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Supporting Information

One-dimensional magnetism in a facile spin 1/2 Heisenberg antiferromagnet with a low saturation field

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List of Tables

Table 1: Crystal data and structure refinement for $(C_5H_7N_2)_2[Cu(C_2O_4)_2]\cdot 2H_2O$ (**CuD**)

Identification code	shelx
Emperical formula	$C_{14}H_{18}CuN_4O_{10}$
Formula weight	465.86
Temperature	296(2) K
Crystal System	Monoclinic
Space Group	P 21/c
a[Å]	3.7064(3)
b[Å]	20.2976(17)
c[Å]	11.9059(11)
α[deg]	90
β[deg]	90.474(3)
γ[deg]	90
V[Å^3]	895.66(13)
Z	2
Density calculated (mg/m^3)	1.727
Absorption Coefficient	1.285 mm^{-1}
F(000)	478
Crystal Size	0.060 x 0.058 x 0.040 mm^3
Theta range for data collection[deg]	2.637 to 24.989
Index ranges	-22<=h<=22, -8<=k<=8, -8<=l<=8
Reflections collected	1580
Independent reflections	1580 [R(int) = 0.0360]
Completeness to theta = 24.989°	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.950 and 0.927
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1580 / 4 / 149
Goodness-of-fit on F^2	1.058
Final R indices[I>2sigma(I)]	R1 = 0.0257, wR2 = 0.0712
R indices (all data)	R1 = 0.0298, wR2 = 0.0737
Extinction coefficient	n/a
Largest diff. peak and hole	0.280 and -0.212 e.Å-3

Table 2: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^4) for **CuD**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atoms	x	y	z	U(eq)
C(1)	7558(6)	5932(1)	4837(2)	42(1)
C(2)	8852(6)	6238(1)	3918(2)	34(1)
C(3)	9035(5)	6928(1)	3887(2)	26(1)
C(4)	7756(6)	7272(1)	4830(2)	34(1)
C(5)	6501(6)	6935(1)	5723(2)	41(1)
C(6)	1748(5)	5884(1)	8403(2)	26(1)
C(7)	3462(6)	5221(1)	8048(2)	27(1)
Cu	0	5000	10000	28(1)
N(1)	10343(6)	7246(1)	3004(2)	36(1)
N(2)	6424(5)	6276(1)	5729(2)	43(1)
O(1)	3063(4)	4755(1)	8767(1)	35(1)
O(2)	-15(4)	5864(1)	9328(1)	30(1)
O(3)	2179(5)	6368(1)	7817(1)	38(1)
O(4)	5085(5)	5177(1)	7168(1)	39(1)
O(5)	13565(6)	6509(1)	1230(2)	48(1)

Table 3: Cartesian coordinates(Optimized uisng B3LYP/631g++(d,p) level of theory) of **CuD**. Optimized energy E (B3LYP/631g++(d,p)) = -3156.7311 Hatrees

Atoms	x	y	z
Cu	0.000056	-0.000223	-0.000056
O	1.349258	-1.408489	-0.000166
O	1.555928	1.208904	-0.000317
O	-1.555827	-1.209402	0.000155
O	-1.349117	1.408033	0.000060
C	2.553263	-0.975017	-0.000359
C	2.660900	0.588146	-0.000460
C	-2.660790	-0.588611	0.000226
C	-2.553122	0.974548	0.000173
O	3.582235	-1.649237	-0.000537
O	3.786286	1.126623	-0.000635
O	-3.786213	-1.126976	0.000287
O	-3.582090	1.648787	0.000235
C	8.364467	0.740974	-0.000396
C	7.017048	1.003617	-0.000462
C	6.489278	-1.277034	-0.000529
C	7.822122	-1.616114	-0.000451
C	8.808417	-0.603834	-0.000429
H	9.080587	1.552390	-0.000272
H	6.614109	2.008371	-0.000463
H	5.053877	0.295694	-0.000602
H	5.673705	-1.988875	-0.000560
H	8.104672	-2.661734	-0.000404
C	-7.016634	-1.003259	0.000222
C	-8.364091	-0.740798	-0.000086
C	-8.808247	0.603934	-0.000557
C	-7.822089	1.616367	-0.000659
C	-6.489204	1.277494	-0.000314
H	-6.613515	-2.007939	0.000576
H	-9.080033	-1.552373	0.000062
H	-8.104810	2.661940	-0.001053
H	-5.673724	1.989435	-0.000356
H	-5.053761	-0.295014	0.000286
N	-6.105216	-0.012933	0.000120
N	6.105458	0.013437	-0.000557
H	10.438235	-1.853804	0.000070
H	10.827884	-0.162290	0.000484
H	-10.438225	1.853687	-0.000178
H	-10.827687	0.162163	-0.000014
N	10.129319	-0.896621	-0.000608
N	-10.129175	0.896545	-0.001114
O	-11.959609	-1.456450	0.001957
O	11.957925	1.457739	0.002782
H	-12.396800	-1.839139	-0.766004
H	-12.395952	-1.837359	0.771283

