

Supporting Information

Change in molecular shapes of the trinuclear $\text{Cu}^{\text{II}}_2\text{Zn}^{\text{II}}$ complexes on Schiff base reduction: Structural and theoretical investigations

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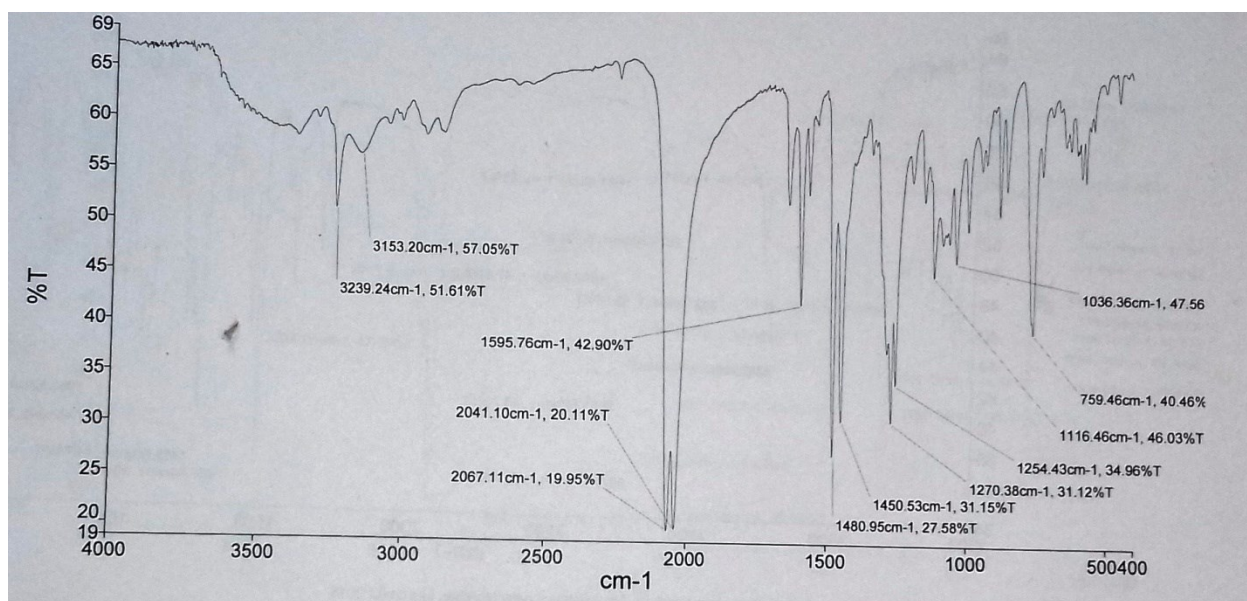


