262548976 -0.4747147403 2.5715726853
 H 4.2292786008 -1.59025024 1.4157433495
 H 4.1379189854 1.6927896563 4.0915037613
 H 6.6455207741 -1.5162906284 2.5976905661
 H 6.5973846094 0.6053524386 4.3073033927
 H 0.7700258833 -2.9932663288 0.8582971448
 H -0.8212156863 -3.1511236449 1.6086195793

O_Br_Cu2+_2f

1 2
 C 0.7770266196 3.2673942062 -0.5657208826
 C 0.4439794607 3.0028567098 0.8999419298
 C -0.4065664446 2.7640549562 -1.4174006259
 C 0.5025829083 1.4767324917 1.0721688728
 N 0.5724169909 0.8219639189 -0.2867949242
 C -0.4871085626 1.2313249795 -1.2379185911
 C 1.8488024234 1.1887497911 -0.9000014268
 H 0.9749140069 4.3209641385 -0.7605260498
 H -0.5368155681 3.4266202756 1.1329978564
 H 1.1740928029 3.4786476935 1.5584840087
 H -0.2607713622 3.0155060558 -2.47039939
 H -1.3116948813 3.2773305377 -1.077130807
 C 2.9349746873 0.3934322142 -0.2090294799
 C 4.1936408276 0.8788636964 0.0288305555
 C 5.1665079501 0.0143017249 0.5973036851
 H 4.4205692269 1.9030836785 -0.2390363725
 C 3.4528689613 -1.6918787287 0.6125313978
 C 4.7474437155 -1.3085775222 0.8805278856
 H 3.1029061242 -2.6952262991 0.8326632191
 H 5.4237353015 -2.0278422743 1.3242891806
 N 2.5398044208 -0.8669460484 0.0753316384
 H 1.8173994246 0.8468659914 -1.9449022807
 C -0.5366098207 0.7636407649 1.9151610406
 C -1.7536779392 1.2986699887 2.2722842897
 C -1.0372591925 -1.25887195 2.8604513433

C -2.7086663574 0.470856762 2.9094080383
 H -2.0015881098 2.3222624168 2.0249304745
 C -2.2925667066 -0.8338052777 3.2483792564
 H -0.7149714511 -2.2771208337 3.0589697204
 H -2.9523397468 -1.5205062898 3.763884825
 N -0.1704168375 -0.5003438577 2.1809799653
 H 1.4605839818 1.2196237798 1.5292966073
 H -0.1929253129 0.7687726529 -2.187431068
 C -1.7614178512 0.5076780104 -0.8618732791
 C -3.0244369469 1.037897854 -0.9752578338
 C -4.1470788415 0.2343778834 -0.6521759483
 H -3.1527508029 2.055792489 -1.3220890831
 C -2.5751531926 -1.530677627 -0.1697615027
 C -3.8785460613 -1.0869432564 -0.2328864848
 H -2.3375416873 -2.5428923624 0.1422414339
 H -4.6768746427 -1.7624467909 0.0468184964
 N -1.520746293 -0.7638964798 -0.4782033628
 Cu 0.4982134374 -1.2092466434 0.0025779114
 Br 0.4009461795 -3.5383745249 0.0743150502
 O 2.0083574583 2.5896797181 -0.8816260248
 N 6.4185011615 0.4345903294 0.8484786186
 C 7.4871878837 -0.4392967549 1.3375915085
 C 6.8711181572 1.8123831948 0.6487349963
 N -5.407764299 0.712832739 -0.7415265684
 C -5.7279336662 2.0708346465 -1.1793907091
 C -6.5988508636 -0.1318992001 -0.624184693
 N -3.9660312286 0.9087011397 3.1489256235
 C -4.9987880554 0.0789468522 3.7635317651
 C -4.4993875555 2.156030754 2.6079332969
 C -6.0153064654 1.9700940592 2.7022642272
 C -6.1847475329 1.0340474051 3.9024095897
 C -7.2465666948 2.1553266761 -1.0157698179
 C -7.7083705516 0.7142110194 -1.2548544916
 C 8.7495426356 0.4073636345 1.1616429071
 C 8.2394666139 1.84139766 1.3331945144
 H 7.524293982 -1.3664043138 0.7566499314
 H 7.3151715471 -0.6999826514 2.3905807107
 H 6.1666902593 2.5203217286 1.0977962712
 H 6.9483549783 2.0382762516 -0.4235692556
 H -5.4267206437 2.2200739869 -2.2259434461
 H -5.2028129306 2.8118095319 -0.5655491315
 H -6.8065806812 -0.3610193641 0.4303634628
 H -6.4536337065 -1.0795275153 -1.1527541717
 H -4.6630538898 -0.3120963102 4.729238968
 H -5.2403991129 -0.7763161496 3.1142549169
 H -4.168507979 2.2974154259 1.5718606186
 H -4.1560431311 3.0168681473 3.1976227274
 H -6.375144641 1.4786473214 1.7922748705
 H -6.5474602178 2.9176502118 2.8127676027
 H -7.1420909785 0.508673834 3.907548068
 H -6.1025086518 1.5977060735 4.8373727566
 H -7.695245991 2.8683335974 -1.7103150073
 H -7.4977742875 2.4740870193 0.0011634178
 H -7.763315766 0.509766813 -2.3288926319
 H -8.6876267563 0.5008716172 -0.821703227
 H 9.1538401644 0.2671670958 0.1537375552
 H 9.5282737681 0.1399667461 1.8786251164
 H 8.9037568481 2.5890049619 0.8950883646
 H 8.1186059811 2.075673172 2.39605748

O_Br_Cu2+_2d

1 2

C 0.3075545555 3.6325848143 -0.4198444412
C -0.2150112773 3.1480401652 0.9329323787
C -0.6910230048 3.1656128427 -1.4931012392
C 0.0564206495 1.6382362297 0.9488765989
N 0.2806959161 1.1530825864 -0.4594304063
C -0.7128145085 1.6200603048 -1.4635352544
C 1.5729044383 1.6987723303 -0.8954809473
H 0.4437920013 4.7124852086 -0.4523237924
H -1.2818489794 3.380874723 1.0138944326
H 0.3022028298 3.6331504508 1.7639024923
H -0.387565661 3.5174196046 -2.4817376128
H -1.6650812785 3.6120708601 -1.2732529683
C 2.6734316472 0.8854762226 -0.2509078361
C 3.8960893267 1.4001160997 0.135372748
C 4.8524514958 0.5140147385 0.6307196835
H 4.0869206794 2.4633580478 0.046237338
C 3.2900108023 -1.2724985177 0.3112119102
C 4.5491464272 -0.8390961286 0.7120990311
H 5.8244979196 0.8799766622 0.9445766853
H 2.9899473833 -2.3143374589 0.3587736519
H 5.2701734775 -1.5570701025 1.0849474587
N 2.3698710161 -0.4237841256 -0.1567400107
H 1.644221886 1.535347273 -1.9808924917
C -0.8864742374 0.7430975152 1.72529688
C -1.8257049539 1.2031241149 2.6359911997
C -1.3523978157 -1.4604771713 2.240902635
C -2.5490367259 0.2661958856 3.3738873956
H -1.9896984995 2.2640278526 2.7866037307
C -2.3097497308 -1.0871026328 3.1791889292
H -1.1279706628 -2.5017966678 2.0264159873
H -3.288821333 0.5971414967 4.0955771768
H -2.8503671992 -1.8429580144 3.7370312348
N -0.6590845203 -0.5644473716 1.540459089
H 1.0301904669 1.4872611628 1.4272683186
H -0.3091612803 1.2666842251 -2.4192616023
C -1.9748624794 0.8061218895 -1.2967283691
C -3.2712361509 1.2784978453 -1.3820132413
C -4.3190488298 0.3585078589 -1.3161849681
H -3.4711213797 2.3362176458 -1.5114359101
C -2.6988134133 -1.3846433755 -1.0939920171
C -4.0314887077 -0.9914025236 -1.178057154
H -5.3471381771 0.6994042674 -1.3815466451
H -2.4052839492 -2.4235176271 -0.9766555998
H -4.8183444577 -1.7353701451 -1.13544288
N -1.6992754274 -0.5053725728 -1.1500148518
Cu 0.3247644347 -0.8943634538 -0.4418931719
Br 0.4117516856 -3.2006580629 -0.6744547087
O 1.6240856018 3.077875028 -0.624008866

O_Br_Cu2+_3b

1 2

C 0.1783654188 3.6386972088 -0.3063032886
C 1.6274290798 3.2380617108 -0.6463028304
C -0.8574692594 3.1492446108 -1.3247474947
C 1.6435094159 1.7119512846 -0.9106132845
N 0.3395501845 1.1669045726 -0.4558851273
C 0.1165997196 1.670521783 0.9319286968
C -0.6984516113 1.6142867434 -1.4235086153
H 0.1029448173 4.714487659 -0.1509363052
H 2.2574077311 3.5081191284 0.207062615

H 1.9870744446 3.7936011266 -1.5159810243
H -0.722492646 3.6197851432 -2.3023632373
H -1.8407781751 3.4366748456 -0.9438782265
C 2.7405707878 0.8629376819 -0.3003934239
C 4.0136822844 1.3378552138 -0.0435322884
C 3.3229889797 -1.2799526445 0.3619634481
C 4.9672827463 0.4407442553 0.4394146605
H 4.2733220094 2.3752898455 -0.2199033514
C 4.6233635496 -0.8894924041 0.6460228685
H 2.9923329659 -2.3044604357 0.4974435543
Cl 6.565292646 0.9914968795 0.7746094594
H 5.3442746233 -1.6071846807 1.018039186
N 2.4019361472 -0.4265452126 -0.0989507342
C -0.9245775165 0.8548171298 1.6643594541
C -2.0024709213 1.415607235 2.3228773767
C -2.856960899 0.5424800085 2.9969771123
H -2.1661808511 2.4859112231 2.3137274565
C -1.4894081186 -1.2786552261 2.2925889067
C -2.6004041822 -0.8240752264 2.9950611602
Cl -4.2353217614 1.1670525272 3.8281071426
H -1.2523275295 -2.3369867623 2.2318273232
H -3.2484018608 -1.5168741539 3.5185011834
N -0.6679472311 -0.4570794496 1.6399031387
H 1.0705279513 1.5009443638 1.4523049527
H 1.6924199005 1.5297692194 -1.9899079139
H -0.2767404297 1.3733104635 -2.405921339
C -1.9016300226 0.7022871757 -1.3131866145
C -3.2088227793 1.1089899822 -1.5032979756
C -4.2086266044 0.1351486107 -1.4871487334
H -3.461198348 2.1491556378 -1.669634552
C -2.5346708669 -1.5153991253 -1.1169373349
C -3.8737738333 -1.1996091007 -1.3001619837
Cl -5.8548303258 0.5995722879 -1.7044270987
H -2.2051693535 -2.5372702129 -0.9572347365
H -4.6296947739 -1.9753441571 -1.2940146449
N -1.5727625993 -0.5894432733 -1.1197584488
Cu 0.3874725126 -0.8938974361 -0.3671196926
Br 0.495191553 -3.2149872051 -0.4696550847
O -0.1902069688 3.0349511486 0.9361756895

O_Br_Cu2+_3e

1 2

C 0.3548029294 3.3771502692 -0.6150243213
C 1.8101574733 2.9267356623 -0.852606385
C -0.6389794245 2.7868902762 -1.6222474401
C 1.8068961151 1.3834896913 -0.9688548265
N 0.4890814823 0.9108369856 -0.4848496732
C 0.2400885729 1.5637993203 0.8375267542
C -0.5319098514 1.2468032445 -1.5101753134
H 0.288905891 4.4649593854 -0.5850101689
H 2.4106156506 3.2657212733 -0.0024509533
H 2.2139285372 3.3929329459 -1.7552561588
H -0.4302764893 3.1223619381 -2.6422545379
H -1.6322106483 3.1482671307 -1.3441778956
C 2.8743967701 0.5751584974 -0.2573757629
C 4.1386319218 1.0586927532 -0.0146093994
C 3.4063835015 -1.4925575441 0.6089163199
C 5.1129474507 0.2165621919 0.5818405756
H 4.3775555422 2.0760995274 -0.296151848
C 4.6947632288 -1.0998170582 0.8888083949
H 3.0626021773 -2.4966214413 0.8342541081

H 5.3649414786 -1.8163758992 1.3440861825
 N 2.4942970241 -0.684463156 0.045207555
 C -0.8125705157 0.8062081059 1.6147734857
 C -2.0725348612 1.3035582254 1.8491401526
 C -3.0328199619 0.455081715 2.4498637433
 H -2.3060739353 2.3082703453 1.5246815077
 C -1.2826712577 -1.2039019752 2.5711748381
 C -2.5818976333 -0.8230796744 2.8479449281
 H -0.9358120103 -2.2010322575 2.8268067322
 H -3.2394291699 -1.5285983124 3.338831676
 N -0.397522077 -0.4239524042 1.9421446844
 H 1.1841077825 1.4613654953 1.3883894163
 H 1.8655172267 1.0985311574 -2.0254631281
 H -0.1210732154 0.854709506 -2.4476172277
 C -1.764182099 0.4047860625 -1.2486342238
 C -3.0502977661 0.8327087889 -1.4805413723
 C -4.1374394408 -0.0346541186 -1.2099828839
 H -3.219569662 1.8353003876 -1.8489109748
 C -2.4835209651 -1.6777562661 -0.5874240881
 C -3.8061762812 -1.3304433366 -0.7557797888
 H -2.2000996279 -2.6686036621 -0.2472659134
 H -4.5654124752 -2.070995346 -0.5431233522
 N -1.465426237 -0.8381008191 -0.8200293518
 Cu 0.5009263813 -1.1278529891 -0.172610387
 Br 0.5423179634 -3.4645488592 -0.073670605
 O -0.0777343014 2.9194908765 0.6670772066
 N 6.3675051784 0.6509346184 0.8401072011
 N -5.4237160057 0.3675981498 -1.3700186755
 N -4.3275329699 0.8442729328 2.6042872169
 C -5.7166438192 1.6674939372 -1.9497889266
 H -6.7962536288 1.7889525563 -2.0313945235
 H -5.3347957795 2.4829374391 -1.322951401
 H -5.287966365 1.7668196698 -2.9544060214
 C -6.5109815084 -0.5531398828 -1.0797363409
 H -6.4642678308 -0.8987237478 -0.0405814435
 H -7.462439538 -0.0408604144 -1.2194869927
 H -6.4919432192 -1.4269521853 -1.7422878391
 C 7.3386342956 -0.2493254315 1.4446540384
 H 7.006039812 -0.5875287646 2.4326826616
 H 7.5168195019 -1.1255536858 0.8108924811
 H 8.2849692705 0.2757995367 1.5683689567
 C 6.7544602397 2.0120879596 0.5065790955
 H 6.6751820788 2.1984970844 -0.5712216652
 H 6.1370884185 2.7443438354 1.04053805
 H 7.7914424757 2.1719069467 0.7992376931
 C -4.7692929976 2.1092914102 2.0487575133
 H -5.8344021806 2.235333498 2.2429664271
 H -4.2436154664 2.9532323543 2.509183481
 H -4.6096311969 2.1475595042 0.9619797207
 C -5.3049866993 -0.0972925258 3.1189594255
 H -5.047590793 -0.4220711627 4.1330110955
 H -6.2813428685 0.3852304813 3.1637497393
 H -5.3860635982 -0.9869007531 2.4789187526

O_Br_Cu2+_3a

1 2
 C 0.1800800188 3.6222784529 -0.3628374453
 C 1.6313791965 3.2154672326 -0.6847041477
 C -0.8480178358 3.1142475273 -1.3793448911
 C 1.6486078717 1.6850434536 -0.9244838087
 N 0.342758396 1.1444887382 -0.4651433579

C 0.1145991631 1.6786448196 0.9120091456
 C -0.6893429339 1.5774326968 -1.4474286754
 H 0.1029446399 4.7001181284 -0.22554206
 H 2.2567465612 3.4998537531 0.167431785
 H 1.9975838324 3.755804879 -1.5610002896
 H -0.7044946145 3.5649095975 -2.3648701241
 H -1.8346528702 3.4098709751 -1.013753705
 C 2.7463822994 0.8506602504 -0.2975105593
 C 4.0199370425 1.332127298 -0.0479801394
 C 3.3309042646 -1.2872179586 0.4056274197
 C 4.9517804461 0.4328602601 0.4483541894
 H 4.3002742842 2.3620212618 -0.2329614555
 C 4.6345123049 -0.8900290857 0.6837538283
 H 2.9974645855 -2.308207932 0.5579624736
 H 5.3705833739 -1.5842222982 1.0692463222
 N 2.4159345304 -0.4372307172 -0.0699330791
 C -0.9250858418 0.8792492708 1.6640665069
 C -1.9885013223 1.4563241128 2.3349477533
 C -2.8152720023 0.5853345827 3.0307363341
 H -2.165623134 2.5239825862 2.3235537788
 C -1.4894458956 -1.2499588928 2.3377843698
 C -2.5836718239 -0.7775705897 3.0599396592
 H -1.2547928234 -2.3089229246 2.2856980354
 H -3.2341330158 -1.4418431147 3.6150781478
 N -0.6841628488 -0.436089583 1.6572775453
 H 1.0682670392 1.5223515097 1.4381311208
 H 1.7023126174 1.4854135982 -2.00051685
 H -0.2628144005 1.3169946808 -2.4228901059
 C -1.8965421475 0.672981773 -1.3299664385
 C -3.2017056953 1.0786101642 -1.5449826802
 C -4.1807103195 0.0955933382 -1.5229416266
 H -3.4739607395 2.1094290166 -1.733573845
 C -2.5364814985 -1.5480248418 -1.1008715703
 C -3.8758054393 -1.233842158 -1.3109080278
 H -2.206472553 -2.5657564789 -0.9183401616
 H -4.6474545489 -1.9933398521 -1.3062219338
 N -1.5803740834 -0.6177620405 -1.1073138142
 Cu 0.39076857 -0.9095029862 -0.3353421847
 Br 0.4901112473 -3.2246446132 -0.3769265922
 O -0.1989086679 3.0380621348 0.8876032739
 N -3.9838138653 1.1370776874 3.7542021027
 O -4.668399098 0.3473847686 4.3750570878
 O -4.1672541895 2.3366836299 3.6617387068
 N -5.591618937 0.4939540087 -1.7377917911
 O -6.4217194618 -0.3921774713 -1.7017703004
 O -5.8007681207 1.6775041021 -1.929443395
 N 6.3239940279 0.9152867733 0.7316762194
 O 6.5442802209 2.0915693305 0.5097189106
 O 7.112614194 0.0984371456 1.1626203392

O_Br_Cu2+_3c

1 2
 C -0.6410690623 -3.3591217076 -0.0452078962
 O -0.2759075286 -2.5794635232 1.0952331571
 C 0.38090428 -3.0070272868 -1.1325879165
 C -0.6159823506 -1.2342776567 0.9060283117
 N -0.8383479248 -0.9412788161 -0.5451007726
 C 0.2259470332 -1.4952656831 -1.4244228579
 C -2.1272006943 -1.5658656821 -0.929216127
 H -0.5495988752 -4.4009747259 0.261128478
 H 0.2285994448 -3.5982595285 -2.0398158795

H 1.3693811839 -3.2504029087 -0.7351073508
 C -3.2404169304 -0.6464860185 -0.4675543172
 C -4.502704506 -1.0943095687 -0.1407792149
 C -5.4929413705 -0.1601904559 0.206400514
 H -4.7171136405 -2.1559283071 -0.1299071114
 C -3.8505713035 1.5558798594 -0.1272714477
 C -5.1416036882 1.1944417715 0.2055038103
 H -3.5390665982 2.5947991857 -0.148835362
 H -5.8674385254 1.965469566 0.4300959315
 N -2.9109239083 0.6616093849 -0.4610533083
 H -2.1600016971 -1.5519876162 -2.0246622497
 C 0.4194079191 -0.2931198732 1.477485737
 C 1.6787934392 -0.7046259547 1.8569009676
 C 0.8775678525 1.903806002 1.8881314028
 C 2.6141498895 0.2794117239 2.2054860715
 H 1.9269939451 -1.7579051023 1.8501081929
 C 2.181950037 1.6090476372 2.2552962333
 H 0.5248642719 2.9306478777 1.8683564485
 H 2.8604470119 2.4125584597 2.5142427753
 N 0.0093924379 0.9793455232 1.471043608
 H -1.5722792148 -1.0092146724 1.3960958393
 H -0.1652345286 -1.3741779537 -2.4410960229
 C 1.4229501106 -0.5672062374 -1.3675822107
 C 2.7364007391 -0.9827311334 -1.4099103943
 C 3.7596707606 -0.0216511142 -1.364754583
 H 2.9756407808 -2.0380787929 -1.4254424295
 C 2.0462853532 1.6536433547 -1.3077798368
 C 3.3885207692 1.3263251543 -1.3352128301
 H 1.7130738836 2.6860147691 -1.2776424182
 H 4.1293325141 2.1153369117 -1.3495552671
 N 1.0746312468 0.7337113972 -1.3131577697
 Cu -0.9181512574 1.1039906009 -0.770321105
 Br -1.0350647358 3.3848205231 -1.221156452
 C -2.0958417094 -3.0322808787 -0.4347416327
 N 5.0914679759 -0.4018205475 -1.3329220908
 N -6.7714228617 -0.5733660886 0.5412091125
 N 3.9414280516 -0.0639391778 2.4413436422
 C 6.1368942718 0.3591059665 -0.8229265434
 C 5.6053124893 -1.6247644878 -1.7508890547
 C 6.9477744102 -1.6232076502 -1.5201858104
 C 7.2827517894 -0.3683766995 -0.9224318252
 C -7.6770815176 0.1370512759 1.323343501
 C -7.3713858355 -1.7691751948 0.1573677382
 C -8.6263262862 -1.8040856865 0.6830852637
 C -8.8159866106 -0.6000430758 1.4319455003
 C 4.5811255995 -1.1895712032 1.9360126391
 C 4.8748846802 0.6901246009 3.1387099357
 C 5.8908214844 -1.1414161225 2.3065209591
 C 6.0754314156 0.0463249863 3.0785089577
 H 5.9549390828 1.3155021084 -0.3584910205
 H 4.9841444467 -2.3504657308 -2.2526539148
 H 7.6297938355 -2.4235872912 -1.7689006728
 H 8.2601850437 -0.0506815056 -0.5897010512
 H -7.4033354391 1.0756956471 1.7794317697
 H -6.874228642 -2.453585459 -0.5123633874
 H -9.346797894 -2.5966066086 0.5413569773
 H -9.6952128988 -0.3207187635 1.994129088
 H 4.0596610388 -1.8915935958 1.3044420969
 H 4.5848529122 1.5833434483 3.6702483572
 H 6.646564318 -1.8643939781 2.0367657934
 H 6.9900966041 0.3759803355 3.5498510223

H -2.4516290704 -3.7189325306 -1.2071116801
 H -2.7196772476 -3.1737654754 0.4534519819

O_Br_Cu2+_3f
 1 2

C 0.4101887121 1.4082441755 4.7481573948
 C -1.0102223526 0.8407789836 4.9432064699
 C 1.4567639197 0.3439746717 4.3946986809
 C -1.3461337665 -0.0187221502 3.7003243193
 N -0.3121825412 0.264724701 2.678423972
 C -0.2224062062 1.7502152603 2.5329095639
 C 0.9593232778 -0.3669712178 3.1142269294
 H 0.7155441688 1.9864102611 5.6206431785
 H -1.6965457014 1.6874160922 5.0439798615
 H -1.0675442125 0.2509769452 5.8619583271
 H 1.6020281953 -0.3701761099 5.2104273507
 H 2.4027190875 0.8664480876 4.2287752693
 C -2.6996773998 0.1235814492 3.031773197
 C -3.8362075802 0.4872679257 3.7136516662
 C -3.8731542261 -0.192367506 1.0711288416
 C -5.0825592467 0.5164405289 3.0352548064
 H -3.7761798006 0.7229987254 4.7691215622
 C -5.0620885033 0.1566717806 1.6670047433
 H -3.8279958005 -0.4700484263 0.0233319403
 H -5.9648405965 0.1633828235 1.0699515466
 N -2.6988986922 -0.2155286829 1.7238770413
 C 0.4673760999 2.0986435056 1.2352188629
 C 1.7471599141 2.5959854329 1.186796645
 C 2.385243344 2.6838968453 -0.0721464498
 H 2.2513624228 2.8571652006 2.1077679965
 C 0.3093677641 1.9147534927 -1.0282817179
 C 1.6006410495 2.3732193455 -1.2048170695
 H -0.2923899289 1.6219727654 -1.8839688204
 H 2.0057822854 2.4459866337 -2.2065393822
 N -0.2610470197 1.7407125878 0.1697469276
 H -1.2611143706 2.0962216002 2.4599523199
 H -1.2444132149 -1.0801448918 3.9532249894
 H 0.6792417882 -1.3944029813 3.3738128912
 C 1.8692047829 -0.5184035952 1.9116526854
 C 3.2417936238 -0.4563231083 1.9774713928
 C 4.0082530379 -0.6679580541 0.8046177678
 H 3.7262804053 -0.228587029 2.9184225893
 C 1.9123306116 -1.0078588724 -0.3376669727
 C 3.2873383391 -0.9458974466 -0.377675008
 H 1.3314777525 -1.2309461093 -1.2267994819
 H 3.7926238404 -1.128634174 -1.3172366247
 N 1.1966824325 -0.8053525415 0.7783869902
 Cu -0.8668765004 -0.4977400081 0.8425618503
 Br -1.4854650365 -1.590796763 -1.1335080391
 O 0.4009673383 2.3232931968 3.6532577902
 N -6.218671446 0.8673503652 3.6633337478
 C -7.5410694485 0.823104907 3.0343500551
 C -6.2745854254 1.339729588 5.0472547022
 N 3.6929632305 3.0142499451 -0.1725849156
 C 4.5813435387 3.1280281045 0.98140305
 C 4.4117941628 3.0658222661 -1.4415996533
 N 5.3576394303 -0.6070991159 0.8175344721
 C 6.1599595126 -0.5018153629 2.0361839734
 C 6.1776705102 -0.8321844885 -0.373987846
 H -7.6942795033 -0.1336166151 2.5250219909
 H -7.6381093879 1.6274493758 2.2928924179