H	12.393620	1.838577	0.772519
H	12.395375	1.841006	-0.764748

Table 4: Cartesian coordinates(Optimized using B3LYP/lan2dnz level of theory) of **CuD**. Optimized energy E (B3LYP/lan2dnz) = -1711.72283 Hatreees

Atoms	x	y	z
Cu	0.00000400	-0.00001100	0.00000900
O	-1.37308800	1.39949100	0.00038300
O	-1.56014200	-1.22106200	0.00025200
O	1.56014600	1.22104000	-0.00014300
O	1.37309700	-1.39951100	-0.00037600
C	-2.61130400	0.95987900	0.00051000
C	-2.70670700	-0.60749100	0.00066700
C	2.70671400	0.60746900	-0.00059400
C	2.61131100	-0.95989800	-0.00059500
O	-3.66716100	1.64675600	0.00071200
O	-3.85320200	-1.16596900	0.00114200
O	3.85320800	1.16594700	-0.00109300
O	3.66716600	-1.64677900	-0.00058600
C	-8.48373700	-0.80675500	-0.00005300
C	-7.12813500	-1.09777800	0.00026100
C	-6.55652900	1.20551400	0.00018000
C	-7.89721500	1.56683200	-0.00014200
C	-8.91035500	0.55962300	-0.00026900
H	-9.21520600	-1.60724400	-0.00014100
H	-6.74636300	-2.11233700	0.00041900
H	-5.14397000	-0.39744400	0.00067800
H	-5.72672000	1.90372900	0.00032500
H	-8.16378100	2.61908000	-0.00030800
C	7.12813300	1.09775500	-0.00027000
C	8.48373700	0.80674400	0.00001500
C	8.91036900	-0.55963000	0.00018000
C	7.89724000	-1.56684900	0.00002700
C	6.55654800	-1.20554500	-0.00027600
H	6.74635300	2.11231000	-0.00039900
H	9.21519400	1.60724500	0.00011100
H	8.16381400	-2.61909500	0.00015200
H	5.72673400	-1.90375900	-0.00040500
H	5.14398500	0.39740200	-0.00069100
N	6.19242300	0.10835900	-0.00041300
N	-6.19241400	-0.10839600	0.00037100
H	-10.53193800	1.84087900	-0.00074600
H	-10.95782000	0.13998700	-0.00065300
H	10.53198100	-1.84085700	0.00060100
H	10.95781100	-0.13995600	0.00059000
N	-10.24043000	0.87309500	-0.00059000
N	10.24044800	-0.87308100	0.00047200
O	12.11950300	1.24217600	0.00048600
O	-12.11960000	-1.24197600	-0.00039000
H	12.51202900	1.63071100	-0.80387200
H	12.51179300	1.63097600	0.80483100