Fig. S1 IR Spectrum of complex 1

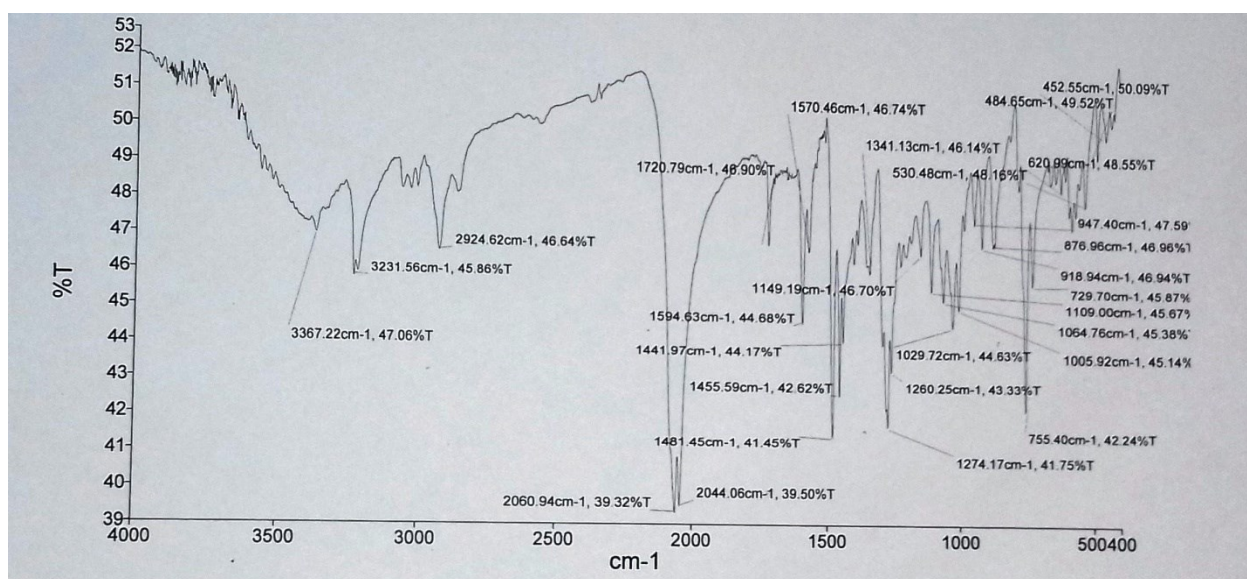


Fig. S2 IR Spectrum of complex **2**

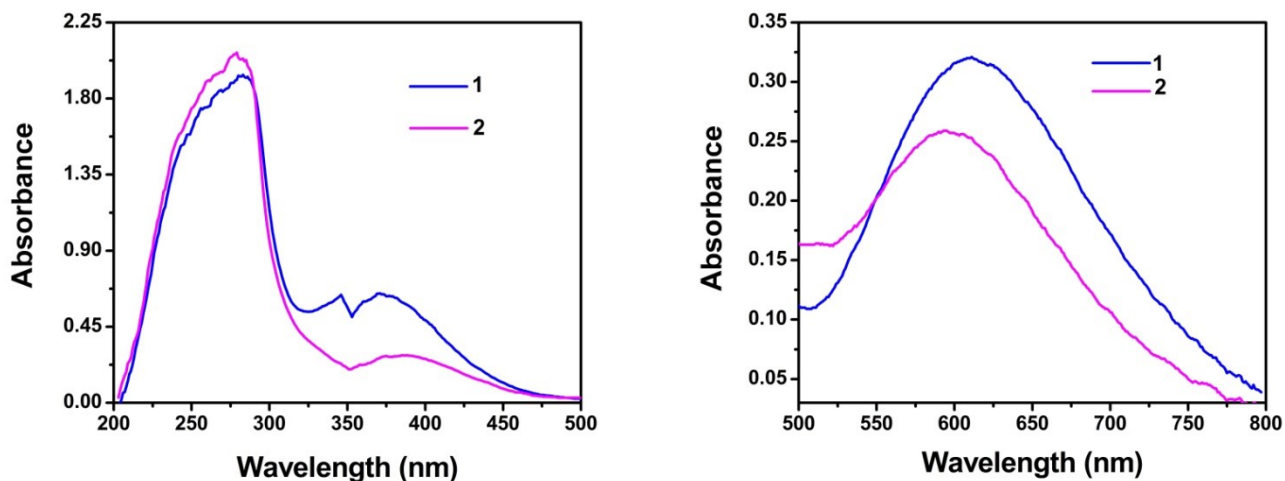


Fig. S3 UV-Vis spectra of trinuclear complexes, **1** and **2** in acetonitrile solution (charge transfer band in the left and d-d transition band at the right side).

Table S1

Hydrogen bonds, distances Å, angles, deg.

A acceptor, D donor

Atoms	D-H	A...H	D...A	D-H...A	Symmetry element
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In **1**

N18-H18...N6	0.83(3)	2.65(9)	3.298(12)	136(11)	$\frac{1}{2}+x, -1/2-y, 1-z$
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N39-H39...O1W		0.85(3)	2.33(7)	3.097(11)	151(12)
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N43-H43...N3		0.84(3)	2.55(4)	3.378(10)	169(12)	$-1/2+x, 1/2-y, 1-z$
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In **2**

N18A-H18A...N1B		0.84(2)	2.57(3)	3.387(7)	165(9)
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N22A-H22A...N1B		0.83(2)	2.34(3)	3.168(7)	171(10)
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N22A-H22A...N2B	0.83(2) 2.55(4) 3.346(6) 160(9)
N39A-H39A...N6A	0.84(2) 2.38(4) 3.194(9) 165(10) x, 1/2-y, z-1/2
N43A-H43A...N6A	0.85(2) 2.43(4) 3.250(10) 164(10) x, 1/2-y, z-1/2
N18B-H18B... N1A	0.84(2) 2.42(4) 3.212(7) 158(9)
N22B-H22B...N1A	0.83(2) 2.61(4) 3.400(7) 159(9)
N39B-H39B...N6B	0.84(2) 2.36(6) 3.095(9) 146(10) x, 1/2-y, 1/2+z
N43B-H43B...N6B	0.84(2) 2.55(5) 3.308(9) 151(9) x, 1/2-y, 1/2+z

