Supporting Information

Two S = 1/2 One-Dimensional Barium Copper Phosphates Showing Antiferromagnetic and Ferromagnetic Intrachain Interactions

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Table S1 Slected bond lengths [Å] and angles [°] for **1** and **2**.

$BaCu_2(PO_4)_2(H_2O)$

Ba1—O1	2.727 (2)	Ba1—O3	3.132 (3)	Ba1—O3^{v}	2.899 (2)
Ba1—O7^{i}	2.754 (2)	Ba1—O6^{iii}	2.785 (2)	Ba1—O5^{ii}	3.007 (2)
Ba1—O8^{ii}	2.770 (2)	Ba1—O2^{iv}	2.850 (2)	Ba1—O4^{v}	3.109 (3)
Ba1—O8^{i}	3.147 (2)	Ba1—O8^{iii}	3.214 (2)		
Cu1—O1	1.912 (2)	Cu1—O6^{v}	1.912 (2)	Cu1—O4^{v}	1.998 (2)
Cu1—O5	2.014 (2)	Cu1—O9	2.490 (2)		
Cu2—O2	1.987 (2)	Cu2—O4^{vi}	2.005 (2)	Cu2—O9	2.259 (2)
Cu2—O7^{vi}	1.922 (2)	Cu2—O5	1.961 (2)		
P1—O1	1.546 (2)	P1—O2	1.528 (2)	P1—O3	1.505 (2)
P1—O4	1.584 (2)				
P2—O5	1.578 (2)	P2—O6	1.541 (2)	P2—O7	1.541 (2)
P2—O8	1.492 (2)				
Cu1—Cu2	3.192(4)	Cu1—Cu2^{ii}	3.259(3)		
Cu1^{vii}—O4—Cu2^{iii}	109.04 (7)	Cu2—O5—Cu1	106.82 (4)	Cu2—O9—Cu1	84.32 (4)

Symmetry codes: (i) 1/2-x, 1-y, 1/2+z; (ii) 1-x, 1/2+y, 1/2-z; (iii) -x, 1/2+y, 1/2-z; (iv) 1/2+x, 1/2-y, 1-z; (v) 1+x, y, z; (vi) -x, -1/2+y, 1/2-z; (vii) -1+x, y, z.

$Ba_2Cu(HPO_4)(PO_4)(OH)$

Ba1—O1	2.878 (4)	Ba1—O2	3.155 (3)	Ba1—O2^{v}	3.155 (3)
Ba1—O1^{i}	2.878 (4)	Ba1—O3^{ii}	2.755 (6)	Ba1—O4	2.735 (4)
Ba1—O4^{i}	2.735 (4)	Ba1—O4^{iii}	2.926 (4)	Ba1—O4^{iv}	2.926 (4)
Ba1—O7	2.718 (5)				
Ba2—O1	2.893 (4)	Ba2—O1^{i}	2.893 (4)	Ba2—O2^{ii}	2.588 (6)
Ba2—O3	3.210 (3)	Ba2—O3^{v}	3.210 (3)	Ba2—O4^{vii}	2.825 (4)
Ba2—O4^{viii}	2.825 (4)	Ba2—O5^{vi}	2.755 (5)	Ba2—O6^{vi}	3.082 (6)
Ba2—O6^{viii}	3.202 (3)	Ba2—O6^{ix}	3.202 (3)		
Cu1—O1	2.004 (4)	Cu1—O1^{vi}	2.004 (4)	Cu1—O7	1.915 (3)
Cu1—O7^{vi}	1.915 (3)	Cu1—O5	2.486 (2)	Cu1—O5^{x}	2.486 (2)
P1—O1	1.550 (4)	P1—O1^{xi}	1.550 (4)	P1—O2	1.531 (6)
P1—O3	1.535 (6)				
P2—O4	1.528 (4)	P2—O4^{xi}	1.528 (4)	P2—O5	1.513 (5)
P2—O6	1.636 (6)	Cu1—Cu1^{x}	2.934 (6)		
Cu1^{x}—O7—Cu1	100.0 (2)	Cu1^{xii}—O5—Cu1	72.35 (2)		