H -5.5171149337 2.1109429809 5.2240266563
H -6.0904699717 0.5099526337 5.7436331891
H 4.3836653704 2.3227899083 1.6995078198
H 4.4327301603 4.0868442221 1.4957120972
H 3.9107052376 3.7336353477 -2.1496906445
H 4.4603866581 2.06403615 -1.8959152938
H 5.7451878563 -1.1309592478 2.8304663539
H 6.1796602272 0.5366174098 2.3970601343
H 5.8914253484 -0.1421166375 -1.1761243447
H 6.042079152 -1.8577895582 -0.7432952787
C -7.6981781013 1.8848628288 5.1822668258
C 7.5474790433 -0.977369545 1.5975554441
C 7.6082665619 -0.5947439216 0.1153999426
C 5.9795824092 3.017095549 0.370577304
C 5.7980157907 3.5748127898 -1.0440763356
C -8.5014119938 1.0160906942 4.2096117061
H -7.7261007422 2.9327249957 4.8657051864
H -8.0645265166 1.831486489 6.2094413982
H 7.6162955232 -2.0642414559 1.709209586
H 8.3460214014 -0.5261400898 2.1899467783
H 7.8775657434 0.4610653004 0.0055647786
H 8.335747564 -1.1830951983 -0.4472424242
H 6.2660612149 1.9615247356 0.3207779876
H 6.7348414107 3.5497587563 0.9525472206
H 5.8009432307 4.6693911573 -1.0230324825
H 6.57496365 3.2485469425 -1.7389887676
H -8.7299439002 0.0475478613 4.6664331807
H -9.4427340642 1.475216582 3.9013511931

O_Br_Cu2+_3D

1 2
C 0.2192875446 3.6423313216 -0.1901707611
C 1.6546320477 3.2322693654 -0.5752830307
C -0.8461383814 3.1929770891 -1.1965638548
C 1.6464312767 1.7127941255 -0.877400901
N 0.34464543 1.1743499003 -0.4086638784
C 0.1623606938 1.6430531607 0.9969122049
C -0.706376362 1.6600322664 -1.3427466921
H 0.1622205579 4.7148984448 -0.0059689954
H 2.308965373 3.4728194008 0.26853827
H 1.9999165859 3.8054901373 -1.4394420401
H -0.7301638048 3.6904376146 -2.1633966333
H -1.817057021 3.4775873125 -0.7830377035
C 2.7460054458 0.8378195834 -0.3106259818
C 4.0350013168 1.2817475902 -0.0672196055
C 3.3070491136 -1.3317270701 0.2923427441
C 4.9871750098 0.3654821077 0.3760872329
H 4.2982091797 2.3214540922 -0.2283280259
C 4.6191366157 -0.9602870763 0.5581115207
H 2.957835906 -2.3522632261 0.409188142
H 6.0039435419 0.68864231 0.5735495676
H 5.3298194169 -1.7034683353 0.8997340546
N 2.3936650126 -0.4517497932 -0.1314545154
C -0.8614352235 0.8210360923 1.7460195251
C -1.881260283 1.367237158 2.5053211233
C -2.7069153443 0.4889769445 3.2069614029
H -2.0148102677 2.4413339161 2.5482839067
C -1.430896524 -1.3311254064 2.3217217077
C -2.4772935204 -0.8786900381 3.1211923371
H -3.5180601651 0.8732256622 3.816997336
H -1.2174798681 -2.3887588789 2.1946262067

H -3.0967014271 -1.588257203 3.6578556036
N -0.6390882543 -0.4945238316 1.6519889801
H 1.1307584648 1.4547620668 1.4833794308
H 1.6692327483 1.5578969431 -1.9617770794
H -0.3022339171 1.4459123993 -2.3387076039
C -1.9196142822 0.7611474459 -1.2430363528
C -3.2273637111 1.1791853177 -1.4191251403
C -4.2396822918 0.2204611576 -1.4307096807
H -3.4598694195 2.2288011312 -1.5575177902
C -2.5727142387 -1.4583016619 -1.1012967439
C -3.9091820133 -1.1180936465 -1.2756196532
H -5.2731179943 0.5219489398 -1.5668635886
H -2.2469886983 -2.4849977799 -0.9675280312
H -4.6660998194 -1.8934890068 -1.2878611034
N -1.6047757101 -0.5391297802 -1.085801994
Cu 0.3646304106 -0.8866782669 -0.3726707756
Br 0.4480422726 -3.2075284523 -0.556230113
O -0.1292454223 3.0116684566 1.0439269723

O_Cu1+_4a

1 1
C -0.1740323254 0.0507636802 2.848592861
C -0.1081183307 -1.4261180141 2.4037473812
C 1.1095597794 0.7845066553 2.3985229968
C 0.323323385 -1.3826465784 0.913487476
N -0.0252095483 -0.0458741283 0.4168483428
C -1.350110213 0.3152135429 0.8612933083
C 0.9352300497 0.9670760408 0.8688462811
H -0.3347584412 0.1348805666 3.9229557668
H -1.0915824048 -1.8861944453 2.5410327165
H 0.607575465 -1.9740933688 3.0234721518
H 1.9884836045 0.1850722766 2.6608193089
H 1.1969917245 1.7493993593 2.9036767632
C 2.1036927405 0.8986119248 -0.0836500557
N 1.93329705 0.5222833918 -1.3457559142
H 0.4502068964 1.9353877188 0.7001996614
C -0.2495822187 -2.3679391062 -0.0777860095
N -0.4905129514 -3.685997529 0.1243921055
N -0.487520299 -2.034618795 -1.3407580833
C -1.8618670238 1.3905784401 -0.0622290662
N -2.7689019774 2.3539791271 0.2078646984
N -1.5111914839 1.4023366471 -1.3428848225
H -1.9942559529 -0.5687328886 0.7478280485
H 1.4157376775 -1.461938357 0.8503035091
Cu -0.0482222834 -0.0387087271 -1.8201314
O -1.3049889455 0.695978682 2.2326555365
N 3.3816964844 1.2942029331 0.1312673105
C 3.1506217099 0.6653271827 -1.9583712309
C 4.05822041 1.1431355793 -1.0596818058
C 3.9677932534 1.8085666775 1.3597648295
H 3.2923244748 0.41887031 -2.9993150048
H 5.1059001256 1.3857527222 -1.1495328936
H 3.277353508 2.4981407644 1.8477568959
H 4.8765629015 2.3553920135 1.1070741768
H 4.2220655778 0.9963028032 2.0452413386
C -2.9940038812 3.0300758418 -0.9695334498
C -2.2130584371 2.4302212314 -1.915824759
C -3.3778107179 2.6693733228 1.4945718503
H -3.677277364 3.8637635665 -1.0206771664
H -2.1134938988 2.6686087758 -2.9634686306
H -3.6292912788 1.7505284596 2.0233059656

H -4.2882520517 3.2406627736 1.3117917455
H -2.6919797039 3.2557355656 2.1086897183
C -0.9185802612 -4.2090797413 -1.0759396562
C -0.3171818027 -4.4473532606 1.3519935298
H -1.1846876934 -5.2500112084 -1.1769212272
H 0.6174520513 -4.1667609432 1.8411107995
H -0.2659128471 -5.5064713532 1.0984891241
H -1.1531478691 -4.2866599023 2.0369692033
C -0.912223261 -3.177245955 -1.9673789893
H -1.1825434018 -3.1817142751 -3.0119652363

O_Cu1+_4b

1 1
C 0.1116681049 0.0434286953 3.3855204629
O 1.3377437099 0.5178232506 2.7777568608
C -1.0704227389 0.9403497737 2.9353909863
C 1.071635102 0.8114689506 1.4236925946
N -0.0316546035 0.0154196311 0.9728768473
C 0.1484208344 -1.362466806 1.4013291556
C -1.2841590048 0.5777862822 1.4471440032
H 0.2748587961 0.1069348827 4.4598669139
H -0.8024790818 1.9928605812 3.0717236743
H -1.9583966955 0.7340589657 3.5390644461
N -1.6218003878 1.6498009922 0.5167383427
C -1.270957465 1.5622433365 -0.8087992846
H -2.0444818616 -0.202944733 1.3515669594
N 2.1942595435 0.5134166423 0.5528721775
C 1.9706964246 0.2930043466 -0.7841269938
N -0.653303616 -2.1764537839 0.4974163516
C -0.7411739429 -1.8341363389 -0.8294614506
H 1.1986639294 -1.6084154326 1.230327913
H 0.8169626708 1.8713491873 1.3092041233
Cu -0.0055317343 0.0247132661 -1.2661114257
C -0.135340846 -1.4150439977 2.9176802402
H 0.5413038489 -2.1084819214 3.4213711503
H -1.1651312888 -1.7123537525 3.1463379441
N -1.4234145037 -2.8670686213 -1.3655287735
C -1.2453333084 -3.399042113 0.7593216267
C -1.7397624635 -3.8328843 -0.4218968295
N -1.8588229643 2.6487797772 -1.3509440637
C -2.4217059476 2.7503821634 0.7701840158
C -2.5658476665 3.3864377035 -0.4136923955
N 3.2195739249 0.1988028449 -1.283317046
C 3.5407489584 0.5742461361 0.8621649345
H -1.2638293528 -3.8490022603 1.7395935701
H -2.2867642035 -4.7289936726 -0.6705458054
H -2.8112296797 2.9845974426 1.7485865382
H -3.0961489719 4.2910158374 -0.6678542827
H 3.9007110968 0.7420361603 1.8643691583
C -1.748194547 3.0108750659 -2.7543703864
C 3.5127038398 -0.0627872549 -2.6825467395
C -1.7922201387 -2.9498616359 -2.7690522033
H -1.1353599793 2.2569522331 -3.2480898365
H -1.2720909893 3.9893128071 -2.8549550404
H -2.7384014562 3.0369873339 -3.2157977523
H 2.5650714766 -0.1475846968 -3.2141158041
H 4.0710266481 -0.9968261375 -2.7827989719
H 4.0964542339 0.7587674507 -3.1048452062
H -1.4158789176 -2.0569395714 -3.2678248585
H -2.8793188311 -2.9932124437 -2.8717061832
H -1.3465485019 -3.8378816144 -3.2238785844

C 4.1906992878 0.3661685743 -0.3046797911
H 5.2459332593 0.3156707736 -0.5236212819

O_Cu1+_1b

1 1
C 0.2115245487 0.2510558204 3.1072268932
C -1.2704638084 0.4097386987 2.7115842241
C 0.717083944 -1.1439835747 2.6805262835
C -1.3526062366 -0.0343211933 1.2298981035
N 0.0056022773 0.0483134356 0.6813354133
C 0.6182053961 1.2998311029 1.0676426084
C 0.8406759754 -1.0667568692 1.1404734566
H 0.3608047151 0.430456329 4.1711188709
H -1.5623587201 1.4567969749 2.8439641816
H -1.9071500013 -0.2008815105 3.3579261845
H 0.0011897531 -1.9070244893 3.008220376
H 1.6818130034 -1.3670192353 3.1417983874
C 0.5330129419 -2.2933126953 0.2975289122
C 0.6096036328 -3.577559352 0.8143064823
C 0.384779756 -4.6552926914 -0.0389855363
H 0.8485357531 -3.7460537429 1.8579930736
C 0.0356935476 -3.1040038586 -1.8043761532
C 0.0915505969 -4.4229208886 -1.3761020191
Cl 0.4699118249 -6.2681666647 0.5709182253
H -0.1910368833 -2.8752117011 -2.8403771114
H -0.0894515081 -5.2385578034 -2.0655585663
N 0.248447643 -2.0557347959 -1.0012640532
H 1.873343577 -0.7904320725 0.8954776231
C -2.3133892774 0.7059453392 0.308585907
C -3.4839946904 1.2682456775 0.796624937
C -2.8539837315 1.3159075068 -1.849983408
C -4.3606097557 1.8729994426 -0.0998991059
H -3.719663232 1.2346127935 1.8541332197
C -4.0466406568 1.9018862026 -1.4525347614
H -2.5664841344 1.3176598024 -2.8959948582
Cl -5.8260053512 2.5826198593 0.4737177041
H -4.7050408418 2.3665892006 -2.1763333229
N -1.999125983 0.7280858533 -1.0039636864
C 1.7922744891 1.6000844727 0.149823986
C 2.9445721107 2.1998779114 0.6268253752
C 3.9518367529 2.4985592247 -0.287375545
H 3.0475603139 2.4206280141 1.6823300918
C 2.5853301901 1.5842402502 -2.0090939282
C 3.7738963335 2.1934797674 -1.6316203561
Cl 5.4132551026 3.2426405617 0.2518637575
H 2.4097398225 1.3201750249 -3.0464818024
H 4.5384520001 2.4163903147 -2.3659812961
N 1.6060432178 1.2837921087 -1.1477126299
H -0.127956222 2.0954268554 0.9169226134
H -1.6423175833 -1.0916715921 1.1807874091
Cu -0.0669484196 0.0034393025 -1.4444727771
O 0.9982078175 1.2493668831 2.4300466167

O_Cu1+_1e

1 1
C 0.236058572 0.2668451457 3.0064002814
C -1.2468344685 0.4081166141 2.6074483092
C 0.7449762005 -1.1381213797 2.6188326988
C -1.329259494 -0.067983823 1.1356245653
N 0.0302115047 -0.0047939749 0.5925529014
C 0.6477221935 1.2537074268 0.9342229726

C 0.8607263332 -1.1103487707 1.0762425145
 H 0.3826638181 0.473035928 4.0666542293
 H -1.541815094 1.4573372781 2.7137498031
 H -1.881135764 -0.1892784715 3.2693213283
 H 0.0320545928 -1.8928776812 2.9719484083
 H 1.7122733351 -1.3439866818 3.0838737224
 C 0.5417627803 -2.361314348 0.2721786366
 C 0.6059775126 -3.6188037884 0.8366129214
 C 0.3780624432 -4.7691591051 0.044159008
 H 0.847632222 -3.7104352901 1.8876307662
 C 0.0454102271 -3.2371150851 -1.7857902975
 C 0.0878124114 -4.53349542 -1.3173634558
 H -0.178004748 -3.0500881847 -2.8316133746
 H -0.1034930378 -5.3442043719 -2.0079459719
 N 0.2641172833 -2.1493382691 -1.0336140217
 H 1.8921787444 -0.8438355008 0.8165968795
 C -2.2851236127 0.6569285547 0.1950133192
 C -3.4367302575 1.2463035974 0.6768270898
 C -2.8320021148 1.2048113061 -1.9615187028
 C -4.3533660146 1.8571579372 -0.21102194
 H -3.6298527682 1.224737051 1.7416847083
 C -4.0065524918 1.8166629284 -1.579385704
 H -2.558731484 1.1739392661 -3.0116236769
 H -4.6365621458 2.2567697957 -2.3410399928
 N -1.9652515825 0.6254886525 -1.1173176326
 C 1.8273415882 1.5149833606 0.0110305793
 C 2.97916873 2.1030770161 0.4807423283
 C 4.0347056848 2.3917573479 -0.4170718053
 H 3.0442814756 2.3266956868 1.5370913228
 C 2.6221858249 1.4437871147 -2.1295309773
 C 3.8126848358 2.0396306542 -1.7674000103
 H 2.4522941693 1.1634204408 -3.164397088
 H 4.5562788778 2.2203710178 -2.5324648661
 N 1.6227646377 1.1688596316 -1.2786978968
 H -0.094718534 2.0461522353 0.7552134485
 H -1.6203032857 -1.125638816 1.1089921434
 Cu -0.0431499927 -0.111346577 -1.5437590253
 O 1.0163141085 1.2512600652 2.3081064826
 N 5.188680477 2.9713756843 -0.0004139651
 N 0.4342971017 -6.0216188902 0.5650320865
 N -5.4938564566 2.4470295546 0.2290633758
 C 6.2439066827 3.2570827689 -0.9571590234
 H 6.6034186945 2.3408703424 -1.4408192894
 H 5.9041546177 3.954015783 -1.7329598968
 H 7.0851999959 3.715171571 -0.4378180209
 C 5.3594371568 3.3288148489 1.3975384056
 H 4.6011253116 4.0513800519 1.722376041
 H 5.3032594933 2.4463369301 2.0461551763
 H 6.339818423 3.7845516965 1.5336170241
 C -6.4055589761 3.0616192003 -0.7213483085
 H -6.7841268839 2.3285798226 -1.4437153532
 H -7.258441044 3.4756630847 -0.1843073959
 H -5.9213178655 3.8786691938 -1.2695651163
 C -5.8037740061 2.4667733846 1.647494733
 H -5.0304723731 2.99407161 2.2197082732
 H -6.748048831 2.9881699493 1.8013775731
 H -5.909215671 1.4517849471 2.0501969843
 C 0.7496927258 -6.2139183265 1.9692762875
 H 0.7398505851 -7.279456754 2.1968725749
 H 1.7454959217 -5.8248707202 2.2156490174
 H 0.010979575 -5.7249549144 2.6162113203

C 0.205276345 -7.1733856428 -0.2912515194
 H 0.2917305132 -8.0838263316 0.3011316189
 H -0.7988181466 -7.1503439019 -0.7313016898
 H 0.9433334176 -7.2241654563 -1.1008558423

 O_Cu1+_1a
 1 1
 C 0.2246686879 0.2405109836 3.107109333
 C -1.2580023854 0.4070676172 2.7173733253
 C 0.7235360766 -1.1551931171 2.6746142746
 C -1.3469453538 -0.0356103373 1.2357890506
 N 0.0089450207 0.0459345601 0.6788824655
 C 0.6245616262 1.2960453458 1.070848386
 C 0.8443880391 -1.0713728144 1.13493574
 H 0.3798814796 0.4180176671 4.1701257811
 H -1.5460204538 1.4547775516 2.852936628
 H -1.8951475395 -0.2016654545 3.3646281281
 H 0.0062403959 -1.9172954023 3.0010773978
 H 1.6883985678 -1.3840665636 3.1322677249
 C 0.5349989359 -2.2941536672 0.2887340202
 C 0.6089225354 -3.5822865102 0.7986298291
 C 0.3802598101 -4.6340194713 -0.0733008262
 H 0.8430633052 -3.7797858334 1.8375848624
 C 0.0355664294 -3.0940891953 -1.8268248859
 C 0.0899351369 -4.417913437 -1.4057447178
 H -0.1894588959 -2.8547534208 -2.8603291727
 H -0.0878348043 -5.2430049395 -2.0837690741
 N 0.2497730993 -2.0563727352 -1.010830813
 H 1.8774484212 -0.796142382 0.8897494438
 C -2.3102264241 0.7069915476 0.3205224179
 C -3.4790794599 1.2722936168 0.8120315179
 C -2.8561386335 1.3202901159 -1.8453744947
 C -4.3372543598 1.8709039586 -0.0943755145
 H -3.7310231627 1.2513207178 1.865391504
 C -4.0486191205 1.9099161488 -1.4444444535
 H -2.5679545832 1.3188574013 -2.8907332948
 H -4.7209462636 2.3806712613 -2.1503941584
 N -2.0055947327 0.7328395052 -0.995073598
 C 1.7931669336 1.6018752769 0.1486152951
 C 2.9490803792 2.2030647197 0.6196529137
 C 3.9304159269 2.4957150174 -0.3129127034
 H 3.0790724237 2.4290787201 1.6706503642
 C 2.5726353476 1.59298218 -2.0246382566
 C 3.7644253303 2.2048988003 -1.6539447296
 H 2.3857123182 1.3300799261 -3.0598588242
 H 4.534962928 2.439834551 -2.3772737311
 N 1.6055580267 1.2909458093 -1.1502530144
 H -0.121852207 2.0933098258 0.9279068294
 H -1.6399587039 -1.0921844596 1.1873177766
 Cu -0.0713995209 0.0066439729 -1.4400147479
 O 1.0142646504 1.2365142469 2.4265121115
 N 5.18737943 3.1315730731 0.1412852681
 O 6.0148997025 3.3823437703 -0.7139577723
 O 5.2909750535 3.3496718673 1.3336528399
 N 0.4467812918 -6.0193486653 0.4428448354
 O 0.2529801349 -6.9128744988 -0.3581342142
 O 0.6883600857 -6.1508403986 1.6286825955
 N -5.5899188598 2.483206102 0.4017113364
 O -5.7914870536 2.4231254106 1.600657775
 O -6.3150550122 2.996372035 -0.427938774

O_Cu1+_1c

1 1

C -0.2427964846 0.0373151188 2.8653178075
C 0.1866030076 -1.3828535935 2.4446580659
C 0.817119183 1.0591927205 2.4004717381
C 0.5636527954 -1.2748550007 0.9460481646
N -0.0735185841 -0.058167509 0.4324343196
C -1.4484051279 0.0049160749 0.8718685409
C 0.6371598541 1.1484010628 0.8664630296
H -0.4215594343 0.0965211463 3.9384004489
H -0.6516253041 -2.0679502765 2.6091204778
H 1.0266733531 -1.7258670022 3.0554529948
H 1.8139913879 0.7044998514 2.6879978208
H 0.6556777581 2.0307974284 2.8733310592
C 1.8505242758 1.3563720434 -0.025314132
C 3.0206665232 1.918878752 0.4510027953
C 4.0854315396 2.1526179431 -0.4293054436
H 3.1184234468 2.157705328 1.5031096559
C 2.7114160542 1.2245443374 -2.1535538332
C 3.912916347 1.7919564609 -1.7678276769
N 5.2718841386 2.7196270329 0.0205122814
H 2.5520205894 0.9393397732 -3.1882792867
H 4.6837813395 1.9739188389 -2.5062562889
N 1.6873119565 1.0055608108 -1.3198467961
H -0.0361420984 1.9868340174 0.6510076132
C 0.2275969874 -2.4456124412 0.0310686729
C 0.1828741192 -3.7406544374 0.5166125453
C -0.2154461818 -3.1732298926 -2.1051001114
C -0.0646288786 -4.8032867424 -0.3613035518
H 0.3149779381 -3.9261941172 1.5758137867
C -0.2666333099 -4.4973155023 -1.7097702914
H -0.3672772806 -2.9104885927 -3.146769938
N -0.1111325647 -6.1138095271 0.0983127849
H -0.4330585391 -5.2729757967 -2.4468338941
N 0.029344759 -2.1528766602 -1.2721809254
C -2.2244626462 0.9700041265 -0.0094933323
C -3.2138868725 1.7772841205 0.5128393867
C -3.9439191529 2.6037825628 -0.3517608198
H -3.4192435202 1.7372564199 1.5750240859
C -2.620828551 1.7122058533 -2.1412819937
C -3.6291607692 2.5579546888 -1.7137315573
N -4.9435142907 3.4381854867 0.1321671348
H -2.3526291761 1.6711505362 -3.1917555223
H -4.1328970919 3.1934073181 -2.4313322496
N -1.9117159632 0.9256424513 -1.3214047433
H -1.8875268567 -0.9949573059 0.733166409
H 1.6458865424 -1.1189966331 0.8520403454
Cu -0.0909417191 -0.0936450039 -1.7002046651
O -1.4988264396 0.3630897152 2.2431085837
C -0.809301215 -7.1578706806 -0.495007724
C 0.5289794727 -6.6036373532 1.2297751847
C -0.6157189654 -8.2802309838 0.2530018259
C 0.2419044097 -7.9310505592 1.3415077499
C -6.0104671833 3.9412542476 -0.601854524
C -5.0457870724 3.9146735866 1.4333377132
C -6.7699006291 4.7144215119 0.2236405832
C -6.1522243247 4.7055761896 1.512647537
C 6.5227761062 2.5521290486 -0.5594630989
C 5.4107118435 3.5482258946 1.126878826
C 7.4305537657 3.2573259629 0.1723491851
C 6.7233267803 3.8977643107 1.2361704857

H -1.4283509342 -6.9907313589 -1.3629552364
H 1.1833958489 -5.9761335267 1.8149836136
H -1.0470365245 -9.2509005623 0.0554691906
H 0.6129158656 -8.593377448 2.1102721005
H -6.1637521001 3.6547798292 -1.6307010934
H -4.2900696332 3.6902140039 2.1699081219
H -7.6796407448 5.2268266072 -0.054041652
H -6.4870570914 5.2340107534 2.393558488
H 6.6598796811 1.8979957147 -1.4067177523
H 4.5505290069 3.8662020242 1.6956978045
H 8.4924604681 3.3072906577 -0.0203015053
H 7.140286111 4.5535661439 1.9868006801