Table S2

Cartesian Coordinates

1A

Zn	0.0001740	5.5614798	-0.0002059
Cu	-2.0444944	7.2283358	-1.1197446
O	-0.8297291	5.9161559	-2.0253069
O	-2.1369702	5.6504683	0.1069147
N	-1.8608929	8.5204506	-2.6146597
N	-3.2973229	8.2133204	0.0723734
N	0.0413133	3.4755518	-0.0470718
N	0.2447072	2.7257014	-0.9724824
C	-0.3346185	7.1697321	-4.0162576
C	-2.8328382	5.4464703	1.2032814
C	-4.4152922	6.1580933	2.9347367
H	-5.0714547	6.9292237	3.3457884
C	-2.6996290	4.2119646	1.8857131
H	-1.9989513	3.4879768	1.4671776
C	-0.2068214	6.0175564	-3.1752408
C	-1.1231672	8.3099214	-3.6690349

C	-3.7047758	6.4402460	1.7410687
C	-3.5094327	9.6360838	-0.2015448
H	-2.6173451	10.1778709	0.1600881
H	-4.3718705	9.9994114	0.3831740
C	-3.4108622	3.9728104	3.0484877
H	-3.2778905	3.0233494	3.5693935
C	-4.2800427	4.9446170	3.5835790
H	-4.8248794	4.7477651	4.5062873
C	-3.7216808	9.9210567	-1.6870334
H	-4.1404566	10.9341500	-1.7867687
H	-4.4622323	9.2197162	-2.1026061
C	0.3854174	7.2168964	-5.2398210
H	0.2857798	8.1069885	-5.8659158
C	-2.4315724	9.8700954	-2.4963586
H	-2.6018343	10.2848026	-3.5047423
H	-1.6809595	10.5108582	-2.0003850
C	0.6254163	4.9570985	-3.6143477
H	0.7128067	4.0733512	-2.9849845
C	1.3094690	5.0398124	-4.8134270
H	1.9516368	4.2104885	-5.1127780
C	1.2005716	6.1767966	-5.6403071
H	1.7524509	6.2335070	-6.5780184
C	-3.8354274	7.7426475	1.1606769
N	0.4693535	1.9674570	-1.8257472
H	-4.4663108	8.4392374	1.7374495
H	-1.0751007	9.1311011	-4.4047028
Cu	2.0445719	3.8947375	1.1199202
O	0.8294348	5.2069260	2.0249056
O	2.1375057	5.4724849	-0.1068136
N	1.8605895	2.6028989	2.6150498

N	3.2974573	2.9093908	-0.0718059
N	-0.0408703	7.6474059	0.0462092
N	-0.2433788	8.3974646	0.9716503
C	0.3343017	3.9540290	4.0162419
C	2.8332265	5.6760459	-1.2033737
C	4.4151644	4.9636411	-2.9349731
H	5.0710575	4.1922549	-3.3459720
C	2.7001798	6.9104276	-1.8860549
H	1.9997408	7.6346711	-1.4675650
C	0.2064866	5.1059196	3.1748467
C	1.1228303	2.8137321	3.6693458
C	3.7048117	4.6819335	-1.7410970
C	3.5095211	1.4866783	0.2024669
H	2.6175215	0.9448027	-0.1592537
H	4.3720826	1.1232466	-0.3820050
C	3.4112911	7.1491658	-3.0489934
H	3.2784592	8.0985492	-3.5700780
C	4.2801249	6.1770243	-3.5840343
H	4.8248217	6.3735324	-4.5068972
C	3.7214662	1.2020167	1.6880437
H	4.1401823	0.1889269	1.7880808
H	4.4619728	1.9034134	2.1036001
C	-0.3857249	3.9072515	5.2398221
H	-0.2860292	3.0173923	5.8662377
C	2.4312042	1.2532007	2.4971077
H	2.6012625	0.8386827	3.5056013
H	1.6806580	0.6123850	2.0011055
C	-0.6258802	6.1664519	3.6135277
H	-0.7133664	7.0499414	2.9838084
C	-1.3099559	6.0841021	4.8126183

H	-1.9522026	6.9134755	5.1116614
C	-1.2009486	4.9474403	5.6399305
H	-1.7527868	4.8910534	6.5776856
C	3.8353930	3.3796816	-1.1603620
N	-0.4672121	9.1559229	1.8249336
H	4.4660948	2.6828434	-1.7370333
H	1.0747003	1.9927379	4.4052150