Symmetry codes: (i) x, 3/2-y, z; (ii) 1-x, 1-y, -z; (iii) -x, 1-y, -z; (iv) -x, 1/2+y, -z; (v) x, 1+y, z; (vi) 1-x, 1-y, 1-z; (vii) 1+x, 3/2-y, z; (viii) 1+x, y, z; (ix) 1+x, 1+y, z; (x) 1-x, 1/2+y, 1-z; (xi) x, 1/2-y, z; (xii) 1-x, y-1/2, 1-z.

Table S2 Atomic site parameters for **1** and **2**.

$BaCu_2(PO_4)_2(H_2O)$				
atoms	*x*	*y*	*z*	*U*
Ba1	0.50269 (3)	0.520739 (17)	0.463829 (11)	0.00913 (5)
Cu1	0.51885 (9)	0.25142 (3)	0.26005 (2)	0.00782 (8)
Cu2	0.10029 (7)	0.01181 (4)	0.27986 (3)	0.00689 (8)
P1	0.01741 (18)	0.30149 (7)	0.37728 (5)	0.00576 (15)
P2	0.01363 (18)	0.22221 (7)	0.13268 (5)	0.00561 (14)
O1	0.2846 (4)	0.3458 (2)	0.33972 (16)	0.0103 (5)
O2	-0.0115 (5)	0.14526 (19)	0.37514 (13)	0.0095 (4)
O3	-0.0236 (5)	0.3611 (2)	0.47147 (14)	0.0131 (5)
O4	-0.1942 (4)	0.3658 (2)	0.31131 (7)	0.0081 (5)
O5	0.2265 (4)	0.1541 (2)	0.19567 (6)	0.0063 (5)
O6	-0.2525 (4)	0.1767 (2)	0.16968 (17)	0.0101 (5)
O7	0.0541 (4)	0.3789 (2)	0.13935 (14)	0.0089 (5)
O8	0.0471 (4)	0.1755 (2)	0.03588 (15)	0.0114 (5)
O9	0.4839 (4)	0.0370 (2)	0.35244 (16)	0.0163 (5)
H9A	0.618 (7)	-0.011 (4)	0.353 (2)	0.020 (fixed)
H9B	0.476 (7)	0.055 (4)	0.407 (3)	0.020 (fixed)
$Ba_2Cu(HPO_4)(PO_4)(OH)$				
atoms	*x*	*y*	*z*	*U*
Ba1	0.21405 (5)	0.7500	0.09602 (5)	0.00650 (13)
Ba2	0.78511 (5)	0.7500	0.26916 (5)	0.00907 (13)
Cu1	0.5000	0.5000	0.5000	0.00736 (19)
P1	0.4899 (2)	0.2500	0.1825 (2)	0.0052 (3)
P2	0.0637 (2)	0.2500	0.3034 (2)	0.0050 (3)
O1	0.5049 (5)	0.4696 (6)	0.2819 (4)	0.0084 (7)
O2	0.3166 (7)	0.2500	0.0384 (6)	0.0165 (12)
O3	0.6489 (7)	0.2500	0.1362 (7)	0.0146 (11)
O4	0.0198 (4)	0.4641 (6)	0.1996 (4)	0.0108 (7)
O5	0.2414 (7)	0.2500	0.4375 (6)	0.0100 (10)
O6	-0.0730 (7)	0.2500	0.3932 (7)	0.0137 (11)
O7	0.3424 (6)	0.7500	0.4202 (6)	0.0083 (10)
H6	-0.1760	0.2500	0.3651	0.020 (fixed)
H7	0.2460	0.7500	0.4370	0.020 (fixed)

Table S3 The geometries of hydrogen bonds for **1** and **2**.