O_Cu1+_1f

1 1

C 0.0398109093 0.0348035906 3.1496381366
C -1.4333689673 0.1539052931 2.7094806741
C 0.6029334794 -1.3331075455 2.7081375175
C -1.4546727395 -0.246310573 1.2131836647
N -0.0811381025 -0.1167956178 0.7200186765
C 0.4875152988 1.1390450722 1.1452821384
C 0.7658098942 -1.2224934078 1.173474763
H 0.1462967746 0.1894750596 4.2234430147
H -1.7638582526 1.1870883139 2.8594820061
H -2.0697906403 -0.4954891704 3.3182748043
H -0.0974535631 -2.1251287831 2.9991870556
H 1.5610970143 -1.5348950003 3.1934925078
C 0.5083010543 -2.4385757623 0.2972681419
C 0.5850948985 -3.7212173564 0.7986858489
C 0.410737225 -4.8317722107 -0.0610455621
H 0.7806655287 -3.8704633199 1.8535206165
C 0.0971711767 -3.2183417656 -1.819863684
C 0.155972056 -4.5356188561 -1.4176356188
H -0.0950818557 -2.980883411 -2.8617035988
H 0.0188286848 -5.319836368 -2.1515143253
N 0.2669002397 -2.1663700222 -1.0053716436
H 1.796541885 -0.9144939488 0.9612295236
C -2.4007607179 0.5010299219 0.2805239596
C -3.5832519722 1.032856243 0.7530155331
C -2.8959483278 1.1412805774 -1.8654150319
C -4.4868950012 1.6610140378 -0.1356878886
H -3.8222197815 0.945325202 1.8060140119
C -4.0990813136 1.7000322471 -1.4929134922
H -2.5860942319 1.172764895 -2.90535939
H -4.7181985558 2.1732977761 -2.2446452311
N -2.0394231839 0.5449425129 -1.0213844758
C 1.6879103005 1.4802795447 0.2768623563
C 2.8062135104 2.0750533319 0.8130522287
C 3.8766900106 2.4410695204 -0.0372939978
H 2.8355895288 2.2581771735 1.8794835556
C 2.549029621 1.5464501807 -1.8405948937
C 3.70913525 2.1559124642 -1.4109070958
H 2.4189163134 1.312775098 -2.8927366458
H 4.4810894764 2.3892172032 -2.1335780393
N 1.5332818118 1.1981202145 -1.0360121927
H -0.2721006124 1.9184577778 0.9820234605
H -1.7132489296 -1.3087807899 1.1219896663
Cu -0.0831134458 -0.1139410147 -1.4204253215
O 0.8116778411 1.0760916638 2.529314948
N -5.6512658577 2.1929573614 0.2927878482
N 0.4823781217 -6.1007695497 0.3946813861

N 4.9929425395 3.0285775902 0.4423700329
 C 0.8487142827 -6.454029012 1.7645489428
 C 0.213801671 -7.2748920408 -0.4344573181
 C 1.0834308779 -7.9649898401 1.6940506342
 C 0.1338313579 -8.4172505995 0.5805163223
 C 5.2414867998 3.2599229391 1.8643218839
 C 6.0791440778 3.5193924227 -0.4042258007
 C 6.715657272 3.6685417642 1.9062150943
 C 6.9283581028 4.3571777579 0.5546001513
 C -6.0436364465 2.2672706482 1.6985987861
 C -6.6562130432 2.7674759389 -0.6008714102
 C -7.255020375 3.2028569722 1.6829621787
 C -7.8755354096 2.9518269747 0.3052070256
 H 0.0352864112 -6.2022863203 2.4599704084
 H 1.746396481 -5.9109258085 2.0798599674
 H 1.0261502512 -7.4307863873 -1.1579442519
 H -0.720126539 -7.1500038228 -0.9927142857
 H 0.8922774503 -8.458410093 2.6492725805
 H 2.1216973168 -8.1662951751 1.4100485535
 H -0.8878819327 -8.5017972408 0.9656254694
 H 0.4113112032 -9.3787336081 0.1436742682
 H 5.0454922939 2.3526857184 2.4457840113
 H 4.5881132979 4.056866666 2.2460961579
 H 5.6849854507 4.1134328692 -1.2357119198
 H 6.6503189677 2.6800275756 -0.8249496724
 H 7.3467999802 2.7764708206 1.9791610073
 H 6.9420042315 4.3136625222 2.7577199089
 H 7.9768583932 4.3961312747 0.2520854915
 H 6.5468792933 5.3831027528 0.5890573959
 H -5.2245276806 2.661174533 2.3104187459
 H -6.3064003713 1.2705010677 2.0804046058
 H -6.8608182444 2.093034504 -1.4391254627
 H -6.3061326549 3.725331655 -1.0102260934
 H -6.9218619862 4.2429234381 1.7635465519
 H -7.9427074161 3.0029409415 2.507309316
 H -8.5205063312 3.7665351007 -0.0302726897
 H -8.4702514252 2.0323976971 0.3199934969

O_Cu1+_1d

1 1
 C -0.149010174 0.022539348 3.1213155772
 C 0.2760536526 -1.3917433989 2.6766153668
 C 0.9056571714 1.0509701187 2.6587489148
 C 0.6381785132 -1.2628005318 1.1761141411
 N -0.0062012735 -0.0398910203 0.6850308049
 C -1.3766185377 0.0149130504 1.141613604
 C 0.7073056784 1.1622070675 1.1285217439
 H -0.3167024977 0.0674373067 4.1968157262
 H -0.5593778376 -2.0806766921 2.8394500297
 H 1.1223844074 -1.7430247275 3.2738001479
 H 1.9066785308 0.6937153369 2.9281709654
 H 0.7497131305 2.0156893358 3.1471161626
 C 1.9117529368 1.3848909933 0.2288377295
 C 3.0891295397 1.9602061894 0.686753752
 C 4.1240902214 2.2001049556 -0.2127686626
 H 3.1948312683 2.2268825938 1.7327517189
 C 2.7405042377 1.28367692 -1.9259244625
 C 3.9482892248 1.8554391458 -1.5455795897
 H 5.0515805759 2.649828435 0.1261700511
 H 2.5597103991 0.9980055895 -2.9570579259
 H 4.7255928817 2.0218206905 -2.2823427561

N 1.7402056742 1.0504763786 -1.0688901108
 H 0.0293313242 2.0020296538 0.9341261089
 C 0.2929392663 -2.4225606365 0.2511680221
 C 0.2637613656 -3.7343422967 0.7068762095
 C -0.1646365674 -3.1131257733 -1.906297096
 C 0.0095649983 -4.7636788801 -0.1939416691
 H 0.4434143334 -3.9507416677 1.7544993572
 C -0.2094484891 -4.4484064713 -1.5280327481
 H -0.3326127814 -2.8204626626 -2.9375240317
 H -0.0170192196 -5.7942724828 0.1444011849
 H -0.4137363485 -5.214863861 -2.2665903359
 N 0.0808576482 -2.1165413036 -1.0466839763
 C -2.1672372086 0.9874612854 0.281851967
 C -3.160228213 1.7951230953 0.8125236646
 C -3.8833196351 2.615482846 -0.0489283927
 H -3.3499482827 1.7754564409 1.8792272712
 C -2.5689224915 1.7593433829 -1.8515052247
 C -3.5865478499 2.5939774147 -1.4056717149
 H -4.6666311235 3.2601777588 0.3359906538
 H -2.2986297599 1.7191962854 -2.9015286121
 H -4.1254007562 3.2140276842 -2.1128368781
 N -1.8643897761 0.969233066 -1.0324563024
 H -1.8138967436 -0.9852194102 0.99702017
 H 1.7192469889 -1.1037365743 1.0741530779
 Cu -0.043188238 -0.0484642589 -1.4392408191
 O -1.4114701645 0.3574902808 2.5164571855

O_Cu1+_4c

-2 1
 C -0.0941782855 0.0346113285 3.0211849236
 C 0.3501873339 -1.3726212106 2.560905685
 C 0.9425542678 1.0782242569 2.5454558852
 C 0.6610797405 -1.2452583381 1.0468196294
 N 0.0053210333 -0.0135967722 0.5937837544
 C -1.359413809 0.0417268547 1.0496819886
 C 0.7372102647 1.1870408726 1.0124468904
 H -0.2237187812 0.066618663 4.109803851
 H -0.4635292778 -2.0862574836 2.7377795927
 H 1.224804651 -1.7029803149 3.1374571291
 H 1.9589785384 0.7438291764 2.7953088365
 H 0.7694402112 2.0419987057 3.0385369868
 C 1.946659519 1.3428899592 0.1324239523
 N 1.8089279609 1.0525704113 -1.1965321669
 H 0.0438622106 2.0148522899 0.8236216835
 C 0.2373060333 -2.3750737606 0.1456979835
 N 0.0367407777 -2.1096712832 -1.1806503594
 C -2.1276135294 1.0203012969 0.2078242955
 N -1.8408908313 1.0473340458 -1.1300170029
 H -1.7714093055 -0.9712481522 0.934691882
 H 1.7352547113 -1.0590056806 0.9169902166
 Cu -0.0196243278 -0.0129755428 -1.5924122296
 O -1.3720410566 0.3568761895 2.4717544414
 C -2.6960436841 1.9542607436 -1.6684913553
 C -3.1582197755 1.8962243923 0.5238726471
 C -3.5312765009 2.5067425184 -0.6996991353
 C 3.0168610629 1.314005706 -1.7594630219
 C 3.2335674209 1.7884319004 0.4180080798
 C 3.9317330018 1.7756333384 -0.8165028201
 C -0.2829017472 -3.2994547881 -1.7523731361
 C 0.0484841755 -3.7264036567 0.4199462596
 C -0.2860214415 -4.3316122727 -0.8177703559

H -2.6594724643 2.1718802998 -2.7323577557
H -3.5717480749 2.069142684 1.5116048659
H -4.2965396285 3.2637841551 -0.8524130317
H 3.1714585194 1.1433525747 -2.8213315449
H 3.6115957594 2.0956827468 1.3893537043
H 4.9690519688 2.0499153533 -0.9912011243
H -0.5090137891 -3.3499256057 -2.8138128428
H 0.1509700046 -4.2105094068 1.38735298
H -0.5164728566 -5.3782061945 -1.0000302613

O_Cu2+_4a

2 2
C -0.1196715865 -0.0278052439 2.8509635506
C 0.4935523807 1.3118186077 2.3996450544
O -1.4228323824 -0.1326856039 2.231397753
C 0.2127409597 1.3907484199 0.8810374998
N 0.0199363643 -0.0122504205 0.3943459178
C 1.106629268 -0.9091618912 0.9004374036
C -1.2877374316 -0.5140493727 0.8930453209
H -0.2981113192 -0.0614350336 3.9240303554
H 1.5627344365 1.3360681425 2.6333427432
H 0.0153563385 2.1473943661 2.9140610665
C -2.3363955757 0.0320050835 -0.0383439085
N -3.6503376209 0.2221941827 0.1546894494
N -2.0025493535 0.2740665477 -1.3067986691
H -1.2649050949 -1.609210087 0.7975422655
C 1.1936088983 2.0143933153 -0.0743952767
N 2.0010634413 3.0778190286 0.0885785289
N 1.2595161602 1.5683678386 -1.329369927
C 1.1918099679 -2.0430879494 -0.0865736217
N 1.739753088 -3.2627120083 0.0640903859
N 0.7692789756 -1.8746745424 -1.339472615
H 2.0340485897 -0.3292977421 0.8305978061
H -0.7536499468 1.885207228 0.7350630002
Cu -0.0046349551 -0.0073932911 -1.5816690352
C 0.7739011381 -1.1913099924 2.3864450631
H 1.6836901217 -1.2244157991 2.9906201014
H 0.248162172 -2.1405376948 2.5227086832
C 1.0446543751 -3.0377681454 -2.013445806
C 2.3392438322 -3.8364506175 1.2682629326
H 0.7958079261 -3.1738099786 -3.0544211074
H 1.5690182608 -4.2548762406 1.9192852612
H 2.910694543 -3.0747578464 1.8000944314
H 3.0236160963 -4.6296775585 0.9684424149
C -3.1553754695 0.6455148725 -1.9510004763
C -4.1821431787 0.6166658315 -1.0524615299
C -4.4257398075 0.0170483728 1.3811636064
H -3.1718229198 0.9125042955 -2.9962781471
H -5.2316741682 0.8454317251 -1.159635271
H -3.7469572164 -0.173670679 2.2101043304
H -5.0976644039 -0.8320952795 1.2447439439
H -5.0064323167 0.9168883389 1.5883929199
C 2.6213569993 3.308806382 -1.1208413698
C 2.1568232828 2.3681337835 -1.9911113397
C 2.2051560456 3.8772348262 1.2962734846
H 3.3290577217 4.1135065026 -1.2496521606
H 2.405231218 2.2195763966 -3.0304963116
H 1.2580975382 4.012006316 1.8195888707
H 2.5758084285 4.8585695479 1.0012279571
H 2.9361696692 3.4012792873 1.9530289805
C 1.6476804917 -3.9050072892 -1.1517968497

H 2.0157860189 -4.9100589317 -1.2909476602

O_Cu2+_4b

2 2
C 0.0922799615 -0.1426555113 3.4092669959
C -1.3697744596 -0.0933465549 2.8893131995
O 0.7378906888 -1.3049283407 2.8188690088
C -1.2316892772 -0.389786846 1.380866084
N 0.1335904341 -0.017409002 0.9877307761
C 0.4587106011 1.3147925153 1.4996875319
C 1.0444160495 -1.0213524613 1.48928545
H 0.1428627057 -0.2979732536 4.4844780359
H -1.8141251146 0.8858992203 3.0971102268
H -1.9817994256 -0.8542252567 3.3766364668
N 0.8621710495 -2.1763921614 0.6094718525
C 0.5228687134 -2.0005407192 -0.7047470874
H 2.0765096658 -0.6651811736 1.3860002411
N -2.1042968202 0.2744948799 0.4173319859
C -1.7133716308 0.4003566091 -0.8831691405
N 1.4015159075 1.8996680381 0.5481559666
C 1.3035008335 1.6114610659 -0.7850809415
H -0.456762462 1.9084519206 1.4341308274
H -1.3318679523 -1.4649011234 1.2271929184
Cu 0.2635763598 -0.0583211998 -1.181153508
C 0.8540994186 1.1381002146 2.9770251602
H 0.5434537236 1.992496391 3.5831518022
H 1.9299926349 0.9941290759 3.1159647032
N 0.4968476869 -3.2418125733 -1.2104758549
C 1.0567417042 -3.506450969 0.9070752234
C 0.8223825621 -4.1794234908 -0.2479823658
H 1.3314188915 -3.8508868405 1.8918374907
H 0.8594712036 -5.2362596626 -0.4643230444
N 2.1422067813 2.4715308375 -1.38162075
C 2.7513932835 3.2960025527 -0.454945634
C 2.275565864 2.9435245747 0.7651032609
N -2.7826234809 0.9031608239 -1.5137874543
C -3.4172357713 0.6736552448 0.5829797892
C -3.8417755735 1.0771794965 -0.6378507872
H 3.471006672 4.0488805602 -0.7385817177
H 2.487772249 3.3420045969 1.745283539
H -3.9308316925 0.6350980236 1.5311494172
H -4.7938184391 1.473116608 -0.9568012579
C 0.1746318105 -3.5741074137 -2.5965706294
C 2.4153454491 2.5187366884 -2.8165689467
H -0.1272245661 -2.6621389919 -3.1108591293
H -0.6460967285 -4.2929200554 -2.6187609698
H 1.0520982801 -3.9994285557 -3.0870543969
H 1.7077638937 1.8662389297 -3.327852643
H 3.4348782023 2.1812671413 -3.0123981535
H 2.2889804796 3.5409671495 -3.1766319804
C -2.8393556814 1.2372981711 -2.9341188393
H -1.8775125827 0.9953109068 -3.3855461688
H -3.0423990135 2.3029242689 -3.0554242822
H -3.6255130888 0.6550556517 -3.4181722706

O_Cu2+_1b

2 2
C 0.2066138693 -0.1500458905 -3.5326288007
O 1.043061857 -1.1283923649 -2.8736921074
C -1.2601915543 -0.3693345709 -3.125498697
C 0.6619584005 -1.2820634808 -1.5426759217

N 0.0187379385 -0.0242777909 -1.0889280146
 C 0.8416372462 1.1348832037 -1.5399212041
 C -1.3662407741 0.0454694485 -1.637826459
 H 0.3554323008 -0.3048882511 -4.5994575026
 H -1.5291892653 -1.4192375505 -3.2761258643
 H -1.9214579071 0.2385542616 -3.7476179095
 C -2.2842970749 -0.7532268442 -0.7316413876
 C -3.4665930737 -1.3073276114 -1.183727192
 C -4.2924618528 -1.9651544093 -0.2671312735
 H -3.7587693882 -1.2304365756 -2.2251331061
 C -2.6980908358 -1.4748516643 1.435666468
 C -3.9012450002 -2.0506539978 1.0678961992
 H -2.3542198085 -1.52727049 2.4631990682
 H -4.5162093573 -2.5565717314 1.8027791336
 N -1.9025078087 -0.8339417806 0.5641308184
 H -1.6716010739 1.0957307361 -1.5629250182
 C 1.8244344932 -1.5942459615 -0.6219010357
 C 2.9537987804 -2.251840811 -1.0604284718
 C 2.5876510919 -1.5326299787 1.5618201047
 H 3.0662007674 -2.5153411495 -2.1059201434
 C 3.7482143541 -2.2044022064 1.216945541
 H 2.413328222 -1.2228045048 2.586591073
 H 4.4919063688 -2.4348519119 1.9706955361
 N 1.6353103253 -1.2277610101 0.6656233412
 C 0.5068357825 2.320894348 -0.6590146712
 C 0.6042434509 3.6286811919 -1.0918812732
 C 0.3577586505 4.657080963 -0.1763086465
 H 0.877552792 3.8614349034 -2.1150189858
 C -0.0669960337 3.0008610895 1.4850658039
 C 0.0163217348 4.3378517268 1.136394188
 H -0.337357697 2.7114934131 2.4950252596
 H -0.1829019312 5.11067781 1.8693508064
 N 0.1752188595 2.0072286272 0.6159568389
 H 1.8804909478 0.8616069413 -1.322795565
 H -0.0896512253 -2.0790674975 -1.432808434
 Cu -0.0337078181 -0.0303531474 0.8364986446
 C 0.6746652975 1.243124042 -3.0723095072
 H 1.6265140675 1.5090145335 -3.5357904933
 H -0.0651499413 1.9992562869 -3.3563601196
 C 3.9382866711 -2.5642151917 -0.1170299269
 Cl 5.3608905499 -3.3795297873 -0.6019563246
 Cl -5.7658013114 -2.6595910207 -0.7884672408
 Cl 0.473145913 6.2895956564 -0.6731075275

O_Cu2+_1e

2 2
 C 0.1839695242 -0.1555746912 -3.4825171952
 O 0.9700212595 -1.178911365 -2.8382415297
 C -1.2901074504 -0.3012983903 -3.0693272865
 C 0.601965594 -1.3077534682 -1.494300757
 N 0.0138113814 -0.0273038548 -1.0417010487
 C 0.8814112712 1.0979404741 -1.4887881073
 C -1.3695920999 0.1030436939 -1.5787612708
 H 0.3175677707 -0.3103533464 -4.5517953407
 H -1.610616072 -1.335924651 -3.2242250591
 H -1.9226498006 0.3429659988 -3.6849985603
 C -2.315219191 -0.6654031713 -0.672458227
 C -3.503018865 -1.1768098302 -1.1331135279
 C -4.3985195904 -1.823859802 -0.2346482655
 H -3.7527512892 -1.0692662362 -2.1807472739
 C -2.7586996933 -1.368540819 1.4807238897

C -3.9681083893 -1.9025159379 1.1172166129
 H -2.4247120595 -1.43441815 2.5111834962
 H -4.5719268368 -2.3802334307 1.8767618045
 N -1.9242049738 -0.746953235 0.6230552353
 H -1.6265542498 1.1649675073 -1.4907059144
 C 1.7597170709 -1.661017702 -0.582033521
 C 2.857736404 -2.3391324649 -1.0372617142
 C 2.5342039321 -1.6431882524 1.5850937995
 C 3.8783376922 -2.717573287 -0.1180161295
 H 2.9191463625 -2.57468968 -2.091423067
 C 3.6654270301 -2.3366680059 1.2352828544
 H 2.3791370001 -1.3416833366 2.615916525
 H 4.3819585588 -2.5764399104 2.0091785897
 N 1.5693076621 -1.2957221927 0.7095742618
 C 0.5912866678 2.2971642586 -0.6078131986
 C 0.7260192429 3.5882476277 -1.0526591066
 C 0.5283813339 4.6762097822 -0.1546874443
 H 1.0018946979 3.7654381195 -2.0841180023
 C 0.0571953576 3.0026158912 1.5237884278
 C 0.1776337632 4.3240190114 1.1761711394
 H -0.2162258181 2.7318976077 2.5385444863
 H -0.000477188 5.0760373493 1.9327606045
 N 0.26116142 1.980427312 0.6692854271
 H 1.9063607674 0.7802662378 -1.2673398671
 H -0.1803237846 -2.0723590837 -1.374361226
 Cu -0.0314596113 -0.0344220902 0.8865343387
 C 0.7214582429 1.2113611037 -3.0202143047
 H 1.6844339184 1.4297999834 -3.4857992944
 H 0.0187958097 2.0028944151 -3.3024829459
 N 4.9709957752 -3.3908597355 -0.5095233787
 N 0.6627595747 5.9537476374 -0.5452863298
 N -5.5730940278 -2.3303142572 -0.642144462
 C -5.9744356812 -2.2294506568 -2.0408416305
 H -5.2620320885 -2.7448149479 -2.6945664785
 H -6.9473156229 -2.7006625185 -2.1687164368
 H -6.0626153795 -1.1828664621 -2.3528801492
 C -6.4625832737 -2.9833090333 0.3151869479
 H -6.7654957716 -2.2901554311 1.1069943122
 H -7.3602044583 -3.3173763539 -0.20208544
 H -5.9832566991 -3.8597126792 0.7640100207
 C 5.9914754922 -3.7662008699 0.4654722967
 H 6.7917214464 -4.3008087877 -0.0431612049
 H 6.4246879991 -2.8807184732 0.942518723
 H 5.5773452568 -4.4263255504 1.2350028314
 C 0.457487181 7.0389140798 0.4107979361
 H 0.6151549559 7.9917633385 -0.0913504433
 H -0.5640347922 7.0281005623 0.8052810706
 H 1.1677061195 6.9712693582 1.2416306024
 C 5.1414372264 -3.7676552364 -1.909234749
 H 6.080549413 -4.3063861522 -2.0220625391
 H 4.3312133676 -4.4250595849 -2.2425970728
 H 5.1785415938 -2.8832887018 -2.5544347928
 C 1.0301338986 6.2697687805 -1.9210198924
 H 2.011085704 5.8528892517 -2.174878857
 H 0.2816434536 5.8924691624 -2.6266374229
 H 1.0846065642 7.3506932725 -2.0374557684

O_Cu2+_1a

2 2
 C 0.1920959416 -0.1428052911 -3.494496429
 O 1.0467483113 -1.1090679317 -2.8370142664

C -1.2695034339 -0.3838960751 -3.0810084969
 C 0.668352527 -1.2745420498 -1.5096596556
 N 0.0135852208 -0.0235375074 -1.0478739743
 C 0.8218333441 1.1451800883 -1.5028674781
 C -1.3744223558 0.0311170222 -1.5924940106
 H 0.3395616312 -0.2959435309 -4.5616608691
 H -1.5257053252 -1.4371105451 -3.2311422601
 H -1.9425047202 0.2146617563 -3.6995169712
 C -2.2803482102 -0.77698168 -0.6839630834
 C -3.4621236285 -1.3431999453 -1.1297725586
 C -4.2502894569 -1.9977306657 -0.1955326745
 H -3.7841328793 -1.2854620696 -2.1635921121
 C -2.6750882358 -1.504823935 1.4941090639
 C -3.8796107342 -2.0932325179 1.1323069508
 H -2.3211741552 -1.5519614661 2.5182183741
 H -4.5030794462 -2.6095727824 1.8529484474
 N -1.8973183756 -0.8597170942 0.611709659
 H -1.6926319994 1.0777343905 -1.5182398717
 C 1.8362521097 -1.5810869709 -0.5942449537
 C 2.9701035149 -2.2350816787 -1.0361311763
 C 2.6060673738 -1.5147581827 1.595989432
 H 3.1057407582 -2.508335372 -2.0765378372
 C 3.77227383 -2.1846708199 1.2476598407
 H 2.4290686935 -1.2032392087 2.619512393
 H 4.5325694371 -2.4229165398 1.9823596527
 N 1.6571204293 -1.2180188132 0.6954995116
 C 0.4814627722 2.326076773 -0.6186998365
 C 0.5637482784 3.6384226989 -1.0484274591
 C 0.3109221276 4.633212366 -0.1152509507
 H 0.8228770906 3.9043770059 -2.0670944058
 C -0.0853451015 2.9948792139 1.5401168775
 C -0.0151710705 4.3385421858 1.1945472828
 H -0.3456706562 2.6956070408 2.5495563606
 H -0.2106614938 5.1249485793 1.9142638192
 N 0.1597035034 2.01392586 0.6596169958
 H 1.8656412916 0.8834966167 -1.2946263292
 H -0.0752807365 -2.0796508075 -1.4015224872
 Cu -0.0295015099 -0.0332192354 0.8768451289
 C 0.6434119782 1.2559629854 -3.0344378744
 H 1.5890139739 1.5363754467 -3.5020774456
 H -0.1074986279 2.0032787676 -3.3125733587
 C 3.9336663189 -2.52834843 -0.0819959168
 N 0.3893263581 6.0528577271 -0.547737666
 O 0.6549738776 6.2405829859 -1.7185004222
 O 0.1785943949 6.8866769748 0.3065430377
 N -5.5250272275 -2.6151276039 -0.6455719311
 O -5.7820454481 -2.50768273 -1.8282802865
 O -6.1849049959 -3.1668911453 0.2085673507
 N 5.173657007 -3.2283117414 -0.5080763736
 O 5.2631202436 -3.4826367728 -1.6921707934
 O 5.9772174856 -3.4759153456 0.3659620371