1B

Zn	8.7771922	2.9059437	9.4960545
Cu	5.9215582	3.2760781	11.5024533
Cu	6.4527377	4.7850038	8.2370716
N	8.5142061	0.9404655	9.3836356
N	11.1458492	4.2696641	10.3520372
O	6.0568122	2.8472656	9.5946989
C	4.9475276	0.5935363	6.9846076
H	5.3568336	0.1152733	6.0929529
O	7.6946122	5.3525053	9.6229077
O	8.0459172	3.7040690	7.7058044
C	6.2985874	3.9773246	5.4361854
O	7.8965929	3.0501751	11.4656988
C	8.2423845	3.4405083	4.0527090
H	7.5930133	3.5532819	3.1810821
C	10.5041470	2.7764555	14.7008514
H	11.2196354	2.7458347	15.5217034
N	11.6956611	4.9507069	11.1169204
N	5.6208206	4.3439365	6.4861248
N	5.9995348	4.0385214	13.3253161
N	3.9178987	3.1583168	11.3365894
C	5.2822239	2.0239109	8.9254599

C	8.5064766	6.2157616	11.6504992
H	9.4713253	5.7526147	11.4491498
C	8.3370516	3.4444255	13.7975192
C	3.1014814	0.9675479	8.4814457
H	2.0625437	0.8052341	8.7787604
N	7.6731185	0.4806566	10.1203635
C	3.9196480	1.7893262	9.2977090
C	3.5309718	5.6016052	7.0149633
H	4.0110403	6.5224785	6.6487164
H	2.4735116	5.6416331	6.7119471
C	6.1866858	6.6426971	10.9915412
C	7.4628420	6.0435647	10.6996364
N	4.9280861	5.7352496	9.0809143
C	9.9177937	2.2229724	12.4034642
H	10.1640448	1.7538691	11.4516049
C	9.8755170	3.1341129	6.3082451
H	10.5020967	3.0316608	7.1954674
C	9.2752294	3.3860778	14.8589257
H	8.9993872	3.8282684	15.8192074
C	10.3760235	2.9210028	5.0339044
H	11.4215853	2.6299037	4.9185526
C	3.3307332	2.4256589	10.4305123
C	7.6948035	3.6775154	5.3390990
C	6.0337725	7.4222350	12.1694681
H	5.0660108	7.8965403	12.3558158
C	5.0347723	6.4365497	10.1749404
C	8.6834802	2.9022660	12.5210383
N	10.6199873	3.5559083	9.5347436
C	8.5281745	3.5225011	6.4926516
C	9.5655062	3.0752544	3.8909723

H	9.9747966	2.9025247	2.8960889
C	5.7718331	1.3960377	7.7525466
H	6.8161256	1.5592836	7.4988878
C	10.8086113	2.1794454	13.4633109
H	11.7638049	1.6702302	13.3278376
C	7.0645745	4.0246410	14.0753741
C	7.0657384	7.5749595	13.0719469
H	6.9311868	8.1706701	13.9745896
C	3.0370908	3.8552070	12.2754158
H	2.9515644	4.9039529	11.9335114
H	2.0241285	3.4174712	12.2296621
C	3.5980981	0.3756289	7.3357858
H	2.9628574	-0.2608706	6.7205047
C	8.3064535	6.9538793	12.7995819
H	9.1309949	7.0562138	13.5074925
C	4.8148886	4.6883449	13.8858305
H	4.9848426	4.9030826	14.9544505
H	4.6873026	5.6589891	13.3787798
C	4.1642522	4.3798611	6.3534192
H	3.8883482	4.3408883	5.2852318
H	3.7706094	3.4609397	6.8250628
C	3.5808325	5.5549332	8.5395940
H	3.2184044	4.5675730	8.8747141
H	2.9047757	6.3176243	8.9658272
C	3.5501613	3.8519918	13.7104867
H	2.7630769	4.2755183	14.3530361
H	3.7291846	2.8190608	14.0465313
N	6.8582031	0.0236837	10.8116957
H	5.7309011	3.8489855	4.4993595
H	6.9739390	4.4878173	15.0707819

H	2.2383547	2.2990527	10.5225734
H	4.1109178	6.9087102	10.5524460

1A'