compound	D–H···A	$d_{D–H}$ (Å)	$d_{H···A}$ (Å)	$d_{D···A}$ (Å)	∠D–H···A (°)
1	O9–H9A···O3	0.81	1.95	2.75	167.25
	O9–H9A···O7	0.84	2.01	2.84	167.93
2	O7–H7···O6	0.87	2.48	3.29	154.23
	O6–H6···O3	0.80	2.03	2.58	126.22

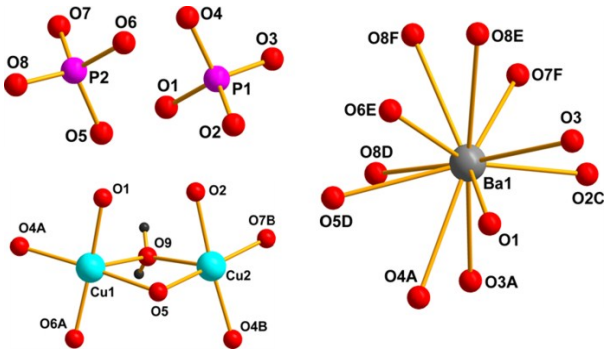

Fig. S1 The coordination condition in compound **1**. Symmetry codes: (A) 1+x, y, z; (B) -x, -0.5+y, 0.5-z; (C) 0.5+x, 0.5-y, 1-z; (D) 1-x, 0.5+y, 0.5-z; (E) –x, 0.5+y, 0.5-z; (F) 0.5-x, 1-y, 0.5+z.

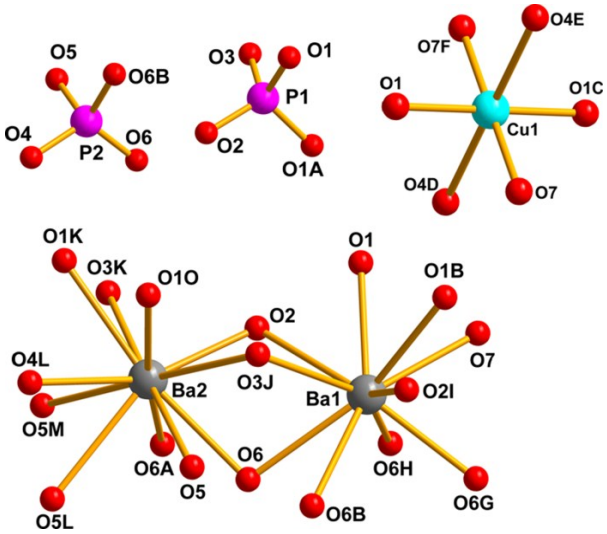

Fig. S2 The coordination condition in compound **2**. Symmetry codes: (A) x, -0.5-y, z; (B) x, 0.5-y, z; (C) 1-x, -y, 2-z; (D) –x, -0.5+y, 1-z; (E) 1+x, y, 1+z; (F) 1-x, -0.5+y, 2-z; (G) –x, 0.5+y, 1-z; (H) –x, -y, 1-z; (I) x, 1+y, z; (J) 1-x, 0.5+y, 1-z; (K) 1-x, -0.5+y, 1-z; (L) –x, -0.5+y, -z; (M) x, -1+y, z.