O_Cu2+_1c

2 2
 C 0.1771232117 -0.1062546746 -2.9202484853
 C -1.0130270336 -0.9750817816 -2.4801482929
 C -0.043740775 1.349192607 -2.4682039621
 C -1.2651329014 -0.6481696577 -0.9889262215
 N 0.003971552 -0.0592039021 -0.4749729038
 C 1.1499756888 -0.8743997671 -0.9412952413
 C 0.1807294699 1.3457042653 -0.9400404153

H 0.3556182854 -0.1830018864 -3.9911818266
 H -0.7676041942 -2.0310526328 -2.628354981
 H -1.8938114847 -0.7462412366 -3.085007206
 H -1.0550511561 1.6732962404 -2.7366076904
 H 0.6681628126 2.0205698715 -2.9520056642
 C -0.6543854609 2.2450585968 -0.0513716409
 C -1.1970837545 3.4293770908 -0.4925422435
 C -1.8987948298 4.255762041 0.4109152262
 H -1.0968743024 3.7110854764 -1.53304549
 C -1.450990837 2.5955894985 2.0900586147
 C -2.015713815 3.8003204431 1.7366863141
 N -2.4456924155 5.4454968332 0.0071387948
 H -1.5321585955 2.2332881928 3.1094677885
 H -2.5156551344 4.3884852363 2.4948233866
 N -0.771097773 1.817464479 1.2292887485
 H 1.230542704 1.5897777284 -0.7422349218
 C -1.6830776222 -1.7768395354 -0.064185261
 C -2.4638492207 -2.8239402201 -0.4974783583
 C -1.6575688232 -2.6003734692 2.0955643025
 C -2.8775776146 -3.8141030094 0.4182833464
 H -2.7371927425 -2.8925621771 -1.5428340103
 C -2.4460382921 -3.673867719 1.7501560427
 H -1.3180283296 -2.4797290244 3.1188743269
 N -3.6592265397 -4.8671880835 0.0220886998
 H -2.7414898213 -4.3769437561 2.5176447298
 N -1.2758702313 -1.6515049754 1.2212840852
 C 2.3423682499 -0.5915829235 -0.0499727851
 C 3.6293750279 -0.6268533607 -0.524111373
 C 4.6981459709 -0.4237919091 0.3756444281
 H 3.7930091164 -0.7845727987 -1.5822200528
 C 3.0396673179 -0.1515528239 2.1011898307
 C 4.3632739452 -0.1878494947 1.7230103927
 N 5.9994414624 -0.4533573636 -0.0494421303
 H 2.7719735275 0.0380312564 3.1352030482
 H 5.1250396674 -0.0530164999 2.4793040979
 N 2.0226743136 -0.3504696212 1.2430201046
 H 0.8613929234 -1.928425693 -0.8099522429
 H -2.0217743614 0.1401257759 -0.9006930549
 Cu 0.0003490653 -0.0711106868 1.452789674
 O 1.3838921088 -0.583441866 -2.2869946151
 C -3.4338176369 6.168707704 0.6862715659
 C -2.1168334671 6.152763209 -1.1559562839
 C -3.714268099 7.2833483259 -0.0334886543
 C -2.870972803 7.2794360444 -1.1950577507
 C 6.455701986 -0.9650625202 -1.2712974968
 C 7.1102904446 0.0198129944 0.6607244971
 C 8.2165040423 -0.1852365351 -0.0958160794
 C 7.8028961759 -0.8193141222 -1.3158621606
 C -4.4125659622 -4.9395014862 -1.1562275165
 C -3.8431042302 -6.0643918479 0.7250597662
 C -5.0469872201 -6.1379525791 -1.1815494957
 C -4.6764507279 -6.8556188058 0.0051153755
 H -3.88679387 5.7915370259 1.589291329
 H -1.3258784542 5.8236359784 -1.8109809541
 H -4.4499062475 8.031100818 0.2248916069
 H -2.82744853 8.0406300518 -1.9605166337
 H 5.7852092877 -1.4396777124 -1.9695893151
 H 7.0034178934 0.5078929296 1.6161215414
 H 9.2249839955 0.090829291 0.1759567927
 H 8.4445403961 -1.1379797269 -2.1244921683
 H -4.4816125504 -4.1029871641 -1.8332814236

H -3.3155305396 -6.2644552826 1.6440098253
H -5.7209424233 -6.478004658 -1.954435985
H -4.9922098197 -7.8516750155 0.2794247051

O_Cu2+_1f

2 2
C 0.1598098594 -0.1619261144 -3.3382604014
O 0.9253091148 -1.2046378107 -2.7010983526
C -1.3152719523 -0.2754820576 -2.9184896639
C 0.5621634784 -1.3275749019 -1.3546292045
N 0.0041380698 -0.0360405078 -0.8969692306
C 0.893538202 1.0713426299 -1.3448953956
C -1.3786425314 0.1255901342 -1.4263399581
H 0.2846131881 -0.3166128415 -4.408673736
H -1.6595676114 -1.3021850575 -3.0749030912
H -1.9361826255 0.3847132731 -3.5291318138
C -2.3358610337 -0.6255878684 -0.5179374344
C -3.5334151922 -1.1156064732 -0.9742964521
C -4.432807965 -1.7516549147 -0.0711958999
H -3.7880178959 -1.0163742295 -2.0222710257
C -2.7801884071 -1.328638578 1.6375805547
C -3.9986315105 -1.8429442565 1.2791710968
H -2.4426134107 -1.3982127799 2.666710009
H -4.6176436153 -2.3034728946 2.0379846997
N -1.9400365017 -0.7173168984 0.7764648043
H -1.6120282538 1.1925125564 -1.3334566977
C 1.7167380664 -1.7072981833 -0.4494000169
C 2.7991712302 -2.4042843322 -0.9111242655
C 2.5040627217 -1.7044454418 1.7158671842
C 3.8162762367 -2.8010315181 0.0047981361
H 2.8641477094 -2.633164489 -1.9671825353
C 3.6206717126 -2.4166220723 1.3601843658
H 2.3567326082 -1.4030039006 2.747923293
H 4.3368182178 -2.6833790559 2.126505708
N 1.5399402575 -1.3400736573 0.8447030785
C 0.6319498636 2.2747646632 -0.4609788316
C 0.7874908836 3.5631762169 -0.9043829984
C 0.6096184321 4.6515555953 -0.0021592775
H 1.050462563 3.7456339524 -1.938972364
C 0.1142170021 2.9863419014 1.6751095072
C 0.254378448 4.3054868712 1.329633495
H -0.1574336558 2.7168084093 2.6907364863
H 0.1036875199 5.0647959328 2.085793912
N 0.3001894601 1.9618114866 0.8176446801
H 1.9122424203 0.7313404109 -1.127911026
H -0.2358341646 -2.0752724321 -1.2319184019
Cu -0.031882599 -0.0463603622 1.0313762643
C 0.7299854894 1.191387253 -2.8753661359
H 1.6957092643 1.3889988256 -3.3445550746
H 0.0441858811 1.9991383503 -3.1530432594
N -5.6101448859 -2.2360512863 -0.4719720764
C -6.5316914603 -2.9764696225 0.4034881356
C -6.1416320792 -2.0881993015 -1.8335905321
N 4.8872935203 -3.491477684 -0.390110807
C 5.9991154535 -3.8596567793 0.4991652313
C 5.0856989445 -3.9905871218 -1.758324745
N 0.7644730197 5.9198067848 -0.3888257193
C 0.5121958942 7.0781327629 0.4819187056
C 0.5478581234 8.2648017946 -0.4823384207
C 1.533777758 7.8129009587 -1.5633463447
C 7.0712040518 -4.3749358857 -0.4626003549

C 6.2569120613 -4.9646488278 -1.6177080773
C -7.559077244 -3.557922006 -0.5689652803
C -7.6017816209 -2.5250375211 -1.6986426785
C 1.2230564045 6.3234716088 -1.724949558
H -6.9943283865 -2.2902899892 1.1239887658
H -5.9941374377 -3.7527171128 0.9561572316
H -5.5860777526 -2.7349507134 -2.5252287385
H -6.0472282319 -1.051548908 -2.1722110084
H 5.6732790099 -4.6374638789 1.2012984159
H 6.3350198256 -2.9905200791 1.0727344712
H 5.3276911571 -3.1565935482 -2.4295564938
H 4.1775130657 -4.4796675261 -2.1235974023
H 1.2970880102 7.1492152738 1.2454245061
H -0.4546825406 6.9765133796 0.9837941864
H 0.8525424664 9.1868851512 0.015435734
H -0.4451405069 8.4252050513 -0.9142622293
H 2.5641528868 7.9425452537 -1.2174348274
H 1.4209318416 8.3589085259 -2.5015364808
H 7.7298409173 -5.1040034477 0.012354042
H 7.6871114834 -3.5418785685 -0.816201678
H 5.8843679315 -5.95915309 -1.3524014183
H 6.8286334675 -5.0536346863 -2.5430670514
H -8.5294648059 -3.7123545683 -0.0942460346
H -7.2097792674 -4.5237008911 -0.9478163421
H -8.2209117863 -1.6698109014 -1.4097997617
H -7.9965042196 -2.9280405262 -2.6329079334
H 0.427925045 6.1518980566 -2.4623028893
H 2.1039809119 5.7445850361 -2.0198992721

O_Cu2+_1d

2 2
C -3.6340317281 0.6886359812 0.0284276306
O -3.2342223964 -0.329271219 0.9738926471
C -2.8919047216 1.999863764 0.3378873938
C -1.8562345044 -0.2907268655 1.181180043
N -1.2159537988 0.2814783324 -0.0287676574
C -1.8091335386 -0.3511884207 -1.2419540754
C -1.4087823049 1.7602382645 -0.0353466893
H -4.710112934 0.7975318862 0.1490551271
H -3.0104030958 2.2471831048 1.3971731413
H -3.3131669598 2.8210587851 -0.2469419143
C -0.3380787698 2.3914412415 0.834373577
C -0.4989676817 3.6233542062 1.4461277892
C 0.5646309628 4.1626110902 2.1680169979
H -1.4361467822 4.1622245361 1.3579708806
C 1.841338222 2.2186696652 1.6283179719
C 1.754089669 3.4498772449 2.2608431553
H 0.4609165866 5.1277105831 2.6526332659
H 2.7469405312 1.6235484451 1.6813090228
H 2.6024617126 3.8334214644 2.8153354812
N 0.8218963317 1.7008915678 0.9260128288
H -1.2254933112 2.0864233827 -1.0658535428
C -1.2561771243 -1.6548312089 1.4544511453
C -1.9665222164 -2.6791508818 2.0503595346
C 0.6870669487 -2.9184255577 1.3948788209
C -1.2979272094 -3.8705385451 2.3315125988
H -3.0156458432 -2.5429459446 2.2869137025
C 0.0483785256 -3.98912261 2.0051375695
H 1.7320039258 -2.9756160799 1.1091828752
H -1.8249116848 -4.6943875286 2.801149261
H 0.6010844046 -4.8984484171 2.210422564

N 0.0493992575 -1.769572081 1.1234724719
C -0.8323731764 -0.1859391069 -2.3877058924
C -1.2180874209 -0.1169820221 -3.7151325872
C -0.2335505224 -0.0537682764 -4.7008574074
H -2.2690052241 -0.1233689073 -3.98320251
C 1.4168202216 -0.1179375388 -2.9761812515
C 1.1045482324 -0.0546999324 -4.3266476755
H -0.5129881458 -0.0037958238 -5.7479749865
H 2.4476892023 -0.1131432924 -2.6379429449
H 1.8984436128 -0.004805047 -5.0625531628
N 0.4725611831 -0.187284293 -2.0263239426
H -1.8619631199 -1.4228604168 -1.0189310698
H -1.5994517445 0.3760334647 2.0188232669
Cu 0.6617398329 -0.1364778059 0.0245364541
C -3.2500005559 0.1903273497 -1.3773464938
H -3.9206467478 -0.605243251 -1.7072447044
H -3.3172760998 1.0125967136 -2.0978187102

O_Cu2+_4c

-1 2
C -3.6813423795 -0.070231227 0.0743685289
O -3.1118132502 -1.2445720738 0.6659757429
C -3.1963825876 1.1910289928 0.8152062281
C -1.7255974311 -1.0354534658 0.9229733568
N -1.2448593645 0.0152516867 0.0046504321
C -1.7100605634 -0.2674201761 -1.3824224344
C -1.69813466 1.3535147121 0.4746146562
H -4.7637200744 -0.1905463097 0.1640763969
H -3.3429877966 1.0677719954 1.8932934705
H -3.7712520014 2.0647306003 0.4907339197
C -0.7639046431 1.7774379828 1.5675890302
N 0.54542084 1.3868665532 1.4519411795
H -1.5873098888 2.0085875136 -0.3979073721
C -0.8624334788 -2.2402343716 0.7210088549
N 0.4565366615 -1.9863587587 0.4406029577
C -0.8228767853 0.5120797347 -2.303356973
N 0.4985868725 0.5982051139 -1.945938961
H -1.5421340048 -1.3419798547 -1.5125067533
H -1.6071519358 -0.6265540645 1.9365596785
Cu 0.710530606 -0.020306139 -0.0120686071
C -3.2308841326 -0.0040269575 -1.3986075525
H -3.7418308171 -0.7664918988 -1.993094634
H -3.4616402937 0.9786946693 -1.8271253269
C 1.0647337711 -3.198909923 0.3379468913
C 0.1532289601 -4.220829219 0.5587135934
C -1.0967420996 -3.5994247856 0.8053891615
C 1.1102163255 1.3374906285 -2.9108040573
C 0.2013383057 1.7140209854 -3.8874718978
C -1.0538077304 1.1859916626 -3.4897009336
C 1.1958910889 1.8960789097 2.5329840704
C 0.3232582508 2.617813125 3.3327502728
C -0.948405896 2.5355533626 2.7110598737
H 0.3596953898 -5.2845619036 0.5351889351
H -2.0460500024 -4.0753637251 1.0156893585
H 0.4117280512 2.3013454138 -4.7736989635
H -2.0001267566 1.273085028 -4.0115049453
H 0.5679874163 3.1332617163 4.2541428357
H -1.8763527929 2.9834927836 3.0481212968
H 2.1201511132 -3.2667037103 0.1007216106
H 2.1680314032 1.5641643868 -2.8428163175
H 2.2529563109 1.7057710066 2.6790333964

O_1b

O 1
C -0.1803101493 -0.0201793441 2.7850305417
C -0.8853847404 1.2315655499 2.2508714617
O -0.8149621118 -1.1771255985 2.2409165765
C -0.9511744554 1.0476492555 0.7140960593
N -0.0431252779 -0.0346414087 0.3054887619
C 1.3041796334 0.2162712354 0.8278224709
C -0.5358461098 -1.2876532505 0.8552277717
H -0.2806706385 -0.1110815666 3.8678118022
H -0.3354643911 2.1379848821 2.5250604206
H -1.8891426973 1.314701576 2.6725554601
C -1.7526502681 -1.7539576709 0.0713294762
C -1.5838199063 -1.9174621058 -1.3073728283
C -2.6771349663 -2.3448968861 -2.0387234055
H -0.6232406179 -1.7009353196 -1.7638815515
C -3.932835982 -2.3936333667 -0.025409195
C -3.8874566003 -2.5937732336 -1.3989058606
H -4.8588346951 -2.5731850126 0.5160237494
H -4.7590155307 -2.9281571807 -1.9492803371
N -2.8958831 -1.9817290766 0.7099290774
H 0.2563445165 -2.0358161563 0.7064706418
C -0.6994334417 2.3021032503 -0.099329117
C -0.1578535539 2.2065067622 -1.3844490927
C -0.8947463091 4.5722102056 -0.2619438361
C 0.0088247017 3.3802863256 -2.1014244408
H 0.1307030196 1.2398555734 -1.7819625236
C -0.3649893148 4.5983502576 -1.5463813243
H -1.2002581648 5.5002515739 0.2158634711
H -0.2448038921 5.5287227983 -2.0886137245
N -1.0587332756 3.4609628987 0.4572633928
C 2.3606999472 -0.5803388237 0.0780842509
C 3.6489489504 -0.6728946287 0.6128016796
C 4.6119969919 -1.3590633842 -0.1095095653
H 3.8936138964 -0.2173091327 1.5658815732
C 2.9732351998 -1.7920394351 -1.7633115723
C 4.2836270537 -1.9406294365 -1.3276587806
H 2.6652927971 -2.2313643861 -2.7091062228
H 5.0150899531 -2.4867724235 -1.9111144149
N 2.0285328435 -1.1300504937 -1.0925858987
H 1.5220043158 1.2719976283 0.6247096849
H -1.9594886451 0.7074468662 0.4502436812
C 1.2966767657 -0.0089296386 2.3662512727
H 1.8421595427 0.7790915344 2.8957844649
H 1.7475323525 -0.9710675721 2.6331198294
Cl 0.6922574808 3.3293741219 -3.7042764677
Cl -2.541730659 -2.5686688011 -3.7627474765
Cl 6.2325495327 -1.4941969622 0.5138900636

O_1e

O 1
C -0.0620969747 0.4938618546 2.8998525798
C -0.9111395073 1.5104979118 2.1290879908
O -0.4736861348 -0.8259827682 2.5403459837
C -0.8728336108 1.043339325 0.6533521121
N 0.2384324014 0.0901529805 0.4681223906
C 1.4989080081 0.6650659758 0.9979971748
C -0.0740269811 -1.122526854 1.1994228708
H -0.2196436628 0.5665576381 3.9779581999
H -0.5066361664 2.5223565666 2.242965581

H -1.9378128455 1.5242428897 2.5004091815
 C -1.1379271044 -1.9556408753 0.4983194439
 C -1.352717443 -1.7675024328 -0.8599270393
 C -2.319880295 -2.5386746102 -1.526758321
 H -0.7753019726 -1.0065479733 -1.367324427
 C -2.6753927878 -3.6096629748 0.5975307533
 C -2.9991967339 -3.493121761 -0.7460962347
 H -3.1919881646 -4.3534207287 1.2024623147
 H -3.7673922038 -4.1332736596 -1.1627975674
 N -1.7693386078 -2.8700274348 1.2394028021
 H 0.8409747651 -1.7312604884 1.2353244881
 C -0.8608957415 2.1607445047 -0.368847867
 C -0.0856623865 2.0636106701 -1.5145968999
 C -1.7360538315 4.1458618951 -1.0271071814
 C -0.1198796677 3.0987300931 -2.4678955682
 H 0.5636334901 1.2051465684 -1.6249045802
 C -1.0065606956 4.1611581644 -2.2060356221
 H -2.4133863391 4.9714903698 -0.8132452936
 H -1.1212159133 4.9946434724 -2.8884141025
 N -1.6808602248 3.1869918386 -0.1019464195
 C 2.682038397 -0.0378733632 0.3478996976
 C 3.393032297 -1.0507575035 0.9742233041
 C 4.4427267306 -1.7086450724 0.3000289068
 H 3.1305985431 -1.3426182362 1.9815706122
 C 3.9449240591 -0.244097587 -1.5358903689
 C 4.7120654102 -1.2700668107 -1.0091366227
 H 4.1498980467 0.10325397 -2.5478855096
 H 5.4951199228 -1.7109411559 -1.6131462154
 N 2.9501498028 0.3747771899 -0.9022965531
 H 1.5368407407 1.6917042795 0.6252041418
 H -1.7871442438 0.472882504 0.4610581068
 C 1.4184907797 0.6832094068 2.5438186782
 H 1.7979032824 1.6284429007 2.9457790851
 H 1.9885027056 -0.1229577897 3.0141047788
 N 0.6759023297 3.0664276828 -3.5849912033
 N -2.5788638303 -2.3546176837 -2.8631331213
 N 5.1548393195 -2.7175080971 0.8931484961
 C -3.6819569612 -3.0608159978 -3.4774041968
 H -3.543681911 -4.1462573525 -3.4048487179
 H -4.6492822072 -2.8067793928 -3.0191695745
 H -3.7281503781 -2.8052408834 -4.5372339783
 C -1.9712665429 -1.2327569478 -3.5518533847
 H -2.335840441 -1.2036978238 -4.5799594729
 H -2.2070693267 -0.2719261348 -3.0726155572
 H -0.8793590906 -1.3331291544 -3.5859125762
 C 1.5128017463 1.9086453502 -3.8320808031
 H 2.1164937041 1.6756345802 -2.9488398884
 H 0.9254013091 1.0130229087 -4.0890153625
 H 2.1874292616 2.1275986912 -4.6625238134
 C 0.4611210624 4.0299718183 -4.6418158567
 H 1.1596686536 3.8313850792 -5.4563480989
 H -0.5602492254 3.9834679749 -5.0475738575
 H 0.6422295095 5.0533848671 -4.2904576078
 C 4.7486757093 -3.2186516105 2.1910542175
 H 3.720619753 -3.6061993254 2.1803390618
 H 5.414703831 -4.0301760532 2.486689885
 H 4.8144883748 -2.4376125625 2.958237658
 C 6.1551891172 -3.4313146418 0.1275485832
 H 5.7230668247 -3.9406735555 -0.7455131889
 H 6.9425899278 -2.753625324 -0.224100539
 H 6.6252303385 -4.1835993015 0.7622341128

O_1a

O 1

C -0.2037620479 -0.0349646333 2.8082517732
 C -0.888654254 1.232443829 2.283872762
 O -0.8598021335 -1.1743557433 2.2497447506
 C -0.9650328309 1.0548425641 0.7465942444
 N -0.0643508643 -0.0290139132 0.3260387294
 C 1.2835506917 0.207234048 0.8544096231
 C -0.5638523926 -1.2838064835 0.8702323281
 H -0.307050528 -0.1353160254 3.8895705645
 H -0.3203375497 2.1269599772 2.5600494629
 H -1.8887168792 1.3327103899 2.7100326306
 C -1.766690236 -1.747911574 0.0674072421
 C -1.5466782363 -2.0197170506 -1.2870213745
 C -2.6343890184 -2.4400683795 -2.0229003325
 H -0.5634775614 -1.8906482039 -1.7262796765
 C -3.9828235501 -2.2716358679 -0.0915156605
 C -3.8876360397 -2.5777089389 -1.4425034264
 H -4.9380395706 -2.3560440025 0.4197913105
 H -4.7403088031 -2.9061328428 -2.0223512753
 N -2.9518378127 -1.8645180472 0.6569835471
 H 0.2286196422 -2.0316694546 0.7268529151
 C -0.7119469026 2.3105121698 -0.0624637424
 C -0.1517049234 2.2280871456 -1.3407970492
 C -0.9228206757 4.5889273345 -0.2131352738
 C 0.0116051364 3.4133259902 -2.0316786309
 H 0.1506601505 1.2750264964 -1.7579849943
 C -0.3740531497 4.6285839706 -1.48964117
 H -1.2437947713 5.5075103103 0.2709141866
 H -0.2453214025 5.5533545242 -2.0366448448
 N -1.0847947211 3.4669588203 0.4903086284
 C 2.3372454595 -0.5845075464 0.098691895
 C 3.6531105031 -0.5859746975 0.5705045655
 C 4.5938621296 -1.2773421984 -0.167365368
 H 3.9408991527 -0.0661662107 1.4763980659
 C 2.9131187779 -1.8914175958 -1.700402534
 C 4.2502673242 -1.9508483158 -1.3278800735
 H 2.5717933263 -2.4000215518 -2.5977517259
 H 4.9889452649 -2.4923504409 -1.9040568473
 N 1.9790410591 -1.229365026 -1.0136410527
 H 1.5095759796 1.2645450047 0.6698757927
 H -1.9775527294 0.7221127197 0.4896085219
 C 1.2737901142 -0.0427479311 2.3897780641
 H 1.8318929906 0.728520889 2.9299608109
 H 1.7121920805 -1.014541309 2.6414720133
 N 0.6175637588 3.3846155341 -3.3773313449
 O 0.7080405133 4.4458866548 -3.9718987455
 O 0.9897170844 2.304884742 -3.8024080887
 N 5.9949263591 -1.2979738033 0.2955355474
 O 6.7962838624 -1.9234344591 -0.3765096576
 O 6.255600737 -0.6886906572 1.3193019344
 N -2.4609692946 -2.7510768579 -3.4539386225
 O -3.456168223 -3.0734799842 -4.0812640692
 O -1.3350749964 -2.6686133688 -3.9143963291