H	-12.51201700	-1.63041700	0.80406700
H	-12.51203200	-1.63083000	-0.80463900

Table 5: Cartesian coordinates(Optimized using B3LYP/631g++(d,p)+lan2dnz level of theory) of **CuD**. Optimized energy E (B3LYP/631g++(d,p)+lan2dnz) = -3156.722906 Hatreees

Atoms	x	y	z
Cu	0.00003000	0.00009600	0.00004100
O	-1.36579400	1.41202300	-0.00011200
O	-1.57264500	-1.21012400	0.00023700
O	1.57268800	1.21031200	-0.00019000
O	1.36583800	-1.41184900	0.00021000
C	-2.56877700	0.97654200	-0.00003600
C	-2.67638700	-0.58748500	0.00015900
C	2.67644000	0.58767000	-0.00015800
C	2.56881600	-0.97635600	0.00008400
O	-3.59790900	1.65031700	-0.00011200
O	-3.80189000	-1.12521900	0.00022000
O	3.80195000	1.12535900	-0.00028100
O	3.59795800	-1.65012700	0.00013500
C	-8.38041700	-0.74138900	-0.00046500
C	-7.03298800	-1.00383100	-0.00034800
C	-6.50568700	1.27703200	0.00039400
C	-7.83855000	1.61586800	0.00029500
C	-8.82464100	0.60334700	-0.00014100
H	-9.09636800	-1.55295800	-0.00080400
H	-6.62979000	-2.00847100	-0.00057800
H	-5.07036600	-0.29490400	0.00016500
H	-5.69029000	1.98906200	0.00073500
H	-8.12130300	2.66142800	0.00055100
C	7.03285400	1.00352700	-0.00058500
C	8.38030300	0.74120300	-0.00062500
C	8.82465000	-0.60349500	-0.00033300
C	7.83865400	-1.61611300	-0.00000100
C	6.50576200	-1.27740100	0.00002600
H	6.62953600	2.00811700	-0.00079400
H	9.09618200	1.55283500	-0.00087400
H	8.12150700	-2.66164500	0.00022300
H	5.69042600	-1.98949700	0.00027800
H	5.07039900	0.29439100	-0.00023400
N	6.12167200	0.01296500	-0.00026500
N	-6.12170000	-0.01336700	0.00007500
H	-10.45476100	1.85289900	0.00041600
H	-10.84394500	0.16127500	-0.00011100
H	10.45488400	-1.85289500	0.00043900
H	10.84391100	-0.16123400	-0.00001600
N	-10.14556900	0.89579900	-0.00035100
N	10.14560200	-0.89582300	-0.00051500
O	11.97339700	1.45901000	0.00079000
O	-11.97364500	-1.45888100	0.00064600
H	12.41035400	1.84142400	-0.76744700
H	12.40923000	1.84112400	0.76981500

H	-12.40946600	-1.84059000	0.76987900
H	-12.41083800	-1.84143900	-0.76738400

Table 6: Comparision of bond length (in Angstroms), bond angles(in degress) and torsional angle (in degress) of **CuD** from experimental and DFT calculation (B3LYP/6311++g(d,p), B3LYP/LanL2DZ and B3LYP/6311++g(d,p)+LanL2DZ(dual basis))