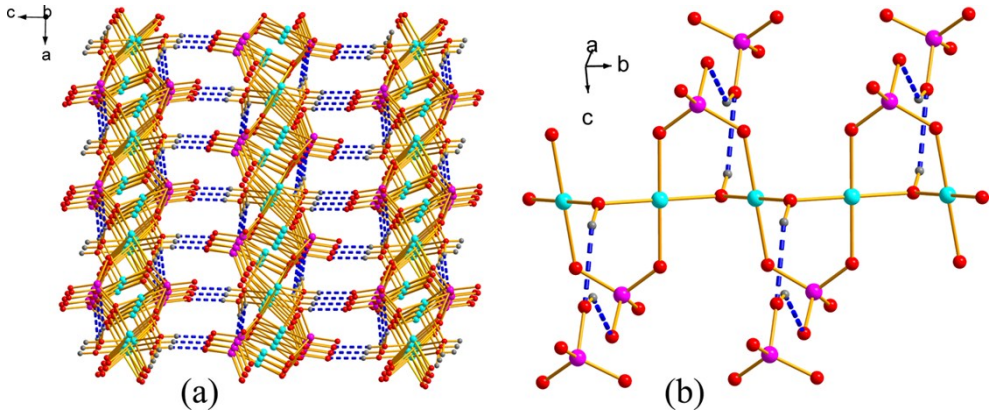

Fig. S3 The hydrogen bonds (blue dashed lines) in (a) **1** and (b) **2**. Cu, Turquoise; P, Pink; O, red; H, gray. The Ba atoms in both compounds are omitted for clearity.

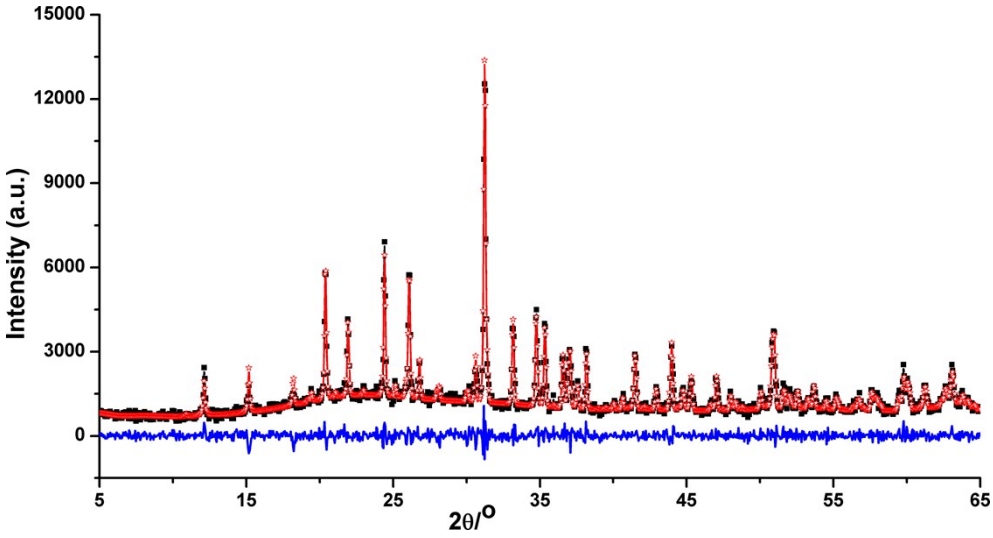

Fig. S4 The experimental XRD patterns for compound **1** fitted by Rietveld method. The fitting crystal contants are a = 5.158 Å, b = 9.736 Å, c = 14.569 Å, $\alpha = \beta = \gamma = 90^{o}$ with space group $P2_12_12_1$. Black, sample; red, calculated; blue, difference.

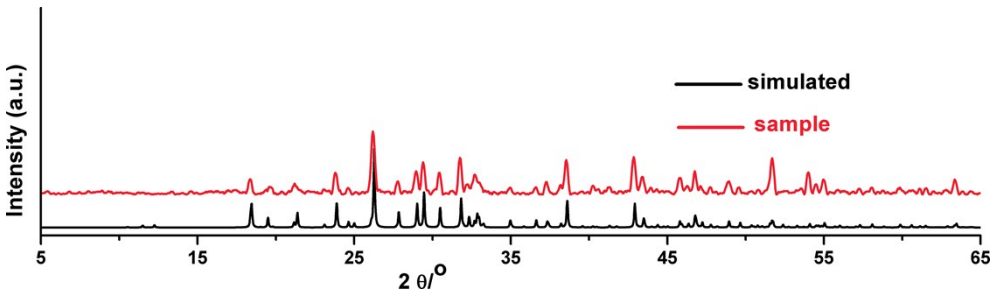

Fig. S5 Powder X-ray patterns of compound **2**.