O_1c

O 1

C 1.2247030312 -2.3012696664 3.0837329184
 C 0.0101047903 -1.5726702134 3.6771558619
 O 0.7827454208 -3.1492186474 2.0177369387

C -0.7476057499 -1.0009101945 2.4575730401
N 0.1477638081 -0.9896525725 1.2909973931
C 1.4100041981 -0.3225418806 1.6263658393
C 0.4141642058 -2.3586648552 0.8968208608
H 1.6978515772 -2.9646924899 3.8093085976
H 0.3240582493 -0.7808782415 4.3661215746
H -0.6222891202 -2.2651548911 4.2367428292
C -0.8031094781 -2.9068306477 0.1668711521
C -1.3908365336 -2.0589791301 -0.7717932201
C -2.5362780298 -2.4825007329 -1.4323390575
H -0.9487964594 -1.0876033957 -0.962224293
C -2.3190696661 -4.5422838484 -0.2437156937
C -3.0145556238 -3.7666384457 -1.1612299854
H -2.6661727549 -5.5482764185 -0.0184301456
H -3.919399165 -4.1416707224 -1.6262360118
N -1.2380384809 -4.1357158641 0.4305581189
H 1.2516856208 -2.3355050656 0.1809682393
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C -1.6088943332 1.1271198679 1.4844602134
C -2.4086936535 1.9058694021 3.9451273619
C -2.2679775985 2.3434604537 1.6030406469
H -1.2483032167 0.7584608588 0.5331456722
C -2.6790562655 2.7484239308 2.8744160817
H -2.7118957436 2.1992412566 4.9477571027
H -3.1692949681 3.7015728849 3.0368610995
N -1.7768399106 0.7324688285 3.8471729099
C 2.0929319556 0.1826767938 0.3633690787
C 3.4793984717 0.195027359 0.2472913293
C 4.06342885 0.7015401997 -0.914183182
H 4.1047820304 -0.1545477251 1.0601471245
C 1.858424288 1.1553109464 -1.692712492
C 3.2281374392 1.1874512774 -1.9172971907
H 1.1789918124 1.5331026342 -2.4537498583
H 3.6263006226 1.556309221 -2.8553564636
N 1.2867319633 0.6717178972 -0.5905895429
H 1.1409047919 0.5741271159 2.1984729293
H -1.5594464434 -1.6930822291 2.2040928827
C 2.2304602961 -1.2756828056 2.532923033
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H 2.9952201174 -1.8197350563 1.9676936426
N -2.504234964 3.1226954471 0.4577882205
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N 5.4588907274 0.7156135735 -1.0645644885
C -3.9240144915 -2.0000912824 -3.4358740556
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C -4.3981054991 -0.8699862438 -4.0447065198
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C 6.33832749 -0.204495728 -0.5261777301
C 6.1830454225 1.6519257465 -1.777448332
C 7.6064940648 0.1455238802 -0.8983803006
C 7.5085604977 1.3293398641 -1.6866193599
C -3.5509048377 4.0037020438 0.2740532746
C -1.7615469203 3.0675891597 -0.70693731
C -2.3339626701 3.9133030021 -1.6175672649
C -3.4735341929 4.503889548 -0.9966552461
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H -4.9928277331 -0.8431905815 -4.946946181
H -4.1615212058 1.2916273952 -3.457517923
H 5.974458134 -1.0564613374 0.0279536793
H 5.6902977047 2.4932207463 -2.2408641491

H 8.5087040442 -0.3929892437 -0.6455022831
H 8.3241494951 1.8851233656 -2.1269128676
H -4.2872444295 4.1569297554 1.0482721517
H -0.8665453288 2.4636857946 -0.7599689718
H -1.9693469783 4.1019880709 -2.6175016294
H -4.1622374028 5.2094720388 -1.4393773379

O_1f

O 1

C -0.0788439728 0.3419146208 2.6897324084
C -0.9253298153 1.4137530417 1.991658877
O -0.5162576985 -0.9496798952 2.2613341482
C -0.9179042242 1.0220582017 0.4945253671
N 0.1850331807 0.0798444776 0.2457920268
C 1.4486039291 0.6189631912 0.7750631405
C -0.1141081873 -1.1732482732 0.9083722664
H -0.2161111587 0.3547553379 3.7729269434
H -0.5025675923 2.4121901105 2.1504044046
H -1.9444420034 1.4229292547 2.3839296183
C -1.170473684 -1.9579507582 0.143283031
C -1.2760921052 -1.7382654724 -1.2228309566
C -2.2386869609 -2.4382788775 -1.9659887248
H -0.6282823409 -1.0002509103 -1.6764684199
C -2.7968313467 -3.5282596147 0.1008790572
C -3.0162812848 -3.3751295548 -1.260151474
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H -3.7669697276 -3.9799071984 -1.7569151267
N -1.9035249799 -2.8446561858 0.8213917564
H 0.8108327203 -1.7713952072 0.9101015101
C -0.9018088186 2.1745996269 -0.4881900642
C -0.219376008 2.0444054916 -1.6890366406
C -1.6697189761 4.234588426 -1.0488766063
C -0.2728759335 3.0872256108 -2.6301459163
H 0.3747473537 1.1536994474 -1.8573179646
C -1.0376450851 4.21722368 -2.2825795065
H -2.2556011325 5.1080633786 -0.7658706475
H -1.1232540861 5.0719374112 -2.9443450841
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C 2.6301633219 -0.0243601449 0.0588006889
C 3.7220967344 -0.5340271483 0.7440590249
C 4.7992603771 -1.1054038863 0.0350268329
H 3.7569493308 -0.479773043 1.8240530672
C 3.5683030629 -0.5579496151 -1.9480264561
C 4.6978815859 -1.1109067871 -1.3671424752
H 3.4819856489 -0.548628225 -3.0342743455
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H 1.4695833519 1.6756748638 0.4845964712
H -1.8373032811 0.4636743349 0.2873948163
C 1.4023256627 0.5201045722 2.3198261517
H 1.8250416553 1.4100825317 2.7980112069
H 1.9410481984 -0.3549116778 2.6974139495
N 0.3918820479 2.9904907763 -3.8166769376
N -2.3970458167 -2.2008898859 -3.3020368045
N 5.8791697891 -1.624996839 0.6824167894
C -3.5269264562 -2.6910807116 -4.0778497379
C -1.6186508263 -1.1951267541 -4.0124128768
C -3.5675369967 -1.7542860562 -5.290718992
C -2.1052944991 -1.326757918 -5.4561668393
C 5.9620696229 -1.768473038 2.1299540024
C 7.049391467 -2.1509971295 -0.0052463185

C 7.1698754378 -2.6882862476 2.3295163764
 C 8.0594442027 -2.3658808486 1.1246387485
 C 0.2946695449 3.9745590538 -4.8819513849
 C 1.2410855259 1.8580787055 -4.1620127287
 C 1.9709672783 2.3392487496 -5.417163825
 C 0.9506534949 3.2738096101 -6.0763608128
 H -4.4539302399 -2.6444688869 -3.493663702
 H -3.3757025179 -3.7379863092 -4.3801079498
 H -0.5441489012 -1.3908865665 -3.9155981244
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 H -3.9802647987 -2.2381314045 -6.1796107149
 H -1.9895072536 -0.3973383482 -6.0199531071
 H -1.5389621324 -2.1105827338 -5.9716143112
 H 5.0411485943 -2.2043701012 2.5342246406
 H 6.1128243964 -0.7927408867 2.6154718945
 H 7.4138193663 -1.4409558236 -0.7568252657
 H 6.8143325959 -3.0945061692 -0.5211417854
 H 6.8490541766 -3.7349746921 2.2902147596
 H 7.6658047401 -2.5222416795 3.2888274753
 H 8.7789939649 -3.1557127533 0.8959392711
 H 8.6168453336 -1.4401414052 1.3050737614
 H 0.826405587 4.9010187516 -4.6159372156
 H -0.7510267041 4.2390201428 -5.0822678609
 H 0.6354958366 0.9603633161 -4.3678875757
 H 1.9197228947 1.6099098551 -3.3391679381
 H 2.2798268388 1.5142367347 -6.0643682852
 H 2.8674224876 2.9015969674 -5.1327508692
 H 0.2010232158 2.685852317 -6.6182067157
 H 1.3993593582 3.9794727842 -6.780056087

O_1d

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 C 1.1551992429 -0.7630821957 0.6862835305
 N -0.0035562782 0.0375837912 0.2595397336
 C -1.2411500875 -0.5636225045 0.7673783341
 C 0.1311516474 1.379861813 0.8037688243
 H 0.1566315337 0.1888513186 3.8253711547
 H 0.8514058825 -1.9608889402 2.5071783237
 H 2.1116951181 -0.7341305248 2.6541018797
 C 1.2008882653 2.1451353981 0.0406100935
 C 1.0143694474 2.2987072142 -1.3369975814
 C 1.9735629534 2.9886203187 -2.0612262033
 H 0.1329635932 1.8655157985 -1.8008775351
 C 3.170411305 3.2875533493 -0.017452396
 C 3.0814686459 3.4986607818 -1.3873109149
 H 1.8643271182 3.1264948003 -3.1331520252
 H 4.0220561094 3.6671739378 0.5436370704
 H 3.8594715586 4.0450788577 -1.9105552518
 N 2.2547789792 2.6238966809 0.6961442678
 H -0.8268898642 1.8907957687 0.631064009
 C 1.249349054 -2.049621066 -0.1116926699
 C 0.7389533281 -2.1180574279 -1.4116669304
 C 2.0191358871 -4.2010666806 -0.22728298
 C 0.8891352626 -3.2998395064 -2.1237078479
 H 0.2257539959 -1.2557680097 -1.8242973075
 C 1.5470835994 -4.3694342049 -1.52352527
 H 2.5369520994 -5.0123814841 0.2806022801

H 0.4979810228 -3.3860948765 -3.1334471832
 H 1.6884933463 -5.3118899771 -2.0422770836
 N 1.8754329676 -3.0740782598 0.4735063072
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 C -4.8632058641 0.0378649039 -0.1890211107
 H -3.847016002 -0.8903356745 1.4671270835
 C -3.3838644912 0.9523577943 -1.8153679318
 C -4.684836866 0.7160099294 -1.3907010627
 H -5.8596990939 -0.1731383879 0.1876255778
 H -3.1975178599 1.4821920978 -2.7473339572
 H -5.5285573237 1.0545937949 -1.9824989742
 N -2.2972318219 0.5642812317 -1.1428339415
 H -1.1638976703 -1.6389530465 0.5648899748
 H 2.0388305078 -0.1700980605 0.4230364316
 C -1.3115147726 -0.3478425483 2.3063756154
 H -1.6237379468 -1.2570367978 2.8311854496
 H -2.0139460968 0.4517894105 2.5662655132

O_Cu1+_2b

1 1
 C 0.6763284338 2.8411445745 0.8020952527
 C -0.0456126987 1.8664075513 1.7461676559
 C -0.1614289853 3.0112832426 -0.4696641064
 C 0.1471497587 0.4786523487 1.1065628874
 N 0.476332674 0.6422837675 -0.3369129282
 C -0.4380543288 1.5944354425 -1.0392858734
 C 1.8139398335 1.2124380621 -0.4344792361
 H 0.8826027589 3.7976161359 1.2808345325
 H -1.0978760315 2.1583174526 1.8227301444
 H 0.3834961533 1.8886223808 2.7506877159
 H 0.3975439632 3.607486626 -1.195874226
 H -1.0697543652 3.5729592444 -0.2419275841
 C 2.9252981301 0.1919959552 -0.221952683
 C 4.1440208732 0.5958228346 0.2981527923
 C 5.1789911757 -0.3332268824 0.353001556
 H 4.2731405757 1.6128918586 0.6471280144
 C 3.7132372066 -1.9473187965 -0.5995267879
 C 4.970109036 -1.6268102921 -0.1148762122
 Cl 6.7132394843 0.1224842746 0.992502122
 H 3.4986388079 -2.9482385805 -0.9563475461
 H 5.7587344959 -2.3690613802 -0.093408424
 N 2.7014450052 -1.0659708515 -0.6550986593
 H 1.9267636477 1.573544322 -1.4681335864
 C -0.9276592147 -0.5849856799 1.2994848594
 C -1.9999163356 -0.4340565068 2.1622674903
 C -1.6009410394 -2.7378175343 0.7594331282
 C -2.9066848304 -1.4832237064 2.2947219736
 H -2.1478343443 0.4840524509 2.7170377516
 C -2.7082266539 -2.6629615767 1.5890695496
 H -1.3985582061 -3.6365942909 0.1877659035
 Cl -4.2755791403 -1.3053281245 3.3287824549
 H -3.3920320418 -3.498114187 1.6784432465
 N -0.7346774595 -1.7300221854 0.608565814
 H 1.0507194311 0.0450353267 1.5547921078
 H -0.1317473915 1.5524905095 -2.0881651209
 C -1.8617277312 1.0619535037 -1.0239823036
 C -2.9185150884 1.687319704 -0.3728867268
 C -4.1638760763 1.0649257912 -0.3881895419
 H -2.8019741475 2.6270040351 0.1520060642
 C -3.2079486345 -0.6612136572 -1.7051103511

C -4.3257596372 -0.1358744744 -1.0613555217
Cl -5.4948431878 1.7901062156 0.4499924148
H -3.2907465609 -1.5914005901 -2.2609975322
H -5.2838934592 -0.6406615503 -1.0955784482
N -2.0057056652 -0.0914376783 -1.6908934707
Cu 0.7755064246 -1.5412874279 -0.654973479
O 1.9628053861 2.2900323423 0.4685549175

O_Cu1+_2e

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C 0.1273355526 -2.5447960654 0.5217231334
C 0.0672862777 -2.5457471794 -1.9784360147
C -0.2118471104 -1.0441133338 0.6097099699
N -0.6821881008 -0.5757601686 -0.7222190259
C 0.2153510414 -1.006919908 -1.8384221054
C -1.9854683503 -1.1673307982 -0.9861858822
H -0.7256640398 -4.1416762007 -0.7151151574
H 1.196691257 -2.731106901 0.3808585446
H -0.1902336705 -3.064237161 1.4293843215
H -0.5450862872 -2.7906963689 -2.8509110799
C -3.1441028406 -0.475538844 -0.2759015542
C -4.2670080206 -1.200996259 0.0494096591
C -5.4092863511 -0.5462269476 0.5702211174
H -4.2456906652 -2.269651777 -0.1129065319
C -4.1354945269 1.4925183696 0.3791523858
C -5.3091620258 0.858264347 0.7126558949
H -4.043819318 2.5658164784 0.5055984977
N -3.0487351061 0.8642674528 -0.1092059802
H -2.1734559222 -1.0362476488 -2.0625533943
C 0.8116482628 -0.0691562662 1.1876290238
C 2.0183040211 -0.4650528683 1.7156962808
C 1.260850012 2.1398327136 1.6779784344
C 2.9361110307 0.4953909226 2.2035387258
H 2.2800016236 -1.5133380431 1.702274083
C 2.4999241259 1.8376729375 2.1963027854
H 0.9148120825 3.1676316161 1.6578131793
H 3.1157282345 2.6422846616 2.5749832344
N 0.4240996902 1.2283386909 1.1641347571
H -1.0882380029 -0.9555557767 1.2646679509
H -0.1870095942 -0.5131121142 -2.7273792713
C 1.6100958815 -0.4260796596 -1.652226878
C 2.738089375 -1.201922605 -1.4388134398
C 3.9743630477 -0.5831578655 -1.1588297229
H 2.6681860673 -2.2803280164 -1.440952588
C 2.8042998864 1.4966928424 -1.4434026417
C 3.9826823791 0.8227287812 -1.1659342381
H 2.8072820635 2.5838194262 -1.4733466528
H 4.8848708533 1.391304969 -0.9797163692
N 1.6300923642 0.9132135329 -1.6810372437
Cu -1.2083445773 1.4685794171 0.1301745226
O -1.976510328 -2.5524704001 -0.6732943597
N 4.1722576428 0.1410114594 2.6371441016
H 1.0194552751 -3.0629489896 -2.1134538212
H -6.1308597029 1.4528279092 1.089188413
N -6.5306411008 -1.2258229172 0.9037250819
N 5.0912291082 -1.319130351 -0.8647912483
C 6.3342299255 -0.640060194 -0.5542762099
H 6.1992884786 0.0432728348 0.2938257107
H 7.0863874643 -1.3772457129 -0.2716628954
H 6.7197414332 -0.0651415643 -1.4066025567

C 5.1027193908 1.1639418595 3.0834098995
H 4.7271546765 1.6934957418 3.9670544645
H 6.0503851807 0.6963065219 3.3496971998
H 5.295800991 1.8974991892 2.2908664311
C 5.0824881427 -2.7568359174 -1.0574901483
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H 4.3883663624 -3.2545398286 -0.3663453003
H 4.8024965501 -3.0281665956 -2.0832162461
C -6.5874399352 -2.6688153452 0.7304146121
H -6.4607788508 -2.95078599 -0.3214845259
H -5.8167539419 -3.1717640364 1.3258775282
H -7.5597752659 -3.0309013641 1.0624869286
C -7.6885849696 -0.5117289191 1.4182817471
H -7.4504077371 0.0138422897 2.3504325147
H -8.0668594811 0.2143295088 0.6890397483
H -8.4851802808 -1.2246360209 1.6279739766
C 4.5776181601 -1.2539494983 2.6292768027
H 5.5880292348 -1.3347756274 3.0297913329
H 3.9191689451 -1.8661882103 3.2567791213
H 4.5807424468 -1.6585457088 1.6091484898

O_Cu1+_2a

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C 0.1983023775 -1.718687298 -2.8411531539
C -0.2326364032 -1.3456579327 0.1059982762
N -0.6222560779 -0.3720521767 -0.9542106127
C 0.3394551285 -0.3609472556 -2.1033824494
C -1.9076629846 -0.7916978357 -1.5050304494
H -0.6725147352 -3.6611006998 -2.3498190571
H 1.1882119291 -2.8480675502 -0.6844971018
H -0.2594222491 -3.5229899118 0.0707468806
H -0.3580550943 -1.5868779336 -3.77291055
H 1.1559368332 -2.1652257893 -3.1150029851
C -3.1032167321 -0.4151675584 -0.6385499173
C -4.2597803897 -1.1806410335 -0.6903392013
C -5.3587050357 -0.7194171062 0.0114146093
H -4.2976196734 -2.101251343 -1.2588330666
C -4.1131178639 1.146961873 0.7474881902
C -5.3171734313 0.459074332 0.7344864552
H -4.0047157288 2.0664656808 1.3105714885
H -6.185064662 0.8168365408 1.2739034592
N -3.0271695393 0.7225211252 0.0807899125
H -2.0353944332 -0.2440933836 -2.4516049944
C 0.7579281872 -0.7027876671 1.0689340098
C 1.9420732063 -1.2998263896 1.4691693086
C 1.171762966 1.1447483976 2.4253241408
C 2.7492196831 -0.6038389162 2.3537643875
H 2.2627185115 -2.262264901 1.0920854089
C 2.3773614841 0.6209282387 2.871948683
H 0.8193438556 2.1076163678 2.7766505921
H 3.0055119181 1.1490691704 3.5780310801
N 0.396179634 0.5122781153 1.5382367671
H -1.1424748655 -1.5001657784 0.7005027448
H -0.0040759403 0.4517509649 -2.7496088939
C 1.7230843468 0.0588713668 -1.6325136179
C 2.8457593835 -0.7592542509 -1.6965016663
C 4.0299615414 -0.2633941072 -1.175820611
H 2.8370111063 -1.7584423363 -2.110274943
C 2.928814086 1.7548394338 -0.6546706443

C 4.106091288 1.0065002479 -0.6414563477
H 2.9231451412 2.7686217544 -0.26450594
H 5.0354366403 1.394750203 -0.2436692174
N 1.7709237187 1.2996226371 -1.1260031118
Cu -1.1590931792 1.2047739967 0.5312266089
O -1.9175482721 -2.1819968626 -1.7447209898
N 5.2280950934 -1.1304038008 -1.177683601
O 6.2462040787 -0.6623596839 -0.7070053712
O 5.0970380155 -2.2482569583 -1.6435043635
N 4.0612792117 -1.1801828738 2.7193113087
O 4.6691372839 -0.6355617205 3.6190429324
O 4.4302320537 -2.1447121209 2.073400825
N -6.6120503543 -1.5083192523 -0.0155796843
O -6.5918015696 -2.5451853536 -0.6506046092
O -7.556014964 -1.0538431678 0.6013709813

O_Cu1+_2c

1 1
C -0.8197339933 -2.855053502 -1.4494691513
C -0.0694205138 -2.5306897646 -0.1511823259
C -0.0666133602 -2.2130348836 -2.6225117624
C -0.3327273881 -1.033118213 0.100741639
N -0.8225783716 -0.3953148841 -1.1522846802
C 0.0090429663 -0.6871191574 -2.3554315909
C -2.1490264501 -0.9154819178 -1.4333021792
H -0.9403344828 -3.9284751274 -1.5923565357
H -0.6038870232 -2.4042784883 -3.5550683728
H 0.9175614841 -2.6798403574 -2.722784322
C -3.2128740959 -0.3042644865 -0.5302837427
C -4.317605296 -1.042450039 -0.1596407119
C -5.3430207543 -0.4259969903 0.5708781824
H -4.3533937104 -2.0917734411 -0.4222284465
C -4.0358535586 1.5824064255 0.5003660412
C -5.1885495947 0.9293674601 0.8885347282
H -3.8896654884 2.6279568876 0.7476081957
H -5.9596061548 1.4789966149 1.4132356065
N -3.0486155915 0.995996998 -0.1978776978
H -2.4018420081 -0.607398582 -2.4584691605
C 0.7610347509 -0.1976338336 0.7539427959
C 1.8397770631 -0.7663541729 1.4032724247
C 1.4785507924 1.924522164 1.312315506
C 2.8016903441 0.0547397059 2.0043111063
H 1.9366819394 -1.8430457763 1.4554993966
C 2.6083052252 1.4388952448 1.940587397
H 1.2955021742 2.9919118247 1.2582008559
H 3.330382103 2.1307845449 2.3554616941
N 0.563195458 1.1388887538 0.7286323695
H -1.1829720609 -0.9730946994 0.7926816915
H -0.4882485693 -0.1495633902 -3.1658261985
C 1.353938856 -0.0016042548 -2.218941922
C 2.5117959704 -0.6489529115 -1.8193771381
C 3.6570236871 0.1096118921 -1.5593246103
H 2.5204043426 -1.7160064758 -1.6326443786
C 2.3976180672 2.0292463694 -2.2171829189
C 3.5988711404 1.4841859861 -1.781935347
H 2.3266856757 3.0959260189 -2.4132962033
H 4.4707286755 2.1129075754 -1.645488749
N 1.2874608752 1.3219254678 -2.4189616353
Cu -1.1402227682 1.5770842465 -0.20081376
O -2.1563930017 -2.330686059 -1.3540972801
N 4.8102555134 -0.4956810223 -1.0542769608

N -6.4678865513 -1.1345015413 0.9602301247
N 3.9076310228 -0.4925881648 2.6361223595
C 5.7471128468 0.1146385615 -0.2363185015
C 5.2102096718 -1.8032565536 -1.2798553794
C 6.3873133228 -2.0091629767 -0.6176358007
C 6.7220124807 -0.7953412892 0.0523797957
C -7.3190316094 -0.800302068 2.0089906598
C -6.9408199105 -2.3028839098 0.3707475132
C -8.0659741994 -2.6887084151 1.0324181558
C -8.3000419298 -1.7412296615 2.0782906448
C 4.4509593531 -1.745673017 2.3833246758
C 4.6552005677 0.1148058031 3.6384752701
C 5.5184795253 -1.9217904512 3.2097107159
C 5.6417624152 -0.7465971898 4.0136526398
H 5.6001565325 1.124506674 0.1153329242
H 4.6643238302 -2.4404465 -1.9593556448
H 6.9616040397 -2.9245299301 -0.62378544
H 7.572736688 -0.6231905981 0.695180707
H -7.1145065931 0.0457608448 2.6463279513
H -6.4656831318 -2.7189530512 -0.503792808
H -8.6726538344 -3.5501513298 0.7934829748
H -9.1004328628 -1.763944433 2.8036101287
H 4.0975606779 -2.3506230527 1.5624444254
H 4.3686706895 1.0723621408 4.0451912806
H 6.1648836616 -2.7872606263 3.2254227528
H 6.3703609358 -0.5680539412 4.7913286743
H 0.9926079604 -2.7608581817 -0.284179657
H -0.4393684675 -3.1311888921 0.6834470082