Zn	-0.0188888	5.5769377	0.1957600
Cu	-1.8621141	7.3979889	-0.8917338
O	-0.8624223	5.9518655	-1.8185967
O	-2.1141649	5.9235430	0.3910761
N	-1.3151658	8.7105700	-2.3379280
N	-3.1575222	8.5109747	0.2399830
N	-0.2330090	3.4510446	0.1615885
N	-0.0222159	2.7134188	-0.7686032
C	-0.5963016	6.9899939	-3.9757740
C	-3.0934730	5.6988345	1.2680794
C	-5.2179007	6.2834258	2.2945061
H	-6.0857743	6.9456691	2.3513085
C	-3.0027308	4.6002554	2.1456228
H	-2.1236320	3.9620050	2.0616230
C	-0.3030777	5.9717257	-3.0311854
C	-1.6061886	8.0548351	-3.6543487
C	-4.2329388	6.5412889	1.3321465
C	-3.3888430	9.9119668	-0.1837408
H	-2.6304904	10.5234243	0.3279693
H	-4.3770875	10.2418640	0.1798911
C	-4.0006986	4.3596099	3.0831255
H	-3.9000235	3.5126319	3.7637113
C	-5.1146800	5.2032385	3.1717345
H	-5.8913209	5.0229780	3.9149331
C	-3.2856948	10.1350852	-1.6940864
H	-3.7032085	11.1273804	-1.9241620

H	-3.9065788	9.4035302	-2.2360546
C	0.0561582	6.9873786	-5.2168441
H	-0.1620438	7.7888216	-5.9277164
C	-1.8433513	10.0880815	-2.2038345
H	-1.7635019	10.6033729	-3.1768714
H	-1.1916824	10.6176125	-1.4935559
C	0.5979042	4.9516267	-3.4014733
H	0.8001671	4.1618273	-2.6817963
C	1.2131246	4.9559354	-4.6459898
H	1.9188662	4.1621131	-4.8934511
C	0.9596748	5.9838286	-5.5624422
H	1.4594786	6.0020486	-6.5307540
C	-4.3986953	7.6817977	0.3629842
N	0.2370659	1.9750962	-1.6360629
H	-5.2306335	8.3239102	0.7003253
H	-2.6269346	7.6421850	-3.5958535
Cu	1.9783989	3.7826901	0.9664558
O	1.0222433	5.1370984	2.0960247
O	2.0694188	5.3699294	-0.1829648
N	1.7062799	2.3721150	2.4072555
N	3.0446710	2.7466425	-0.4529671
N	0.1560630	7.7146654	0.3271958
N	-0.2890493	8.3529951	1.2480932
C	0.9538957	3.9300928	4.1705816
C	2.8499221	5.6514149	-1.2269959
C	4.6459344	5.1011087	-2.7643671
H	5.4416785	4.4200409	-3.0777484
C	2.6270544	6.8381205	-1.9543795
H	1.8261397	7.4892681	-1.6036398
C	0.4834737	4.9509406	3.3011749

C	2.0590977	3.0204020	3.7174166
C	3.9018463	4.7889232	-1.6186940
C	3.3616492	1.3358929	-0.1242735
H	2.5022865	0.7362855	-0.4603137
H	4.2389607	1.0159236	-0.7132184
C	3.3906558	7.1344071	-3.0755082
H	3.1819141	8.0424064	-3.6432007
C	4.3981110	6.2594698	-3.5004691
H	4.9817344	6.4769348	-4.3947668
C	3.6111073	1.0887440	1.3656983
H	4.1249333	0.1214958	1.4752566
H	4.2917607	1.8527945	1.7751095
C	0.3634261	3.7701270	5.4301679
H	0.7237808	2.9724370	6.0854276
C	2.3180903	1.0391567	2.1820975
H	2.4998591	0.5555910	3.1569957
H	1.5804762	0.4260880	1.6440804
C	-0.5587255	5.7899418	3.7458089
H	-0.9155796	6.5721347	3.0763020
C	-1.1147355	5.6249494	5.0084443
H	-1.9262619	6.2838625	5.3201530
C	-0.6634014	4.6106002	5.8612918
H	-1.1097623	4.4729748	6.8461175
C	4.2423165	3.5784494	-0.7931649
N	-0.7697007	8.9881643	2.1030824
H	4.9689476	2.9564298	-1.3439857
H	3.0079824	3.5624427	3.5738314
H	-1.6030150	8.8185642	-4.4513972
H	-0.2948899	8.7302397	-2.2209708
H	-2.6975482	8.5453168	1.1663692

H	-4.6583216	7.3187811	-0.6462429
H	2.2300870	2.2394831	4.4766521
H	4.7183479	3.8683084	0.1594470
H	2.4174181	2.7319927	-1.2721360
H	0.6831165	2.2794548	2.3833224

1B'