	Experimental	6311++g(d,p)	LanL2DZ	6311++g(d,p)+LanL2DZ
bond lengths (Å)				
C(1)-N(2)	1.341(3)	1.346	1.362	1.346
C(1)-C(2)	1.351(3)	1.373	1.386	1.373
C(2)-C(3)	1.403(3)	1.416	1.431	1.416
C(3)-N(1)	1.328(3)	1.353	1.367	1.353
C(3)-C(4)	1.407(3)	1.413	1.367	1.413
C(4)-C(5)	1.351(3)	1.375	1.389	1.375
C(5)-N(2)	1.336(4)	1.346	1.363	1.346
C(6)-O(3)	1.216(3)	1.230	1.260	1.230
C(6)-O(2)	1.286(2)	1.280	1.314	1.279
C(6)-C(7)	1.548(3)	1.567	1.570	1.568
C(7)-O(4)	1.215(3)	1.248	1.275	1.247
C(7)-O(1)	1.285(3)	1.267	1.300	1.267
Cu(1)-O(2)#1	1.9279(14)	1.950	1.961	1.964
Cu(1)-O(2)	1.9279(14)	1.950	1.961	1.964
Cu(1)-O(1)#1	1.9287(14)	1.971	1.981	1.984
Cu(1)-O(1)	1.9287(14)	1.970	1.981	1.984
bond angles (in degrees)				
N(2)-C(1)-C(2)	121.2(2)	121.604	121.287	121.593
C(1)-C(2)-C(3)	119.9(2)	119.299	119.456	119.302
N(1)-C(3)-C(2)	121.6(2)	120.767	120.601	120.764
N(1)-C(3)-C(4)	121.2(2)	121.757	121.907	121.758
C(2)-C(3)-C(4)	117.2(2)	117.476	117.492	117.477
C(5)-C(4)-C(3)	119.8(2)	119.982	120.085	119.979
N(2)-C(5)-C(4)	121.2(2)	120.837	120.572	120.834
O(3)-C(6)-O(2)	125.89(19)	126.966	127.408	126.887
O(3)-C(6)-C(7)	119.29(18)	119.295	119.562	119.276
O(2)-C(6)-C(7)	114.82(17)	113.739	113.030	113.837
O(4)-C(7)-O(1)	125.5(2)	125.103	127.408	125.037
O(4)-C(7)-C(6)	120.45(18)	119.509	119.455	119.472
O(1)-C(7)-C(6)	114.07(18)	115.388	114.670	115.492
O(2)#1-Cu(1)-O(2)	180	180.000	180.000	179.999
O(2)#1-Cu(1)-O(1)#1	85.33(6)	84.079	83.594	83.530
O(2)-Cu(1)-O(1)#1	94.67(6)	95.920	96.406	96.470
O(2)#1-Cu(1)-O(1)	94.67(6)	95.920	96.406	96.470
O(2)-Cu(1)-O(1)	85.33(6)	84.079	83.594	83.531
O(1)#1-Cu(1)-O(1)	180	179.998	179.997	179.999
C(5)-N(2)-C(1)	120.7(2)	120.803	121.107	120.814
C(7)-O(1)-Cu(1)	112.89(14)	112.821	113.798	112.992
C(6)-O(2)-Cu(1)	112.56(12)	113.973	114.908	114.148
torsional angles (in degrees)				
N(2)-C(1)-C(2)-C(3)	0.2(4)	0.000	-0.001	0.000
C(1)-C(2)-C(3)-N(1)	179.0(2)	179.988	-179.999	179.993
C(1)-C(2)-C(3)-C(4)	-1.4(3)	-0.004	0.001	0.000

N(1)-C(3)-C(4)-C(5)	-178.8(2)	-179.987	-180.000	-179.993
C(2)-C(3)-C(4)-C(5)	1.5(3)	0.004	0.000	0.000
C(3)-C(4)-C(5)-N(2)	-0.4(3)	-0.001	-0.001	0.000
O(3)-C(6)-C(7)-O(4)	-3.3(3)	-0.004	0.026	-0.001
O(2)-C(6)-C(7)-O(4)	177.5(2)	179.999	-179.985	179.990
O(3)-C(6)-C(7)-O(1)	175.2(2)	179.997	-179.978	-180.000
O(2)-C(6)-C(7)-O(1)	-4.1(3)	0.001	0.011	0.000
C(4)-C(5)-N(2)-C(1)	-0.8(4)	-0.002	0.001	0.000
C(2)-C(1)-N(2)-C(5)	0.9(4)	0.003	0.000	180.000
O(4)-C(7)-O(1)-Cu(1)	-175.50(18)	-180.000	179.983	180.000
C(6)-C(7)-O(1)-Cu(1)	6.2(2)	-0.002	-0.013	-0.001
O(3)-C(6)-O(2)-Cu(1)	-179.41(18)	-179.996	179.984	-179.999