O_Cu1+_2f

1 1
C 0.6691696715 2.9863773224 0.4398045019
C -0.1256117524 2.0811653697 1.3905475139
C -0.1281760273 3.1408010398 -0.8635817809
C -0.0019999445 0.667049518 0.790305348
N 0.4440013167 0.767619691 -0.6247458918
C -0.3345548958 1.7243279311 -1.4600993758
C 1.8166306581 1.2334134929 -0.6308837479
H 0.8875669268 3.9552449502 0.8891254118
H -1.162447016 2.4302309259 1.4393249759
H 0.2871197699 2.1079526575 2.4024809804
H 0.4298376327 3.7664498198 -1.5654033683
H -1.069564523 3.6580615106 -0.6550030144
C 2.7961915478 0.1345586827 -0.2387079373
C 3.9587483887 0.4483499419 0.423071937
C 4.9280507412 -0.5569894835 0.6605612212
H 4.1153759983 1.4738951845 0.7311654742
C 3.4152695079 -2.0688879354 -0.452164358
C 4.6162961424 -1.8517687669 0.1823378066
H 3.1600018761 -3.0626075087 -0.8045214502
H 5.2947843916 -2.6836976945 0.3224764663
N 2.4932358817 -1.1129802919 -0.6758993537
H 2.0577599979 1.503999009 -1.6688889912
C -1.1708230292 -0.2982778283 0.9524098185
C -2.1399407173 -0.1138868152 1.9172088481
C -2.136358727 -2.2757424082 0.2750392152
C -3.1743727063 -1.0633646069 2.0759661005
H -2.0987722254 0.7617783983 2.5523668126
C -3.1641997913 -2.1574015767 1.1829561868
H -2.0997788699 -3.1241906186 -0.3996708501
H -3.9406462573 -2.9115715833 1.2016272441

N -1.1335930151 -1.3915936805 0.1581612746
 H 0.835458323 0.1780762939 1.3051593212
 H 0.1371694026 1.670612338 -2.443574581
 C -1.7271678056 1.1703750512 -1.6773510254
 C -2.8203971504 1.5567899775 -0.9260440285
 C -4.0225276493 0.8262993695 -1.0270276681
 H -2.7332081372 2.3623738284 -0.2080490067
 C -2.9162563626 -0.4575132839 -2.7312220545
 C -4.0550867135 -0.2030830179 -1.986560373
 H -2.9349020467 -1.2372247739 -3.4892844834
 H -4.953404763 -0.7835129872 -2.1596557275
 N -1.7548416907 0.1829308131 -2.5842332988
 Cu 0.5403160882 -1.4228669609 -0.9131771782
 O 1.9521311586 2.3849389879 0.1915271028
 N -4.1228907202 -0.9332359447 3.0327404803
 N -5.0789909742 1.091438282 -0.2164421626
 N 6.08104597 -0.2893451391 1.3002923865
 C 6.4057036942 1.0151335525 1.8795636693
 C 7.1604095825 -1.2628344939 1.4739487998
 C 7.6560033754 0.7325175547 2.7151796526
 C 8.3365023613 -0.4099789364 1.9550614763
 C -5.0884080156 2.1762760656 0.7532267028
 C -6.2347158781 0.2106274668 -0.0938430523
 C -6.8834531088 0.6528311227 1.2201692337
 C -6.5058549849 2.1332144216 1.3275095224
 C -4.1350291391 0.1513831594 4.0123702587
 C -5.0680437506 -1.9999707149 3.3708799909
 C -5.4178243377 -0.0950413429 4.8071197067
 C -5.5691433289 -1.6189948014 4.7675919053
 H 5.5739666889 1.3866937487 2.4870262436
 H 6.6043978109 1.7482809114 1.0859421536
 H 7.3771759522 -1.7731594854 0.5297904625
 H 6.8768722133 -2.020804797 2.2168814689
 H 7.366402526 0.4005740905 3.7178081091
 H 8.2897044341 1.6153828658 2.8207760684
 H 9.0348444892 -0.9801590343 2.5709549477
 H 8.886782537 -0.0165201762 1.0940143863
 H -4.8640473242 3.1354588364 0.2731081621
 H -4.3285896338 2.0066751502 1.5328010522
 H -5.9153985072 -0.8384631087 -0.0631327616
 H -6.9163375433 0.332526756 -0.9467733801
 H -6.4351232439 0.0965941854 2.0490262422
 H -7.9617154227 0.4802877744 1.234562332
 H -6.5513920596 2.5156934212 2.3504112917
 H -7.175324062 2.7414255216 0.7108469522
 H -4.1384813953 1.1274777995 3.5156255565
 H -3.2450824421 0.1010306688 4.6564206184
 H -4.568408985 -2.9746024027 3.3675952567
 H -5.8858526186 -2.037540432 2.6382512957
 H -6.2663245054 0.3874241384 4.3100935925
 H -5.3554431317 0.3018752017 5.8224290218
 H -6.5938357344 -1.9522759397 4.9437926039
 H -4.9300543926 -2.0790762282 5.5281357363

O_Cu1+_2d

1 1
 C 0.685661938 2.7800229036 1.2774545742
 C 0.1434834751 1.6325637689 2.137551181
 C -0.3743805432 3.0907607212 0.2020328623
 C 0.2660943714 0.3871981871 1.2428808255
 N 0.4285010192 0.8126626546 -0.1732636884

C -0.5454505973 1.8096883683 -0.6546185627
 C 1.7412704724 1.4059361622 -0.3152927318
 H 0.9156360382 3.6653656744 1.86899898
 H -0.8928353594 1.8539788907 2.4146848519
 H 0.7212669592 1.507664263 3.056555423
 H -0.0466481878 3.9221338593 -0.4268858761
 H -1.2909968473 3.4110727888 0.7059050685
 C 2.7982485823 0.3148273015 -0.3468546293
 C 4.045797828 0.4753209898 0.2315652738
 C 4.9876090166 -0.5389860859 0.0790663344
 H 4.2615704957 1.380831643 0.7867035969
 C 3.3678707235 -1.7543460967 -1.1909665083
 C 4.6456301822 -1.6695980733 -0.6513456673
 H 5.9738609313 -0.4433327422 0.5211725658
 H 3.0588482196 -2.6247396883 -1.7599010212
 H 5.3490481639 -2.4803502769 -0.8018193386
 N 2.4501000714 -0.789377827 -1.0452123427
 H 1.7738019713 1.9008705933 -1.2969668854
 C -0.7564853035 -0.7269080174 1.4024262621
 C -1.6251345297 -0.8058159346 2.4821339832
 C -1.4899314936 -2.7703341303 0.6030241384
 C -2.4569161425 -1.9155913339 2.60594664
 H -1.651012885 -0.0191566023 3.2270296609
 C -2.38994544 -2.9195130541 1.6505794485
 H -1.3981943041 -3.5285010542 -0.1681559453
 H -3.1430247076 -1.9927279625 3.443081512
 H -3.0149018198 -3.8030380041 1.7095821354
 N -0.6929199414 -1.705661861 0.4771782543
 H 1.2222617084 -0.0912089637 1.4880667202
 H -0.2151174945 2.039286493 -1.6732883967
 C -1.8800774153 1.1205983774 -0.8611695075
 C -3.0956574706 1.5686297607 -0.3699315918
 C -4.2509051883 0.8497816939 -0.6745470012
 H -3.1531227749 2.4658302891 0.2359325062
 C -2.8859090994 -0.6574832434 -1.922044672
 C -4.1479506874 -0.2826711057 -1.4677783346
 H -5.2149189884 1.179089797 -0.3004950967
 H -2.7603952902 -1.5359437151 -2.5486577266
 H -5.0205410123 -0.866150963 -1.7386110189
 N -1.7738786259 0.0152833348 -1.6278106804
 Cu 0.3730778457 -1.0489389741 -1.1922876402
 O 1.9439021357 2.373807194 0.6989820654

O_Cu2+_2b

2 2
 C -0.4588830387 -3.3360160251 -1.3798113669
 C 0.0914384104 -3.1414757203 0.0359885094
 C 0.5331248671 -2.6597036986 -2.3526512919
 C -0.2057991035 -1.673018392 0.3630666647
 N -0.4409229334 -0.9317545368 -0.9332442526
 C 0.5332897364 -1.1457210969 -2.0257088355
 C -1.7485370309 -1.3541637375 -1.4382694635
 H -0.6026888263 -4.3841074686 -1.6341060962
 H 1.1615513903 -3.3702125704 0.0456423023
 H -0.4032215129 -3.7931887301 0.7593143001
 H 0.2317498697 -2.814865341 -3.3904186252
 H 1.5118557166 -3.1303250781 -2.2231421053
 C -2.7922796949 -0.6321845072 -0.6032114352
 C -4.0475619678 -1.1384922692 -0.3561576146
 C -4.9597995972 -0.3380891016 0.3424870475
 H -4.3131942594 -2.1312204557 -0.7027179838

C -3.2855989062 1.3605766082 0.4875157066
 C -4.573100754 0.9350053031 0.7622500317
 H -2.9447558978 2.3363671007 0.8163864892
 H -5.2579021864 1.5796415276 1.3005322793
 N -2.4010489767 0.6028630935 -0.1836873895
 H -1.8483629305 -0.980194059 -2.4681508561
 C 0.6938448464 -0.9282898023 1.337548171
 C 1.5863034571 -1.5866246154 2.16305458
 C 1.1029446361 1.0909341483 2.3959686714
 C 2.2580199132 -0.8510051803 3.1453199831
 H 1.7571699201 -2.6531028956 2.077443834
 C 2.0079739064 0.5117791883 3.272188075
 H 0.8833742995 2.1520407172 2.4554212427
 H 2.5028335498 1.1073633823 4.0302483843
 N 0.4573999587 0.396259396 1.4518681066
 H -1.1883419566 -1.6509692879 0.8466788774
 H 0.0929947739 -0.6311002766 -2.8882645531
 C 1.7468775366 -0.3001880021 -1.7127942796
 C 3.0470792089 -0.6289225039 -2.0269527737
 C 4.0518815097 0.3214940744 -1.8067415856
 H 3.2904365729 -1.5952741103 -2.4537610905
 C 2.3861395883 1.8167377692 -0.9847098469
 C 3.7141367514 1.5692329893 -1.2859207474
 H 2.0847912274 2.7701644292 -0.5633056276
 H 4.4669048894 2.3298273278 -1.1157142682
 N 1.4160543004 0.9138345581 -1.1925422301
 Cu -0.4416284284 0.9573341709 -0.3993735955
 O -1.7912879049 -2.7522412031 -1.4310864751
 Cl 3.3736771679 -1.6339461665 4.1834247157
 Cl 5.6766016268 -0.0522566403 -2.1822737414
 Cl -6.5304837247 -0.9199823117 0.6730801589

O_Cu2+_2e

2 2
 C -0.4651530381 -3.5700295412 -0.5296576787
 C 0.1255939687 -2.9967462335 0.7627421549
 C 0.4928867104 -3.1768144089 -1.6787327558
 C -0.1750804123 -1.4957446085 0.6865478183
 N -0.4664717051 -1.1430492188 -0.7491595438
 C 0.4694724203 -1.6326687331 -1.7785170325
 C -1.7833847201 -1.679376469 -1.0651719791
 H -0.5973514237 -4.6495161624 -0.4858125623
 H 1.1982751195 -3.2112925444 0.7988727036
 H -0.34007234 -3.4301561337 1.6505465223
 H 0.170407603 -3.6179651137 -2.6241201238
 C -2.7980925894 -0.7617144016 -0.4031982621
 C -4.0135897083 -1.197703655 0.0393485514
 C -4.95657746 -0.2612783117 0.5586738149
 H -4.2324980507 -2.2556065375 -0.0281640432
 C -3.2810071055 1.4351527236 0.1365074217
 C -4.52959581 1.0962251622 0.5878448731
 H -2.9516212833 2.4682547503 0.1742146322
 N -2.3988498681 0.5457349753 -0.3699977
 H -1.9324338743 -1.5910855627 -2.151066323
 C 0.7434467226 -0.503881998 1.3859783544
 C 1.6655185258 -0.9088806845 2.3208733545
 C 1.1574938998 1.7184010313 1.8326530354
 C 2.3868279155 0.0569902597 3.0781207578
 H 1.8141212618 -1.9650770965 2.4989958044
 C 2.0928113397 1.4143064609 2.7923821812
 H 0.9292080723 2.7559050791 1.6090019511

H 2.5816627905 2.2239182264 3.3172745637
 N 0.4733589236 0.7977385802 1.1335271501
 H -1.1408005438 -1.3435312977 1.1802284504
 H -0.018111713 -1.3801767177 -2.7275355667
 C 1.67336415 -0.7165882224 -1.7652336491
 C 2.9538094145 -1.1146450044 -2.0352982224
 C 3.9952825911 -0.1467155967 -2.1485937187
 H 3.1527164202 -2.1663881027 -2.1942496118
 C 2.3027442107 1.5102477629 -1.6678529721
 C 3.6100125306 1.2065415485 -1.9463538558
 H 2.0080436871 2.5418497641 -1.503764162
 H 4.3252263145 2.0150529386 -2.0110390509
 N 1.3203023739 0.5906257033 -1.5875978691
 Cu -0.4673508476 0.8385283229 -0.7341098915
 O -1.805955672 -3.0372349999 -0.6981328354
 N 3.2879719213 -0.3005747024 4.0117651876
 H 1.4832516735 -3.5809699724 -1.4488603428
 H -5.1696590517 1.8816727182 0.966003891
 N -6.1661786524 -0.6402501597 0.9898637524
 N 5.2587652017 -0.4949237687 -2.4336885176
 C 6.2885562808 0.5314307588 -2.5802150104
 H 6.423988818 1.0884715987 -1.647253688
 H 7.234822106 0.0549667322 -2.8299515795
 H 6.0364962084 1.2288563414 -3.3858154465
 C 3.9785472108 0.722439014 4.790637368
 H 3.2694634464 1.3291445852 5.3643070947
 H 4.656237245 0.2406535621 5.4934296801
 H 4.5714386023 1.377653707 4.1434093018
 C 5.6095154919 -1.8955622053 -2.6470083694
 H 6.67740575 -1.9707277108 -2.8439111939
 H 5.3880328354 -2.4962807983 -1.758346809
 H 5.0758911905 -2.3109705342 -3.5089221628
 C -6.5622588833 -2.0454576738 0.9364406332
 H -6.5601888878 -2.4159306351 -0.0940533691
 H -5.8969791773 -2.6650210639 1.5468192706
 H -7.572093003 -2.1464353096 1.3296888349
 C -7.1097633034 0.3519668254 1.5009481906
 H -6.7074858933 0.8574798432 2.3850089609
 H -7.3501611505 1.0958223541 0.7343191421
 H -8.0328911496 -0.1481202657 1.7879312173
 C 3.5419423414 -1.7081741854 4.2911140559
 H 4.3082745599 -1.7880184951 5.0603219954
 H 2.6403361803 -2.2112690106 4.6590001748
 H 3.9065432876 -2.2290174826 3.3985730518

O_Cu2+_2a

2 2
 C -0.4982859584 -3.0250880076 -1.921357803
 C 0.0496282755 -3.0508788961 -0.4921196665
 C 0.4906506966 -2.2040055248 -2.7779153321
 C -0.2528998925 -1.6514590332 0.058619361
 N -0.4861149798 -0.7149868663 -1.1071476189
 C 0.4903652344 -0.7584363386 -2.2202025794
 C -1.7927489422 -1.0601942189 -1.6795958122
 H -0.6418469925 -4.0210041044 -2.3350947124
 H 1.1202791699 -3.2760003707 -0.5144564121
 H -0.4443074597 -3.8074430758 0.1212655249
 H 0.1884968515 -2.1953958658 -3.8269041165
 H 1.4707944473 -2.6863753763 -2.7252319786
 C -2.8443135591 -0.4760381785 -0.7528029969
 C -4.1055368222 -1.0119185815 -0.5946976067

C -4.9940100104 -0.3081021652 0.2067871975
 H -4.3947120131 -1.939908026 -1.0763454629
 C -3.34528718 1.3387874127 0.6249603843
 C -4.6408886118 0.8790697135 0.8213088495
 H -3.0020743735 2.2527333519 1.0972022231
 H -5.348149223 1.4202028206 1.4391732481
 N -2.4635040462 0.6798583096 -0.1436410204
 H -1.8871542188 -0.5342592671 -2.6416606549
 C 0.6460639823 -1.071104128 1.1381131213
 C 1.5349567104 -1.8537001552 1.8554013608
 C 1.0534019324 0.7642381351 2.5043895257
 C 2.1838321642 -1.2629598949 2.9307578913
 H 1.7260565425 -2.8946854946 1.6237499833
 C 1.9538154252 0.0501096758 3.2884454938
 H 0.8330877681 1.8036237525 2.7240102834
 H 2.4569828357 0.4971524627 4.1378870176
 N 0.4187081638 0.2203341962 1.4609207007
 H -1.2365715303 -1.7070108166 0.5375804125
 H 0.0516714444 -0.1163846193 -2.9937706121
 C 1.7047295902 0.0256213076 -1.7810416179
 C 3.0080114832 -0.2485483187 -2.1435160946
 C 3.9818635769 0.6694110536 -1.7731045794
 H 3.2809974061 -1.1326265117 -2.7084667585
 C 2.3397205256 2.0170671184 -0.7377636759
 C 3.6726324498 1.8224884284 -1.0780556955
 H 2.0320212656 2.8935716959 -0.1773547572
 H 4.4414619442 2.5371338759 -0.8079988792
 N 1.3806861934 1.146060883 -1.0789686455
 Cu -0.4948463841 1.0647901116 -0.2978268496
 O -1.8324030221 -2.4405474763 -1.8790763739
 N 5.3964743744 0.3954760171 -2.1391277332
 O 6.2079107308 1.2323145987 -1.8062422689
 O 5.6020117997 -0.644954224 -2.7314850949
 N 3.1510129946 -2.0758301831 3.7121390502
 O 3.6825893554 -1.5236760838 4.6515979782
 O 3.3224468361 -3.2172688803 3.3309616264
 N -6.362730598 -0.8528519986 0.4086499986
 O -6.6014386156 -1.909305181 -0.1397294166
 O -7.104907737 -0.1914770581 1.1031215942

O_Cu2+_2c

2 2

C -0.7603467199 -1.1957908283 2.8890643578
 C -0.2632067619 0.194046111 2.4792197681
 C 0.2919967537 -2.2173505787 2.3999906292
 C -0.5263494041 0.2649523271 0.9703751399
 N -0.6935044263 -1.1414733428 0.4499066358
 C 0.317716805 -2.1392315849 0.8538990693
 C -1.99054715 -1.6234946274 0.9147355963
 H -0.9197675363 -1.2837226164 3.9619647978
 H 0.7980148827 0.2874927843 2.7298186282
 H -0.8071085095 0.9895957605 2.9929699918
 H 0.0314919095 -3.2290641 2.7173296633
 H 1.2505261299 -1.9658225923 2.8631169807
 C -3.0407504635 -0.9517216243 0.046555987
 C -4.3003022979 -0.6551589952 0.4923889092
 C -5.2452780992 -0.1077264887 -0.4061596616
 H -4.5334875532 -0.8309374232 1.534838383
 C -3.5230227771 -0.2026481353 -2.0895978787
 C -4.8141134206 0.1067179116 -1.73144125
 H -3.1815263098 -0.0302960165 -3.104621486

H -5.4828360335 0.4940214632 -2.4882364164
 N -2.6256437114 -0.7320327021 -1.2345023399
 H -2.0436488935 -2.7021501177 0.7058897234
 C 0.3583769615 1.1364906333 0.0914022266
 C 1.2264382316 2.0658097668 0.620217602
 C 0.7864212035 1.8609213014 -2.0569919531
 C 1.9114211729 2.949864451 -0.2390488388
 H 1.3892173017 2.1112700989 1.6886746238
 C 1.6629866431 2.8300169361 -1.6153947004
 H 0.5810194479 1.7542640661 -3.1173795128
 H 2.1176659099 3.500223166 -2.332268955
 N 0.1336099953 1.0256597944 -1.2366911676
 H -1.5241678017 0.6987857527 0.8447962765
 H -0.0743231451 -3.091460235 0.4771017461
 C 1.5373785543 -1.9090499378 -0.0100333311
 C 2.8343778883 -2.0790051025 0.4006500165
 C 3.8883276627 -1.9539693231 -0.5329425571
 H 3.0380620732 -2.2979184087 1.4407189705
 C 2.2080735332 -1.4866842823 -2.1885310334
 C 3.5338911 -1.6542549085 -1.862104185
 H 1.9223006129 -1.2506726069 -3.2083653839
 H 4.2782509524 -1.581380278 -2.643647632
 N 1.2068148215 -1.6151883558 -1.2998668268
 Cu -0.6616587612 -0.9139015379 -1.5098539718
 O -2.0719571966 -1.4048680679 2.2982998621
 N 5.1930290769 -2.1178595381 -0.1560364549
 N -6.5134112577 0.198389745 -0.0026893263
 N 2.7849205897 3.8874643135 0.2570568221
 C 6.3186501344 -1.7272757191 -0.8941276519
 C 5.6429056138 -2.7073155841 1.0337550067
 C 6.9981539173 -2.6874118435 1.0314444862
 C 7.4262421179 -2.0556994269 -0.1854606602
 C -7.4428612603 0.9726349348 -0.7129335596
 C -7.1204827911 -0.2100408662 1.1946800507
 C -8.3797710616 0.28816622 1.222968499
 C -8.5804975781 1.0465295551 0.0186079262
 C 2.8431312105 4.3454059401 1.5772109053
 C 3.7745849768 4.551932645 -0.4736845447
 C 3.8344012606 5.26875762 1.6636926515
 C 4.4326410089 5.3910119052 0.366076612
 H 6.2241338834 -1.2040162558 -1.8319853642
 H 4.9576882445 -3.1488205337 1.7394336337
 H 7.6355749794 -3.0916606189 1.8044223467
 H 8.4461964612 -1.8665373107 -0.4872268006
 H -7.1899163037 1.4409681699 -1.6502831677
 H -6.6184705063 -0.8648620881 1.88831459
 H -9.1026700177 0.1286054774 2.009813746
 H -9.4731544799 1.5881597541 -0.2587236524
 H 2.1259143537 4.0258199637 2.316553965
 H 3.9538880648 4.3247742203 -1.5126113444
 H 4.1058575597 5.8206441143 2.5519216375
 H 5.2622182282 6.0286977005 0.0972110848

O_Cu2+_2f

2 2

C -0.6080405178 3.3269778887 1.1707135142
 C -0.0234682032 2.905835629 -0.1816079282
 C 0.3519095656 2.7994965607 2.263065506
 C -0.327939302 1.4068197974 -0.2785206055
 N -0.6184307857 0.8918049594 1.1068311333
 C 0.3217366001 1.254528522 2.1830976939