Zn	7.9922802	3.4371560	9.6892327
Cu	6.3074229	2.9987453	12.4469687
Cu	6.2877223	4.8390193	7.3056118
N	8.1080680	1.3241378	9.8784304
N	10.0097279	5.3428551	10.3089817
O	5.9463572	3.1907068	10.5124184
C	3.6470523	2.4170767	7.7900140
H	3.6869089	2.0573184	6.7589843
O	6.8042110	5.3585356	9.1046002
O	7.5946339	3.3418483	7.5930939
C	6.5595637	2.9747693	5.0367768
O	8.1522625	3.5457996	11.9000493
C	8.8573567	2.1554293	4.3765566
H	8.4872788	1.9982268	3.3599056
C	11.5555987	2.3636076	13.9967144
H	12.4502590	2.0760916	14.5492549
N	10.3793736	6.1142906	11.0972864
N	6.2608092	4.4317021	5.2650884
N	6.9319087	2.7748001	14.3926532
N	4.2729978	2.7476867	12.7707647
C	4.8179266	2.9884719	9.8588234
C	6.7139755	6.2423322	11.2940664
H	7.7279471	5.8786002	11.4510712

C	9.2973760	3.2548459	13.9682961
C	2.3843402	3.1237153	9.7145522
H	1.4270071	3.3452362	10.1933891
N	7.5536390	0.9699533	10.8734523
C	3.5582396	3.2609411	10.4615934
C	4.6168713	6.2751947	4.8172184
H	5.4795450	6.9612976	4.7603716
H	3.9176997	6.5971815	4.0308264
C	4.7787855	6.4642098	9.8374984
C	6.1080464	6.0088000	10.0369635
N	4.8229270	6.3168856	7.3265301
C	10.3658283	2.5924811	11.8902502
H	10.3284752	2.4788350	10.8093859
C	9.7830237	2.5512418	6.9878243
H	10.1361132	2.7287619	8.0014300
C	10.4400800	2.8636245	14.6697721
H	10.4543941	2.9597982	15.7585555
C	10.6267653	2.0347011	6.0090073
H	11.6567780	1.7891341	6.2730994
C	3.5278872	3.7052755	11.8900877
C	7.9859911	2.6557081	5.3492606
C	4.1151396	7.1378070	10.8742578
H	3.0926250	7.4852606	10.7023405
C	4.0259716	6.1491123	8.5797431
C	9.2466992	3.1374133	12.5546390
N	9.6503536	4.5563333	9.4674023
C	8.4458146	2.8704611	6.6743812
C	10.1782150	1.8375581	4.6965792
H	10.8482512	1.4379003	3.9352769
C	4.8299503	2.5227741	8.5203412

H	5.7923822	2.2325739	8.1019099
C	11.5033561	2.2304220	12.6043586
H	12.3624278	1.8285490	12.0643597
C	8.0662689	3.7240142	14.6699731
C	4.7145510	7.3463612	12.1151221
H	4.1784048	7.8705536	12.9064410
C	3.7712076	2.7971647	14.1593979
H	3.7293870	3.8590313	14.4481950
H	2.7352604	2.4132746	14.1909392
C	2.4126844	2.7321290	8.3717844
H	1.4865275	2.6394928	7.8046361
C	6.0249716	6.8872594	12.3130230
H	6.5250180	7.0496432	13.2701582
C	5.9385522	2.7850449	15.4860010
H	6.3957324	2.3670020	16.4007076
H	5.7017830	3.8395680	15.6986967
C	5.0550248	4.8455738	4.5120404
H	5.2361332	4.7204710	3.4292610
H	4.2515387	4.1452744	4.7888221
C	3.9125602	6.4118734	6.1629114
H	3.1783010	5.5982043	6.2746549
H	3.3514298	7.3622351	6.2111078
C	4.6560046	2.0339007	15.1408867
H	4.0878597	1.8735446	16.0697537
H	4.8950845	1.0339539	14.7417272
N	6.9879615	0.6794804	11.8665262
H	5.8683058	2.4169475	5.6866240
H	8.2440183	3.7761207	15.7572561
H	4.0036796	4.6912353	12.0155819
H	3.6755014	5.1061147	8.5727796

H	6.3332889	2.7177722	3.9882328
H	7.0669126	4.9533878	4.8950126
H	3.1296052	6.7922346	8.5263285
H	2.4816137	3.7855574	12.2322782
H	7.3329488	1.8289481	14.3096139
H	7.7402618	4.7143970	14.3169411
H	4.1311375	1.7976657	12.4017453
H	5.3564550	7.1916935	7.4070223