C -1.9323360719	1.3912936761	1.4856712288	H 3.0913073121	-0.9101831191	-5.2030464234
H -0.735810672	4.4048136293	1.2530329095	H 4.5633387143	-0.8804848468	-4.2051506993
H 1.049821137	3.1200415081	-0.1975491506	H 3.7619580706	2.4155238664	-2.8425032706
H -0.4911274985	3.4402930616	-1.0114109408	H 2.6939147504	2.5864118044	-4.2555172102
H 0.0342309304	3.1296391554	3.2542801732	H 5.6429778539	1.7988103896	-4.1783709322
H 1.3436136415	3.222947052	2.0779722585	H 4.8467652631	2.8930330545	-5.3179778426
C -2.9503751226	0.5605375033	0.7220968751	H 5.3418417274	0.3571093648	-6.1356468913
C -4.1635478927	1.0480879859	0.332967452	H 3.7328888662	1.0236483663	-6.4426800078
C -5.1094191383	0.1767391894	-0.2860500136	H 7.5440626629	1.9857526109	3.6990206773
H -4.3911601442	2.0889485542	0.5272445074	H 7.4974141066	1.3815238491	2.036987828
C -3.4410944569	-1.5615171717	-0.0645878822	H 7.1645505258	-0.2602584556	4.6011691189
C -4.6885797168	-1.1708112769	-0.4719282795	H 8.2808906085	-0.5861432946	3.2689365853
H -3.1115955913	-2.5830147966	-0.2237429704	H -9.1056643473	0.5065672663	-0.2074005192
H -5.3329124343	-1.8974356617	-0.9493254328	H -9.3309240546	0.3176874462	-1.9515284662
N -2.55559446	-0.7374443205	0.5403579356	H -8.7481200998	2.7923869019	-1.0136760653
H -2.0801766137	1.1769930357	2.5539990923	H -7.8469186964	2.2100977301	-2.4202357841
C 0.5888741349	0.5006940482	-1.0873330984			
C 1.5156498259	1.0080186098	-1.9645880219	O_Cu2+_2d		
C 0.9939360381	-1.6582762842	-1.7911286857	2 2		
C 2.2313735857	0.1318113721	-2.8290223862	C 0.4093693854	3.7034956666	-0.3858488249
H 1.6690283464	2.077287768	-2.0295161339	C -0.1457187368	3.2239177583	0.9586326924
C 1.9332949493	-1.2492121386	-2.7057086968	C -0.6113174607	3.2963456546	-1.4722531703
H 0.762280018	-2.7137897971	-1.6867409957	C 0.0963453509	1.7098184105	0.9533724668
H 2.4353430576	-1.9902289921	-3.3142058836	N 0.2961204664	1.2632844717	-0.4775584853
N 0.3109219792	-0.8211247556	-0.9912429455	C -0.6708451347	1.7487088258	-1.486298823
H -1.2942393602	1.3142727641	-0.7855122264	C 1.6188402049	1.7341219933	-0.8920267046
H -0.1644105089	0.8949195521	3.0976512616	H 0.5943123237	4.7755646106	-0.4055553136
C 1.5222956338	0.3428665802	2.0580614174	H -1.2066138111	3.4828283738	1.0298212799
C 2.8047455586	0.7030229915	2.3649837915	H 0.3747846496	3.6827657745	1.8019662292
C 3.8402947572	-0.278261386	2.3631054209	H -0.3068491619	3.6650688868	-2.4537106098
H 3.0151167515	1.7253698013	2.6532848886	H -1.5706218041	3.7629000932	-1.2309306965
C 2.1429865368	-1.8619091086	1.6978836729	C 2.6358435079	0.8070134861	-0.2493795819
C 3.4518198155	-1.5979926173	2.0033167397	C 3.9208283003	1.1838600437	0.0816255023
H 1.8428755392	-2.864547372	1.4102567627	C 4.7955893978	0.2134903322	0.5725741893
H 4.1739088409	-2.4025576687	1.9572811632	H 4.2262554163	2.2163668797	-0.0479234102
N 1.1628108672	-0.9351672797	1.7330635873	C 3.0397709509	-1.3997531841	0.3770055732
Cu -0.6246553483	-1.0758294445	0.8587567605	C 4.3511498724	-1.0962408292	0.7135496725
O -1.9504741083	2.7837615444	1.2811097579	H 5.8131099023	0.4802836695	0.8383283515
N -6.3123232903	0.6028029682	-0.6645399791	H 2.6475748812	-2.404619447	0.491692128
C -7.3586114261	-0.2727828386	-1.2167860226	H 5.0031251779	-1.8772778271	1.0867277625
C -6.7617631785	2.0000435659	-0.5604104602	N 2.193601027	-0.4715765189	-0.0983668271
N 5.0974870423	0.0269847787	2.6857479872	H 1.6994195945	1.5949084378	-1.9803812197
C 5.5603546089	1.3860976652	3.0011393494	C -0.8246126602	0.8062210141	1.7588554141
C 6.1767133086	-0.9655488859	2.8108961929	C -1.6729981614	1.2923144489	2.740412426
N 3.1281934585	0.5908542899	-3.709722332	C -1.3081171787	-1.3860656657	2.347661651
C 3.8089527987	-0.2551984653	-4.6998135726	C -2.3568556797	0.3860430588	3.5514897787
C 3.5177353447	2.0009225399	-3.8262046843	H -1.7917429886	2.3586214041	2.8941490091
C 4.7296092801	1.9627419755	-4.7594001893	C -2.1682018707	-0.9755202077	3.3584687106
C 4.4454830954	0.7546322943	-5.656562586	H -1.1338316191	-2.4396874934	2.154242402
C 7.0832577336	1.2467640804	3.0413908448	H -3.0219646529	0.7464447213	4.3292584006
C 7.293123883	-0.1937849719	3.5162768284	H -2.6730534468	-1.7109403409	3.9739455703
C -8.61304672	0.6015135171	-1.1802138505	N -0.6501956604	-0.5191494028	1.570245596
C -8.0629972919	2.0187080277	-1.364299556	H 1.0814509176	1.548673879	1.4042887225
H -7.4602897779	-1.1763415851	-0.6086835673	H -0.2498933121	1.4217309349	-2.4447658488
H -7.0948479976	-0.5660760604	-2.2405552945	C -1.9181682993	0.9042821777	-1.3590948524
H -6.0061299421	2.6768002686	-0.9703281421	C -3.208876109	1.3320886679	-1.5989318682
H -6.9296564876	2.2583120978	0.4926914033	C -4.2436648905	0.395161441	-1.5923774987
H 5.1559894938	1.7025309855	3.9711972368	H -3.408733251	2.3773161515	-1.8073017252
H 5.2249409827	2.0928315002	2.2355421298	C -2.6350739148	-1.3002360369	-1.1012151338
H 6.483900901	-1.3095036498	1.8152538929	C -3.9523687797	-0.9411112816	-1.3487806327
H 5.8359407539	-1.8293097006	3.3891010475	H -5.2642973099	0.7097049501	-1.783686098

H -2.363249079 -2.3293267761 -0.8897576404
H -4.727249795 -1.6985829599 -1.3464044127
N -1.6382559069 -0.4043616472 -1.1112011202
Cu 0.2186051424 -0.6924466953 -0.3666873922
O 1.7172242056 3.0947500959 -0.5777756382

O_2b

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C 0.7747958927 -0.824987791 -1.995841241
C -0.3969689679 -2.5467018149 -0.6190493863
C 0.5118149905 0.1903325449 -0.8502935463
N 0.5318034083 -0.5214645845 0.4525448899
C -0.4985868109 -1.5666225672 0.5825399076
C 1.8097886448 -1.1933172153 0.5903237824
H 1.1603413344 -2.9680163734 -2.0857445068
H -0.0181643626 -0.8421404896 -2.7503975929
H 1.7034435272 -0.5718303721 -2.5162927592
H -0.3874158249 -3.5863512045 -0.2795124462
H -1.2285687225 -2.4374391842 -1.3247734905
C 2.9833939364 -0.2253692263 0.5869993275
C 3.9410773358 -0.2543855854 -0.423219642
C 4.970609797 0.6747426881 -0.3590441314
H 3.8776469496 -0.9870576031 -1.2170022113
C 4.0248859251 1.496548013 1.6550682658
C 5.0259512489 1.5802965122 0.6899160794
Cl 6.1941509966 0.6993749347 -1.6004542931
H 4.0360860598 2.1757995205 2.5043085193
H 5.818734023 2.3153882428 0.7626653453
N 3.0257765237 0.6190039124 1.6202398634
H 1.8130446732 -1.6979035984 1.5637352032
C -0.7115650542 1.0784041014 -0.9868948597
C -1.8865733601 0.6631766344 -1.6133516589
C -1.6403415247 3.0968677948 -0.4464752578
C -2.9785059495 1.5177619143 -1.5967771726
H -1.9740255318 -0.3145596696 -2.0709941283
C -2.873714276 2.7648667041 -0.9991239391
H -1.4998508932 4.0733639312 0.0115264488
Cl -4.4816723757 1.0127123807 -2.3180733428
H -3.709754875 3.4537441519 -0.974000212
N -0.5842579613 2.2884880062 -0.4341023927
H 1.3412688518 0.8968521292 -0.7935088424
H -0.2133195974 -2.1194683378 1.4860726852
C -1.8901893567 -1.0285690596 0.8937141567
C -3.030368479 -1.7262081489 0.4894827549
C -4.271218973 -1.1915579434 0.806240996
H -2.966424567 -2.6555736069 -0.0634150204
C -3.1553439713 0.5850909482 1.8996785409
C -4.3566974128 -0.0014445441 1.5118632494
Cl -5.7215323966 -2.0176653051 0.3034509189
H -3.1661891856 1.5090799673 2.4735227002
H -5.3122729683 0.4459904555 1.7574733403
N -1.9535073288 0.092006168 1.6157717245
O 1.9919513539 -2.1983379139 -0.4201504185

O_2e

O 1
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C 1.069923526 -1.0140338321 -1.8060811356
C -0.2423981919 -2.627539259 -0.4197891056
C 0.7501954397 0.0680976497 -0.7379649719

N 0.6833437489 -0.5776676929 0.5988922789
C -0.3790549412 -1.5903436128 0.7293869028
C 1.9355496153 -1.2653657347 0.8471048109
H 1.3857850956 -3.1704608866 -1.7653608357
H 0.3360486127 -1.047955611 -2.6179959869
H 2.0442793705 -0.8134459411 -2.2631476887
H -0.2879236804 -3.6510320108 -0.0348811669
H -1.0291127754 -2.5233376189 -1.1763016172
C 3.1356281914 -0.3296984324 0.8534377744
C 4.1144088002 -0.4167154197 -0.123971535
C 5.1991285305 0.480453983 -0.1010121785
H 4.0196089712 -1.1876691228 -0.8755571446
C 4.1830404773 1.3911743487 1.8809426951
C 5.2065208143 1.4212062633 0.9445690136
H 4.1945952271 2.1065362955 2.7015903475
H 5.9902929875 2.1620582363 1.0434297299
N 3.1567908511 0.5426999748 1.8661659619
H 1.872706605 -1.7117760768 1.8462711666
C -0.4616988094 0.9471167695 -0.9913372878
C -1.5945509775 0.4777388938 -1.6418182498
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O_2a

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H -2.020430179 -0.3218604948 -1.9961519687
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O 6.8662578156 1.6151676076 -1.251247441

O_2c

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C 1.1779480481 0.196345433 -0.1141701345
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C -0.0971596644 -1.9155371356 0.1925882305
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H 2.2395224549 0.3511067616 -2.0187344704
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H -0.8605391385 -1.5909963168 -1.868032588
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C 5.7489771608 -0.0825533782 1.8499449673
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O_2f

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O_2d

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O_Cu1+_3b

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 C 5.0308284571 -0.6047496258 0.2295797848
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 H 5.277436893 -2.7498021329 0.1312506094
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 H -4.6831883611 -1.7045092334 -2.0199680072
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O_Cu1+_3e

1 1
 C 0.6043932482 2.8253850994 0.4672543378
 O 0.3281478096 1.9036649209 1.518234521
 C -0.5484407388 2.7026538337 -0.5550274257
 C 0.3721930569 0.5734679455 1.019926068
 N 0.5911570057 0.5572818164 -0.4256644721
 C -0.4149870678 1.3020460774 -1.1959142037
 C 1.9237690637 1.0835698102 -0.7292686511
 H 0.6027006115 3.8132781737 0.9296467745
 H -0.5088081769 3.4927893322 -1.3105770597
 H -1.4784913433 2.822675475 0.0090244455
 C 2.9375925557 -0.0115235809 -0.4155860606
 C 4.1848418369 0.2600768877 0.0976847781
 C 5.1198042768 -0.7858521374 0.3020792608
 H 4.441500281 1.2844617341 0.3325515144
 C 3.4187532705 -2.2547155691 -0.5700213297
 C 4.6862246857 -2.080849418 -0.0584977918
 H 3.0824022585 -3.2473547984 -0.8502124845
 H 5.3229246617 -2.9479911295 0.0548483659
 N 2.5337026416 -1.2631578624 -0.757772272
 H 1.9660906427 1.1929297843 -1.8191231356
 C -0.8824950892 -0.201797871 1.3701049247
 C -1.9463199975 0.4059626601 2.0021655424
 C -1.9877874577 -2.1702689059 1.1574557498
 C -3.1469452255 -0.3155434648 2.1721100121
 H -1.8421825565 1.437697509 2.3081575475
 C -3.1375038622 -1.6540290803 1.730897213
 H -1.9736283897 -3.2050440172 0.8248738516
 H -4.0028193115 -2.2957701668 1.8370352335
 N -0.8646930346 -1.4766310268 0.9553577907
 H 1.2298745572 0.0586227959 1.4717873886
 H 0.0293571015 1.4298542116 -2.1890814073
 C -1.6089325307 0.387969903 -1.4575429502
 C -2.9155156282 0.7617130755 -1.2582875317
 C -3.9648556293 -0.155724113 -1.5111257746
 H -3.1259227266 1.7460993197 -0.8630653024
 C -2.2506018407 -1.6688197348 -2.2605104086
 C -3.5889698659 -1.3897166879 -2.0814346738
 H -1.9484849869 -2.6264566478 -2.6723104132
 H -4.3190637418 -2.1399214607 -2.3543697212
 N -1.2545310862 -0.8344359606 -1.931861873
 Cu 0.5590012332 -1.4400257279 -1.2115103102
 C 2.012374357 2.492224193 -0.0835598317
 H 2.346412787 3.2439129667 -0.8046526042
 H 2.6960641173 2.5179667223 0.7705524943
 N -5.2549037353 0.1378712922 -1.2072634327
 N 6.3527710349 -0.5525351983 0.812304711

N -4.2605450105 0.2699090384 2.7035797728
 C -5.4858024384 -0.4953743633 2.8304659395
 H -5.3785331302 -1.3384307311 3.5254692705
 H -6.2788212504 0.1536889835 3.2026723225
 H -5.8020927704 -0.8867668463 1.8552756303
 C -6.2943285948 -0.8482958035 -1.4473603286
 H -6.1229177537 -1.7647016969 -0.8673689665
 H -7.2586246711 -0.4331500572 -1.1550637088
 H -6.3525224149 -1.1126786181 -2.50904745
 C -5.5751956752 1.36847015 -0.5048264613
 H -6.6476142073 1.4021300618 -0.3132398972
 H -5.0525464178 1.4206487582 0.4595417547
 H -5.3158451755 2.2510628202 -1.1009515642
 C -4.169481436 1.5955503368 3.2887525766
 H -5.1323387793 1.8628324633 3.72433309
 H -3.4132688311 1.6368780539 4.0820386178
 H -3.9192560832 2.3529310732 2.534320649
 C 6.7536753441 0.7982006793 1.1687748101
 H 6.7503961591 1.4616516289 0.2954886793
 H 6.0951925119 1.2207734927 1.9371797695
 H 7.7662308644 0.7770547124 1.5701778243
 C 7.2808111105 -1.6565168438 1.0004603932
 H 6.8783006425 -2.4011165847 1.6972558573
 H 7.5113298023 -2.1503623486 0.0491855405
 H 8.2126391335 -1.274819339 1.4162444747

O_Cu1+_3a

1 1
 C 0.5315422894 3.0718051287 0.4141620421
 O 0.1366302257 2.2186940038 1.4944218543
 C -0.5655137993 2.9249637008 -0.6564955201
 C 0.2950534889 0.8751536173 1.1129149711
 N 0.4888295405 0.7381572873 -0.3340322549
 C -0.4997835577 1.4577762278 -1.150367367
 C 1.8269921039 1.2355546097 -0.6694865134
 H 0.5465329193 4.081712003 0.8226985047
 H -0.426445973 3.6271262999 -1.4830689497
 H -1.514532209 3.1647723194 -0.1687866017
 C 2.8402422782 0.1498103641 -0.3323952294
 C 4.1392863539 0.4462679443 0.049500222
 C 5.0115382737 -0.6113377883 0.2489444534
 H 4.4817286158 1.4648201712 0.1862426927
 C 3.2922511563 -2.1250416397 -0.3155597548
 C 4.6121565686 -1.9202780652 0.0692635443
 H 2.9163926011 -3.1294562373 -0.4744718742
 H 5.2977017385 -2.7439402726 0.2232603185
 N 2.4217080689 -1.1270701779 -0.5115572401
 H 1.8622064957 1.3200430949 -1.7616451879
 C -0.8491508743 0.0135043225 1.6110559953
 C -1.856051996 0.518578255 2.416548808
 C -1.7105883475 -2.1207522166 1.6938751877
 C -2.8181930988 -0.3805958178 2.8481963982
 H -1.8871276582 1.5640783091 2.694616692
 C -2.7655491383 -1.7190950333 2.5078295208
 H -1.6149006617 -3.1563081114 1.3841522915
 H -3.5162168254 -2.4154587599 2.859800525
 N -0.77715764 -1.2777060741 1.2465869394
 H 1.2077424455 0.4715796861 1.577984936
 H -0.0785880044 1.4578024581 -2.162198814
 C -1.753339419 0.6094982093 -1.2987096509
 C -3.0336494996 1.1387453418 -1.3075812754

C -4.086440167 0.2705056447 -1.5515001805
 H -3.2290386858 2.1897341899 -1.1363941069
 C -2.5562495463 -1.5102520328 -1.775502488
 C -3.8758195768 -1.0707281951 -1.799185847
 H -2.3202883127 -2.5520055043 -1.9648277239
 H -4.7014866641 -1.7412634367 -2.0012614036
 N -1.520554625 -0.7043543516 -1.5244886913
 Cu 0.355311354 -1.3548455701 -0.6780047752
 C 1.9495701862 2.6533531554 -0.0479602551
 H 2.3530902926 3.3731463136 -0.7647689966
 H 2.596206618 2.6649648951 0.8354983903
 N -5.4676944289 0.80159546 -1.5483865726
 O -6.3612994214 0.0052054785 -1.7608975641
 O -5.5964245381 1.9918632957 -1.3293181718
 N -3.9316195736 0.1092350853 3.6915772934
 O -4.7411804193 -0.7176580533 4.065909909
 O -3.9500444257 1.3009169378 3.9363017644
 N 6.4027137047 -0.323704514 0.6638089042
 O 6.6982756881 0.8477026162 0.811571639
 O 7.1353360792 -1.2801745744 0.8239192131

O_Cu1+_3c

1 1
 C -0.6268327096 -3.3051639747 -0.66546506
 O -0.309689108 -2.7720541278 0.6218724063
 C 0.4387022645 -2.7462965818 -1.6282809514
 C -0.617741188 -1.3949395592 0.6513352972
 N -0.8266385278 -0.8719015673 -0.7046093808
 C 0.2391146697 -1.208684652 -1.6575965256
 C -2.1044786374 -1.3751835838 -1.2125345124
 H -0.536632494 -4.3875297052 -0.5716723162
 H 0.3499731205 -3.1771588375 -2.629854388
 H 1.4110769123 -3.0399199633 -1.2227173283
 C -3.2178555689 -0.519614065 -0.6187227877
 C -4.4654257374 -1.034136017 -0.3287104862
 C -5.4749669396 -0.1853964719 0.1488357058
 H -4.6515764011 -2.0946483817 -0.446795083
 C -3.8853171955 1.5975520498 0.0002554295
 C -5.1621645157 1.1667429888 0.3101788697
 H -3.6229279015 2.6439876818 0.1111905731
 H -5.9032372994 1.8831226045 0.6415877222
 N -2.9162480509 0.7930697671 -0.4575349617
 H -2.1213600707 -1.1530046246 -2.2859824483
 C 0.4415418969 -0.5815550564 1.3662547141
 C 1.6909483546 -1.090672624 1.6527694437
 C 0.9816412749 1.48188029 2.1716100082
 C 2.6665177206 -0.2196267381 2.1536161526
 H 1.8993213084 -2.1347446362 1.457803866
 C 2.28222489 1.0901652376 2.4521250911
 H 0.6639909746 2.5000714677 2.3780353418
 H 2.9891744291 1.8106056103 2.8451596888
 N 0.0745946063 0.6875037661 1.5980799122
 H -1.5640590995 -1.2398623381 1.1867916583
 H -0.1658086511 -0.9361491378 -2.6392315476
 C 1.4037726184 -0.2440684103 -1.470495883
 C 2.725394466 -0.6339556285 -1.5510172999
 C 3.7413238548 0.3125866636 -1.3624167035
 H 2.9738459566 -1.677084496 -1.6992746194
 C 2.0131970903 1.9483312556 -1.1194090434
 C 3.3607953825 1.6412401462 -1.1598333285
 H 1.69300807 2.9737289369 -0.9681861407

H 4.0958810269 2.4293947578 -1.0562791146
 N 1.0357806795 1.0422480539 -1.256313219
 Cu -0.9156017394 1.2544843647 -0.5744340457
 C -2.0841585099 -2.9145102748 -1.0186537859
 N 5.0769290905 -0.0645460582 -1.3598263569
 N -6.7365516994 -0.6771537242 0.4510393065
 N 3.9844950484 -0.6430541195 2.300360967
 C 6.1015060954 0.6005160895 -0.6999580235
 C 5.6099458091 -1.1910544085 -1.9730319974
 C 6.9479819066 -1.2229555763 -1.714543719
 C 7.2573765734 -0.0919307503 -0.8982851999
 C -7.6368371488 -0.1090057779 1.3448157383
 C -7.3172380927 -1.8207721692 -0.0856594217
 C -8.5582934766 -1.9635398541 0.4569652564
 C -8.7567184765 -0.8835185242 1.3725133095
 C 4.5838322163 -1.6633794289 1.5732931223
 C 4.946216444 -0.0693411985 3.1192670753
 C 5.8977337694 -1.7281089813 1.9271717065
 C 6.1257306011 -0.7233417229 2.916097016
 H 5.8973380722 1.4604262597 -0.0811924843
 H 5.0035304173 -1.8210300755 -2.6055913149
 H 7.6425368321 -1.9641846156 -2.0831164951
 H 8.22353323 0.166584488 -0.4899635009
 H -7.3716077798 0.7619948257 1.9238501179
 H -6.8189731354 -2.3909322468 -0.8543906183
 H -9.2628284884 -2.7476934928 0.220240842
 H -9.6274362656 -0.7097982848 1.9880351657
 H 4.0328913803 -2.2109468067 0.8247769116
 H 4.6871900233 0.7083515682 3.8212899846
 H 6.6283708985 -2.4045185433 1.5087357839
 H 7.0543420656 -0.5202862749 3.429876837
 H -2.4221473848 -3.4399634992 -1.9160336894
 H -2.7153197471 -3.2367112865 -0.1839472392

O_Cu1+_3f

1 1
 C 0.7725292192 3.1525705202 0.5971659043
 O 0.4923995728 2.2455358919 1.6618723457
 C -0.3881510247 3.0151129834 -0.4103388449
 C 0.6070693391 0.9109438593 1.1942506266
 N 0.7575878731 0.8705464987 -0.2602127412
 C -0.288914633 1.5871942063 -1.0004059622
 C 2.0684663952 1.4087844188 -0.6255143825
 H 0.7777311055 4.1465858422 1.0462579976
 H -0.3397657532 3.7757640371 -1.19532459
 H -1.3106404452 3.1739397226 0.1560941946
 C 3.1116902056 0.3288284779 -0.3593747189
 C 4.389654006 0.6320955576 0.0510504344
 C 5.3522036935 -0.3961416231 0.206311986
 H 4.6584433481 1.6655761681 0.2313383237
 C 3.6164188519 -1.9106236396 -0.4954190946
 C 4.9163022357 -1.706733271 -0.0880855164
 H 3.27331636 -2.9150429605 -0.7207151173
 H 5.5774240849 -2.558131922 0.0122989244
 N 2.7028086124 -0.9364528294 -0.638641145
 H 2.0588334868 1.5258511435 -1.7152628965
 C -0.5609063526 0.0481224715 1.6277836637
 C -1.6504116602 0.5773516095 2.2816117888
 C -1.4697011956 -2.034818919 1.5601915654
 C -2.7631532418 -0.2537339468 2.5393754584
 H -1.6395800932 1.6256219436 2.5493614418

C -2.6342730534 -1.6090545825 2.1716621325
 H -1.3649043201 -3.0766484402 1.2685258778
 H -3.4332224549 -2.3199233617 2.3430655294
 N -0.4385431367 -1.2385033154 1.2608040473
 H 1.5211331202 0.4662934442 1.6099855111
 H 0.0978350539 1.6690053754 -2.0222953046
 C -1.5046601146 0.6788898432 -1.1496116116
 C -2.7955958634 1.1051833882 -0.9451312724
 C -3.869449824 0.1931848109 -1.0729135667
 H -2.9770820305 2.1237989209 -0.6279276832
 C -2.2208917504 -1.4234887101 -1.7409949283
 C -3.5441056202 -1.1005725151 -1.5294168303
 H -1.9547373953 -2.4190995987 -2.0819001877
 H -4.3087800914 -1.8449228314 -1.7128768127
 N -1.1945394127 -0.5848321027 -1.5346307729
 Cu 0.6816263208 -1.1765359344 -0.8819218731
 C 2.1729690923 2.8119934386 0.0297025329
 H 2.5019756522 3.5695545692 -0.6875399846
 H 2.8695223509 2.823705114 0.8741771117
 N -3.9022770372 0.2341960467 3.0880976788
 N 6.6103531184 -0.1329802399 0.6106733591
 N -5.1351562266 0.5474524954 -0.7595768499
 C -6.2416474807 -0.4032294454 -0.6685427726
 C -5.5105285207 1.8879990346 -0.3226421117
 C -7.0356270411 1.8200175404 -0.2227759791
 C -7.3003863619 0.3548405938 0.1364439959
 C 7.6633249531 -1.1457578031 0.6936282887
 C 7.0755172902 1.1923000525 1.0185305192
 C 8.4364969655 0.911634962 1.6597501569
 C 8.9357376091 -0.3212839683 0.9002546921
 C -5.0645906989 -0.5931113704 3.3899861346
 C -4.1135195378 1.6421937517 3.4072081539
 C -5.6233839343 1.7336660792 3.6394348096
 C -5.9840717169 0.3449102876 4.1763971458
 H -5.9178218349 -1.3226022038 -0.1676354126
 H -6.6083560483 -0.6717879526 -1.6683227306
 H -5.1747598112 2.6433563373 -1.0412254591
 H -5.0506567663 2.1166152688 0.6501160256
 H -7.4831530242 2.0581845962 -1.1930865336
 H -7.4342736174 2.5228397336 0.5126039963
 H -7.1383974 0.194816562 1.2087405078
 H -8.3150627975 0.0299301207 -0.1022524417
 H 7.6995931409 -1.7422645983 -0.2239065847
 H 7.4775582268 -1.8247510077 1.5371702987
 H 6.3726086669 1.6506038015 1.7226359269
 H 7.1675192853 1.8539660195 0.1458904273
 H 8.3052820638 0.6748150104 2.7208308702
 H 9.1124721943 1.7658335115 1.584566475
 H 9.7044218612 -0.8767909603 1.4412111197
 H 9.3494243354 -0.0264722335 -0.0698550252
 H -4.7793588454 -1.4745420311 3.9746049879
 H -5.5369620069 -0.9461454743 2.4604702175
 H -3.7810021158 2.2830916396 2.5820323008
 H -3.5462666634 1.9306483577 4.3029110999
 H -6.1375076672 1.9148830109 2.6883295847
 H -5.8905592183 2.541639579 4.3237055966
 H -7.0398249609 0.0952509446 4.047765112
 H -5.75176889 0.2825901986 5.2443408588

O_Cu1+_3D

1 1

C 0.5507592245 2.9223050173 1.049739477
 O 0.1867994528 1.8662205554 1.9419935708
 C -0.5768420327 2.9958332991 0.0024924209
 C 0.3260242032 0.6268994238 1.2813128684
 N 0.4842238593 0.8006697978 -0.1639295272
 C -0.5213143662 1.6671715429 -0.7923574151
 C 1.8161045249 1.3537787965 -0.4224624372
 H 0.5792176119 3.8280802018 1.6556138075
 H -0.4653348012 3.8600891542 -0.6586734226
 H -1.5114667827 3.1144133578 0.558157887
 C 2.8321021142 0.2212945276 -0.3391841026
 C 4.14225235 0.4214890207 0.0684427668
 C 5.0379812582 -0.6440970941 0.0361317147
 H 4.4638707292 1.402207892 0.4016482072
 C 3.2673292986 -2.0031583592 -0.8053187016
 C 4.5935158624 -1.8800863321 -0.4105287931
 H 6.0662040582 -0.5055540095 0.3535996902
 H 2.8792324709 -2.9510400058 -1.162460342
 H 5.253354643 -2.7386200816 -0.4558171903
 N 2.3966498535 -0.9861924017 -0.7744156085
 H 1.8244344319 1.6612522523 -1.4743492956
 C -0.8046698488 -0.3242869189 1.6216355195
 C -1.7806109955 -0.0204690456 2.5562607023
 C -1.6641016484 -2.4265634339 1.2723041982
 C -2.7422047822 -0.9861765076 2.8442757623
 H -1.7732426395 0.9477739663 3.0417676923
 C -2.6820814186 -2.2128281135 2.1960089595
 H -1.5824633505 -3.3682928138 0.7378703176
 H -3.5229659051 -0.7827350263 3.5700481983
 H -3.4058631358 -2.9945497861 2.3966983352
 N -0.7424187381 -1.5050878511 0.9835543212
 H 1.2516406657 0.1415131655 1.6260317685
 H -0.1150287831 1.8860919008 -1.7864644315
 C -1.7776483572 0.8660805631 -1.1004095597
 C -3.059930493 1.3818763828 -0.9990539376
 C -4.1400544497 0.6028906953 -1.40789197
 H -3.2193989708 2.3821311924 -0.6127795719
 C -2.5846164601 -1.1065102259 -1.9943774472
 C -3.9001628088 -0.6636305763 -1.9197887157
 H -5.1517362036 0.9878989181 -1.3323432639
 H -2.3496526408 -2.0892821531 -2.3906151459
 H -4.708016344 -1.3014934288 -2.2593175803
 N -1.5426318112 -0.3716595635 -1.5937346176
 Cu 0.3318800022 -1.173979907 -0.9458327914
 C 1.9555318511 2.6156765016 0.472057546
 H 2.3392807602 3.4700989505 -0.0921172442
 H 2.6250985415 2.4487565599 1.322147381

O_Cu2+_3b

2 2
 C -0.25201261 -3.4037088541 -1.1488590532
 C -1.7314103231 -2.9834618288 -1.3447413144
 C 0.7412941824 -2.7230332816 -2.104486345
 C -1.7853474249 -1.4298459265 -1.359934069
 N -0.466549136 -0.9798864549 -0.8678484673
 C -0.2116409441 -1.707708522 0.4224652497
 C 0.5489934227 -1.1962029693 -1.9246546415
 H -0.1567688799 -4.4878104904 -1.1859942474
 H -2.3172435033 -3.405192314 -0.5219987071
 H -2.1227789585 -3.3978035069 -2.2765359097
 H 0.5758372343 -3.0142755347 -3.1446165617

H 1.7430721721 -3.0502046245 -1.8151652714
 C -2.827704035 -0.6655561192 -0.5616920429
 C -4.1181501012 -1.1171705706 -0.3795439555
 C -3.304356522 1.3194403303 0.5665773006
 C -5.0315093482 -0.3021665706 0.2984628222
 H -4.4254052075 -2.0840640168 -0.7628807886
 C -4.616441287 0.9398742691 0.7780927913
 H -2.9394354784 2.2717067704 0.9363221926
 Cl -6.6373888975 -0.832021585 0.5356048213
 H -5.29778178 1.5941195769 1.308984702
 N -2.4220015676 0.5479219477 -0.0928630535
 C 0.7499982011 -0.9830733506 1.3477286519
 C 1.7343540041 -1.6587404595 2.039145463
 C 2.4848430317 -0.9393484603 2.9750140984
 H 1.9029397821 -2.7150719814 1.8677213061
 C 1.2072193374 1.0012259926 2.4296448178
 C 2.2098236034 0.4098415716 3.1843204652
 Cl 3.7266257015 -1.7218786581 3.8589569223
 H 0.9720875456 2.0531515758 2.5547990111
 H 2.7635833991 0.9884968796 3.9143632576
 N 0.4863990358 0.3267327905 1.5254202984
 H -1.1840859824 -1.6992678058 0.9391075899
 H -1.8782607395 -1.0782965659 -2.3933777234
 H 0.0879683037 -0.801350736 -2.8375953162
 C 1.7018349498 -0.2483925682 -1.6655312438
 C 3.0063142161 -0.5001766527 -2.0353240968
 C 3.9596033788 0.5114290941 -1.8741746237
 H 3.2913172841 -1.4568753731 -2.4577478992
 C 2.2468513336 1.9147412852 -0.993171446
 C 3.5713609557 1.7444441145 -1.3517359731
 Cl 5.5850836207 0.2315041648 -2.3207310516
 H 1.906163865 2.8530181959 -0.5677719044
 H 4.2838374518 2.550631853 -1.223312396
 N 1.3249782184 0.9508614838 -1.1476327589
 Cu -0.4850527675 0.9118738343 -0.3113283469
 O 0.1819212629 -3.0114999486 0.1647174471

O_Cu2+_3e

2 2
 C -0.2708318917 -3.5414313121 -0.500096512
 C -1.7555358268 -3.1791004125 -0.7692907998
 C 0.7104054088 -3.0827917791 -1.592777004
 C -1.8193688851 -1.6647386914 -1.1110282433
 N -0.4953584586 -1.1242586817 -0.7562228165
 C -0.2153786354 -1.5383724011 0.6526019809
 C 0.5016729505 -1.5579154705 -1.7562628409
 H -0.1714468696 -4.6085235515 -0.3046948338
 H -2.3299226345 -3.4172658524 0.1315267009
 H -2.1514303559 -3.7865016639 -1.5866597016
 H 0.5435076076 -3.6043140897 -2.5388351385
 H 1.7168796282 -3.3253006389 -1.241850044
 C -2.8469072312 -0.7446701892 -0.4693522917
 C -4.1112347555 -1.1602215565 -0.1484478518
 C -3.3175329491 1.4247899771 0.2070870741
 C -5.0646320565 -0.2365492656 0.3726140521
 H -4.3761222833 -2.1969009988 -0.3131418498
 C -4.6035501847 1.0981832855 0.5438343052
 H -2.9603064175 2.4395372299 0.3482888196
 H -5.2451397637 1.8724706041 0.9416906384
 N -2.4278797999 0.5468018792 -0.3069682653
 C 0.7541828858 -0.6170653959 1.3721467369

C 1.7480813005 -1.1143562131 2.1734475961
 C 2.5362405804 -0.2161744812 2.9469716731
 H 1.8891736362 -2.185574254 2.2171349853
 C 1.2087904363 1.5519624519 1.9672255392
 C 2.2212405542 1.1609302026 2.8118583109
 H 0.9705484521 2.6054694337 1.858251726
 H 2.7554486625 1.9209950252 3.3660446994
 N 0.4608948579 0.6971688095 1.2490625429
 H -1.1772638871 -1.413974511 1.1727027537
 H -1.9341784509 -1.5396939132 -2.1931712616
 H 0.0148775041 -1.3833591998 -2.7227023106
 C 1.6459812182 -0.5634735204 -1.7455592848
 C 2.9331543062 -0.8914067507 -2.0772207331
 C 3.926990619 0.1239828874 -2.1898409456
 H 3.1743844625 -1.926738702 -2.2782920277
 C 2.1853157205 1.6851581274 -1.5873584917
 C 3.4925374343 1.4511745594 -1.9231675094
 H 1.8516312449 2.6953117868 -1.3724348471
 H 4.1698663566 2.2922380848 -1.9800794272
 N 1.2474176099 0.7189192976 -1.508275129
 Cu -0.5099028701 0.8617167758 -0.6199517847
 O 0.1696901318 -2.877505653 0.6930827619
 N -6.3137914213 -0.6062083754 0.6841183643
 N 5.1934260814 -0.1578972757 -2.5302711899
 N 3.5143643874 -0.6530043009 3.7611631654
 C 5.5962684039 -1.5338121893 -2.8036370276
 H 6.6573025241 -1.5543116236 -3.0457287006
 H 5.4377450353 -2.1718938171 -1.9275851162
 H 5.0462881307 -1.9452435875 -3.6570935411
 C 6.1744224991 0.9163834009 -2.6666585141
 H 6.3168434146 1.4420459751 -1.7166488952
 H 7.1310975036 0.4908600577 -2.9641903841
 H 5.8680822787 1.633336525 -3.4354819558
 C -7.2624980127 0.3750033709 1.2079525724
 H -6.9141267525 0.7890706094 2.1598212017
 H -7.4197565394 1.1885158791 0.4924071403
 H -8.2203039677 -0.1120808108 1.3810795722
 C -6.7439790869 -1.9890056586 0.4977514406
 H -6.6808932361 -2.2829376273 -0.5555032804
 H -6.1420541368 -2.6738164024 1.1047010221
 H -7.7814476697 -2.0857777151 0.8122326833
 C 3.777938268 -2.0809639634 3.8925374744
 H 4.604227383 -2.2297117671 4.5857410657
 H 2.9043998096 -2.612769595 4.2858814786
 H 4.0615051421 -2.5202782381 2.9298210619
 C 4.2739801522 0.2961300865 4.5677185785
 H 3.6210814073 0.8416933801 5.2579090329
 H 5.0119203069 -0.245181127 5.1574641002
 H 4.8068887336 1.0137735208 3.9345676991

O_Cu2+_3a

2 2

C -0.301400243 -3.2227882295 -1.5193354658
 C -1.7810040349 -2.7866847126 -1.6693384983
 C 0.6889596667 -2.4520452184 -2.4062725179
 C -1.8355043794 -1.238095002 -1.5381203144
 N -0.5170118695 -0.8345147542 -1.0013181322
 C -0.2627075551 -1.6902610127 0.2124624312
 C 0.4987426823 -0.9494368145 -2.0762488248
 H -0.2049972869 -4.298223827 -1.6594568768
 H -2.3660887017 -3.2849883485 -0.8900152968

H -2.175230608 -3.1096405791 -2.6353640157
 H 0.5192641997 -2.6376644854 -3.4695414575
 H 1.6922514653 -2.8059450818 -2.1562968135
 C -2.8814587827 -0.5555011081 -0.6758004212
 C -4.1765220655 -1.0202027542 -0.5424097947
 C -3.3608044866 1.3239849387 0.634405006
 C -5.0623441495 -0.256982243 0.2037475587
 H -4.5090614127 -1.9437322563 -1.0037191507
 C -4.6798520224 0.9282210832 0.8032101484
 H -2.9923930787 2.2364376192 1.0904613743
 H -5.3814884885 1.5156146094 1.3840346264
 N -2.4843163772 0.6079768404 -0.0889604203
 C 0.6968902997 -1.0651260732 1.2090996996
 C 1.6750625223 -1.8118947107 1.8389396471
 C 2.3982009731 -1.1739089552 2.8373057995
 H 1.863949632 -2.8469033199 1.5802562446
 C 1.1509736371 0.8067619947 2.4908585834
 C 2.1455552344 0.1361833872 3.1964245506
 H 0.9153070228 1.8418314411 2.714372092
 H 2.7067597749 0.6156797846 3.9899969457
 N 0.444193192 0.2218297294 1.5175144834
 H -1.2372531758 -1.7347984912 0.7241387159
 H -1.9267564778 -0.7910995418 -2.5342837874
 H 0.039191145 -0.4655671004 -2.9462883276
 C 1.6540156533 -0.0362264151 -1.7264270375
 C 2.9604813841 -0.2491841916 -2.1240555649
 C 3.8843745724 0.7506700904 -1.8569141053
 H 3.2724476545 -1.1511417845 -2.6382342706
 C 2.1995634882 2.0585288056 -0.8430318709
 C 3.5275677682 1.9262866044 -1.2237165328
 H 1.8551077596 2.9485459297 -0.3271099423
 H 4.2576018723 2.703565973 -1.0302195684
 N 1.2869603459 1.1070706483 -1.0894282041
 Cu -0.5389435618 0.9889739075 -0.271057868
 O 0.1372579629 -2.9559144076 -0.1745185687
 N 3.4724301288 -1.926342649 3.534346472
 O 4.0551443636 -1.3366650838 4.4200385929
 O 3.6714927968 -3.0599408761 3.1452740862
 N 5.2983828075 0.5435341993 -2.2672688183
 O 6.06763216 1.4451759002 -2.0120873658
 O 5.5458100574 -0.5120374441 -2.8147212528
 N -6.4605523024 -0.7376744856 0.3627232536
 O -6.72494735 -1.7944339919 -0.1744713108
 O -7.1988438128 -0.0302475371 1.0136020854

O_Cu2+_3c

2 2

C -0.6397769079 -0.8031015631 2.9609841683
 O -0.2797219226 0.444609973 2.3482177946
 C 0.4439582311 -1.7931893209 2.5023049153
 C -0.6174549856 0.4223750739 0.9992683978
 N -0.7641332465 -0.9919482079 0.5265148813
 C 0.3049702305 -1.9157777401 0.9649127076
 C -2.0685575968 -1.4794716 1.014075328
 H -0.5909217945 -0.6351307553 4.0359770089
 H 0.3370733625 -2.7694207464 2.9818561951
 H 1.4082796834 -1.3720029004 2.7977914042
 C -3.1207039281 -0.9020751234 0.0812427062
 C -4.4257230705 -0.7078738885 0.4597409413
 C -5.371654653 -0.2326129974 -0.4762992298
 H -4.712114533 -0.9037515139 1.4853266503

C -3.5783947545 -0.1752759171 -2.0770333319
 C -4.9028709156 0.0339583542 -1.778003085
 H -3.204818528 0.029348495 -3.0746509962
 H -5.5665344814 0.3769518062 -2.5603174519
 N -2.6826504579 -0.6451522116 -1.185633589
 H -2.0831402572 -2.5631797536 0.8544829877
 C 0.3279081877 1.2449763415 0.1420771753
 C 1.2727319938 2.0697134271 0.7021730108
 C 0.8195759949 1.9534287764 -1.9859813096
 C 2.0407431831 2.8988516542 -0.1415806589
 H 1.4113158273 2.0565972415 1.774828144
 C 1.7794293944 2.8294243078 -1.5206051956
 H 0.6123146052 1.8858703516 -3.0491739704
 H 2.2945810548 3.4682492227 -2.2260304656
 N 0.0903664889 1.163910326 -1.1840096046
 H -1.6136002208 0.8676719793 0.8547113985
 H -0.0824280994 -2.9154632999 0.7363950545
 C 1.4769670973 -1.7572359301 0.0172356742
 C 2.7853602524 -1.9554138107 0.3812969782
 C 3.8036300565 -1.9083621464 -0.5964398886
 H 3.0261359746 -2.1323426879 1.4211768782
 C 2.0753726651 -1.4544339835 -2.2036005364
 C 3.4061210009 -1.6545218081 -1.9234747172
 H 1.7549460234 -1.2515003362 -3.2202531684
 H 4.1197037464 -1.6400619586 -2.7362848774
 N 1.107816317 -1.5099000866 -1.2697971601
 Cu -0.7332560716 -0.7951737701 -1.445028844
 C -2.083429126 -1.18106727 2.5390018001
 N 5.1167256933 -2.1008103181 -0.2644154385
 N -6.6780350992 -0.0361779093 -0.1279359013
 N 3.0009380314 3.7371740131 0.3705156368
 C 6.2228833851 -1.7867756142 -1.0659059231
 C 5.5964802287 -2.6461802678 0.934591694
 C 6.9503189259 -2.6741066118 0.8767969553
 C 7.3477482307 -2.118840981 -0.3868018924
 C -7.6220465503 0.7060911221 -0.8522820468
 C -7.3138042751 -0.5402072654 1.016234181
 C -8.6051525057 -0.1302562692 0.9990782078
 C -8.7972615606 0.669534629 -0.1791541087
 C 3.121853111 4.1302354358 1.707469464
 C 4.028652716 4.3494516018 -0.3534880091
 C 4.1879531576 4.9636790016 1.8107195698
 C 4.7693275677 5.094234833 0.5059230592
 H 6.1069564925 -1.3073729811 -2.0245284809
 H 4.927758144 -3.025293228 1.6904927225
 H 7.6057683289 -3.060972268 1.6435564619
 H 8.3598141081 -1.9808249149 -0.7386519897
 H -7.35250626 1.2384863437 -1.750184931
 H -6.8046762291 -1.1994219726 1.700825116
 H -9.3544402311 -0.3769813107 1.7372622877
 H -9.709751437 1.1644944468 -0.4782535643
 H 2.3988931963 3.8313470199 2.449625819
 H 4.1672546878 4.1585247468 -1.405703649
 H 4.5221869263 5.4500060166 2.7156920817
 H 5.6426366017 5.6743852741 0.2453345534
 H -2.4294234899 -2.0479296398 3.1066562147
 H -2.7385377149 -0.3390689352 2.7838377905

 O_Cu2+_3f
 2 2
 C -0.4079851749 3.3442826006 0.9562496674

C -1.8945600818 2.9696992944 1.1976003515
 C 0.5723537493 2.7906704224 2.0051020351
 C -1.9671114822 1.4324233707 1.4103150483
 N -0.646441707 0.9164090127 1.0115861811
 C -0.3636347101 1.442687077 -0.3577820215
 C 0.3531356483 1.2590885088 2.0430832037
 H -0.302477318 4.4234346347 0.8504629223
 H -2.4690743059 3.286037171 0.3212506855
 H -2.2854041997 3.5084793812 2.0640850393
 H 0.4111041229 3.2339850892 2.9912222215
 H 1.5797165623 3.0542047059 1.6723664501
 C -2.9988791241 0.5759485769 0.6921886966
 C -4.2583386328 1.0249197629 0.4025849685
 C -3.4820623112 -1.5313942386 -0.1578389851
 C -5.2152426393 0.1497449443 -0.191978887
 H -4.5273385912 2.0427654311 0.6576025196
 C -4.764606605 -1.1714607726 -0.468841089
 H -3.1280067269 -2.5321270022 -0.3827441226
 H -5.4129257643 -1.8984030732 -0.9400898228
 N -2.5875961943 -0.7023505026 0.4274931127
 C 0.6043871835 0.5790542376 -1.1469418396
 C 1.6071958708 1.133426095 -1.8966609235
 C 2.3903656103 0.2944249973 -2.7391333095
 H 1.7568115341 2.2044407188 -1.8618696665
 C 1.048062567 -1.539005716 -1.9174788744
 C 2.0687145313 -1.0879684321 -2.7199101354
 H 0.8037864312 -2.5965266647 -1.8925083447
 H 2.6169668846 -1.8000822096 -3.3231944334
 N 0.2999418068 -0.7395121247 -1.1367378128
 H -1.3249936419 1.3647958217 -0.8875714424
 H -2.0833489992 1.2169301344 2.4779788838
 H -0.1353013519 1.00927596 2.9920231173
 C 1.4908963681 0.2616547975 1.9505990476
 C 2.7801440231 0.5537992653 2.3034052666
 C 3.7667043645 -0.4749921484 2.3252819517
 H 3.0393257506 1.56893275 2.5760225184
 C 2.0172940636 -1.9704264522 1.5987508454
 C 3.3268518142 -1.7728067373 1.9447780164
 H 1.6746305893 -2.9570698543 1.3034690676
 H 4.0040916939 -2.6167031422 1.9398382756
 N 1.0834235839 -0.9953917304 1.6090930393
 Cu -0.6721550813 -1.0523443413 0.7099217469
 O 0.0258392218 2.7802565281 -0.2891073237
 N -6.4539293915 0.5489475142 -0.473570765
 C -7.5022354912 -0.3386828647 -1.0035303029
 C -6.9408219174 1.9239757371 -0.2853239263
 N 3.3673386589 0.7879518261 -3.5083327099
 C 3.7705177545 2.1994570879 -3.5154663761
 C 4.1255145781 -0.0099183471 -4.4811016926
 N 5.0277900307 -0.2326764526 2.6850237487
 C 5.5087054824 1.0629049394 3.1864437603
 C 6.0942386962 -1.2460435379 2.6646456286
 H -7.5383982745 -1.2702287712 -0.4313772341
 H -7.2898840405 -0.5783877161 -2.0528311855
 H -6.2336082582 2.6421353629 -0.711664934
 H -7.0541619908 2.1351065812 0.7856302317
 H 3.9264728671 2.5602881648 -2.4937282833
 H 2.9893700839 2.8123863996 -3.983734625
 H 3.4501127644 -0.628280848 -5.0801975911
 H 4.8299272789 -0.6704319492 -3.9590344982
 H 4.8243222057 1.4593453589 3.9427074007

H 5.5736539028 1.7829169084 2.3604723981
H 6.1033385048 -1.7726725753 1.7057009674
H 5.9270776635 -1.9783421645 3.46438902
C -8.2878325361 1.9306853542 -1.0104960648
C 6.8869202127 0.735556712 3.7646752274
C 7.3673762131 -0.4311806724 2.8971827277
C 5.0596216757 2.1990043975 -4.3390649206
C 4.8496240166 1.0434702357 -5.3219115269
C -8.7799267231 0.488890747 -0.8561895717
H -8.1409099926 2.1727397352 -2.0678548698
H -8.9753820123 2.6651595666 -0.5877277275
H 6.7871217553 0.4188547913 4.8075802302
H 7.5577917503 1.5958433369 3.7358034975
H 7.7553511432 -0.0626430752 1.9420978651
H 8.1501834785 -1.0237539905 3.3734925465
H 5.9176738952 1.9953007537 -3.6900683958
H 5.2303819214 3.1565210174 -4.8342690037
H 4.2102435539 1.3615760057 -6.1514531719
H 5.7824363553 0.6631570784 -5.7418247319
H -9.2108835344 0.3365683603 0.1383673625
H -9.532551613 0.2127028456 -1.5964843496

O_Cu2+_3D

2 2
C 0.105139734 3.711672746 -0.3237460315
C 1.5768864513 3.3126111082 -0.6055355496
C -0.9024649806 3.2405994426 -1.3850439124
C 1.6052319385 1.7893225426 -0.9157738001
N 0.2804285209 1.27649384 -0.5092781663
C 0.0446368255 1.750288361 0.8983951442
C -0.7341878149 1.7047678755 -1.5002440048
H 0.0284224711 4.7847079692 -0.154652905
H 2.1729484239 3.5609780293 0.2781720366
H 1.9716729235 3.8904160092 -1.4442280489
H -0.7361335985 3.7222278619 -2.3517644078
H -1.898052582 3.5207624641 -1.0320551936
C 2.6382220593 0.8721709462 -0.2844644678
C 3.9440423267 1.2490648548 -0.0300825198
C 3.0757850994 -1.3031956963 0.44805345
C 4.8394622394 0.3056432074 0.4728987923
H 4.2641768585 2.266216584 -0.2291562992
C 4.3997056388 -0.9908109044 0.7133036001
H 2.6847851436 -2.2978461608 0.6343976752
H 5.8684018513 0.5842644561 0.6748698171
H 5.0643881556 -1.751555798 1.1052592888
N 2.2127749143 -0.3997564365 -0.0462824515
C -0.9165281556 0.8786708498 1.6869878671
C -1.8667111285 1.4166563376 2.5353632707
C -2.6048893009 0.5441232412 3.3359499167
H -2.0102475987 2.4897125704 2.5767216012
C -1.3932807484 -1.276942577 2.3702735682
C -2.3583220441 -0.821000116 3.2609005275
H -3.3555891337 0.9317357305 4.0166732969
H -1.1774336342 -2.3357992296 2.2705312547
H -2.9015071534 -1.5278962683 3.877368481
N -0.683612884 -0.4457588803 1.5984614329
H 1.0227155588 1.6354256087 1.391221769
H 1.6874265941 1.6405104407 -1.9980457832
H -0.2790626289 1.4860787142 -2.4734018661
C -1.9026082296 0.74433856 -1.4246548561
C -3.2061524331 1.0694928694 -1.750653599

C -4.1675346384 0.0597942769 -1.7883754761
H -3.4710445654 2.0936577096 -1.9882321125
C -2.4751664359 -1.5036771923 -1.1661946793
C -3.7961994307 -1.2480297578 -1.4995740043
H -5.1945876705 0.2955387628 -2.0467782199
H -2.1413927493 -2.5053982111 -0.9156760906
H -4.5130058486 -2.0602083954 -1.5265467579
N -1.5473225352 -0.5351205277 -1.1361417061
Cu 0.2667083509 -0.6837964237 -0.3191246288
O -0.3323141561 3.0848886054 0.8936847479

O_3b

O 1
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N 0.5812888979 -0.543994297 0.3063984381
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H 5.8509582221 2.2472380424 1.135364043
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