2

Zn	5.5266852	-0.0608256	21.6062081
Cu	4.9796924	-2.9095575	20.3597498
Cu	3.0493793	1.3359675	20.3954075
O	4.9955613	1.7431046	20.5231668
O	5.5700386	-1.0662427	19.8248076
O	5.3134880	-2.1005569	22.1516440
O	3.5091283	0.1653216	21.9406632
N	5.2180357	-3.5733356	18.3770140
H	6.1802174	-3.9186508	18.2701585
N	4.5905310	-4.7595544	21.2026386
H	5.4843666	-5.2320445	21.3881056
N	2.5256726	-1.5031517	19.6152160
N	1.0965884	1.6864106	21.1026616
H	1.0996356	2.5582855	21.6452375
N	7.1101727	1.6264811	23.1989883
N	2.9383552	2.4606428	18.6903508
H	3.1400264	3.4367303	18.9417447
C	5.5888484	-2.7747815	23.2709398
C	6.2097354	-1.4507494	17.5699999
N	2.7688841	-2.5814695	20.0362383

C	5.7298739	2.4629722	19.6678366
C	4.9295883	-4.0026227	23.5344308
C	3.7582809	0.2791998	24.3232145
H	4.8302849	0.0959174	24.2299000
C	1.5770791	0.5627765	23.2766207
N	7.0619887	0.5552898	22.6327056
C	4.3615415	-5.8607101	18.9624407
H	3.8168663	-6.6931496	18.4915801
H	5.4086093	-6.2004610	19.0571231
C	5.3631676	2.5910730	18.3026075
C	6.4331125	-0.8346844	18.8254618
C	7.0675192	-1.1682623	16.5025360
H	6.8863230	-1.6447236	15.5353354
C	8.1340372	-0.2784570	16.6539561
H	8.7821175	-0.0491231	15.8079275
C	2.9726569	0.3385691	23.1566381
N	2.2999485	-0.4216716	19.1859857
C	6.5223072	-2.2837587	24.2065295
H	7.0225224	-1.3401878	23.9792387
C	7.5425579	0.0148254	18.9877500
H	7.7239684	0.4586366	19.9677619
C	3.9374184	-4.5054604	22.5323954
H	3.4732151	-5.4396913	22.8929560
H	3.1433117	-3.7687803	22.3381072
C	3.7540875	-5.6250853	20.3440190
H	3.5846111	-6.5926720	20.8512228
H	2.7830931	-5.1195617	20.2451584
C	5.2200450	-4.7057712	24.7076197
H	4.7069169	-5.6521782	24.8989315
C	4.2764683	-4.6585516	18.0240166

H	4.4565170	-4.9802375	16.9816053
H	3.2687394	-4.2212841	18.0758310
C	3.1737083	0.4387677	25.5766798
H	3.8013263	0.3827866	26.4671080
C	5.0609421	-2.4031326	17.4472741
H	4.9801938	-2.7698302	16.4090199
H	4.1107399	-1.9215592	17.7189145
C	4.0752575	1.9834880	17.8325534
H	4.0772996	0.8839000	17.8969100
H	3.8863482	2.2655414	16.7830763
C	1.0160449	0.7422486	24.5445733
H	-0.0599168	0.9185829	24.6264852
C	0.4824914	2.8245879	18.9392528
H	0.7171101	3.7968228	19.4085695
H	-0.4077100	2.9987480	18.3155896
C	6.7753628	-2.9904640	25.3793883
H	7.4936569	-2.5903418	26.0974950
C	0.7374137	0.5692357	22.0349706
H	-0.3320614	0.6394552	22.3020093
H	0.8895470	-0.3548724	21.4574475
C	8.3667243	0.3054370	17.9046211
H	9.1958002	1.0006409	18.0403671
C	6.1326345	-4.2070858	25.6397868
H	6.3404945	-4.7599596	26.5560911
C	6.9042049	3.1027826	20.1171579
H	7.1563455	3.0418653	21.1746482
C	7.7268974	3.7800483	19.2216105
H	8.6407396	4.2498877	19.5896791
C	6.1986642	3.2894514	17.4256215
H	5.9123747	3.3673153	16.3736991

C	0.1069284	1.7960758	20.0068645
H	-0.8878148	2.0351860	20.4262900
H	0.0498368	0.7992024	19.5467898
C	1.6256068	2.3950875	18.0182306
H	1.4851050	1.3523880	17.7016232
H	1.6436574	3.0308998	17.1144272
N	7.2217068	2.6385736	23.7530043
C	7.3902210	3.8675014	17.8657149
H	8.0375053	4.3950319	17.1649021
C	1.8006011	0.6792811	25.6987507
H	1.3468946	0.8138265	26.6807194

2'

Zn	5.8076288	-0.0550072	21.4748158
Cu	4.8459946	-2.9395587	20.6043905
Cu	3.3349271	1.3830778	20.0761022
O	5.3058233	1.6382914	20.1199343
O	5.8263025	-1.3254288	19.9000819
O	5.5397733	-2.1026023	22.2593562
O	3.8296045	0.3734810	21.7334217
N	4.6466113	-3.6444651	18.7396738
N	4.1998544	-4.5110942	21.6152782
N	2.7731982	-1.3380389	19.4726696
N	1.3949258	1.2048390	20.5497428
N	6.9095095	1.7670655	23.2309822
N	3.1679862	2.6406045	18.5603377
C	5.8401573	-2.7005254	23.3940121
C	6.0671211	-1.9796090	17.6045812
N	2.6447088	-2.1886853	20.2897519
C	5.9839007	2.6682495	19.6599069

C	5.3154792	-3.9878210	23.7387499
C	3.7542134	-0.1474510	24.0454483
H	4.8419252	-0.1923497	24.0642869
C	1.6958241	0.3074885	22.8237167
N	7.1341029	0.7139643	22.6612701
C	3.7079305	-5.8127318	19.5553732
H	3.0486997	-6.6249223	19.2122849
H	4.7274828	-6.2249817	19.6180525
C	5.4392668	3.5659917	18.6851633
C	6.4049924	-1.1594934	18.7211018
C	6.6487028	-1.6986781	16.3458787
H	6.3621795	-2.3192598	15.4936012
C	7.5636539	-0.6721908	16.1785252
H	7.9981007	-0.4708223	15.1998691
C	3.1175225	0.1889149	22.8323803
N	2.9396165	-0.4713342	18.6799534
C	6.6901282	-2.0549810	24.3252537
H	7.1106579	-1.0901221	24.0336249
C	7.3716149	-0.1501298	18.5411043
H	7.6583540	0.4481372	19.4046310
C	4.4782707	-4.7514679	22.8591140
C	3.2337205	-5.3739137	20.9423812
H	3.0219765	-6.2561916	21.5719455
H	2.3020358	-4.7928328	20.8382497
C	5.6131399	-4.5391161	25.0090652
H	5.1909990	-5.5148361	25.2626494
C	3.6492999	-4.6963844	18.5156200
H	3.7778111	-5.1144126	17.5019474
H	2.6577825	-4.2165534	18.5642935
C	3.0178917	-0.4269147	25.1862368

H	3.5453565	-0.7001885	26.1015245
C	5.1502020	-3.0833454	17.6834961
C	4.1130378	3.4313496	18.1553188
H	3.8860177	4.0831721	17.2945391
C	0.9727750	0.0076293	24.0025149
H	-0.1170080	0.0809937	23.9750003
C	0.6839616	2.6858685	18.6682566
H	0.7607528	3.5597515	19.3345200
H	-0.1830501	2.8526004	18.0108160
C	6.9670182	-2.6320981	25.5545840
H	7.6231424	-2.1052662	26.2501191
C	0.9505488	0.7073301	21.6632525
H	-0.1418204	0.5822248	21.7531366
C	7.9288089	0.0982355	17.2958634
H	8.6546678	0.9063433	17.1919763
C	6.4232744	-3.8793461	25.9155979
H	6.6438493	-4.3209397	26.8869684
C	7.3090867	2.9010788	20.1043972
H	7.7153171	2.2290532	20.8603635
C	8.0610303	3.9498655	19.6006132
H	9.0755129	4.1003307	19.9740876
C	6.2431247	4.6185528	18.1835057
H	5.8133024	5.2844813	17.4310330
C	0.4163586	1.4210532	19.4810815
H	-0.5992667	1.4544661	19.9124894
H	0.4736359	0.5474662	18.8099429
C	1.9307394	2.5875665	17.7876745
H	1.9239784	1.6194841	17.2595872
H	1.9297944	3.3930593	17.0316418
N	6.7636253	2.7641760	23.7972305

C	7.5373171	4.8210019	18.6275718
H	8.1369859	5.6422327	18.2363584
C	1.6132142	-0.3620058	25.1733817
H	1.0393310	-0.5877942	26.0716245
H	4.8623290	-3.5085727	16.7071431
H	4.0249381	-5.6506483	23.3090297