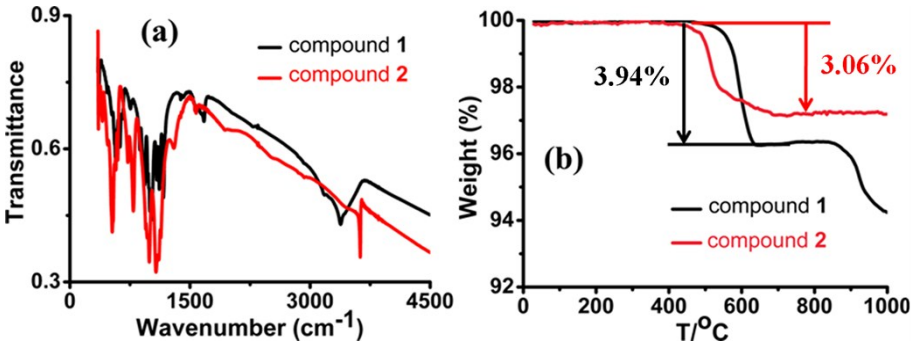

Fig. S6 Infrared spectrums (a) and TG curves (b) for **1** and **2**.

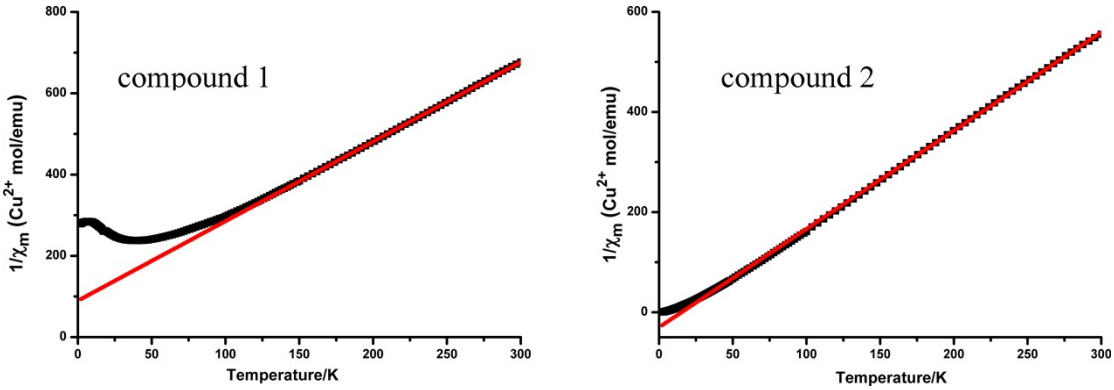

Fig. S7 The χ_m^{-1} vs T curves for compounds **1** and **2**.

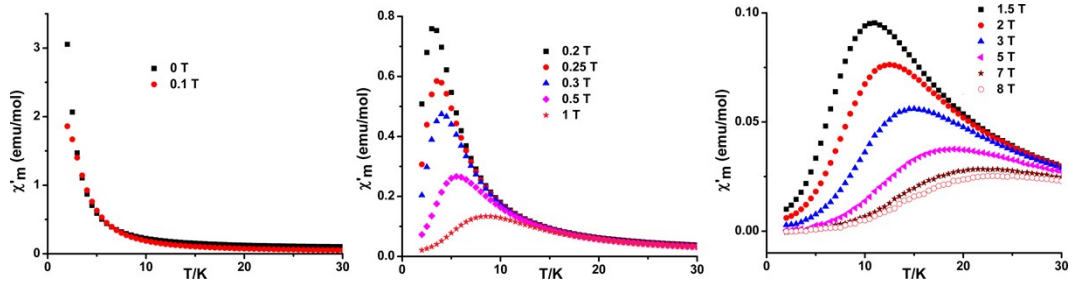

Fig. S8 The χ'_m vs T curves for compound **2** between 2 and 30 K at different static magnetic fields with H_{ac} = 3 Oe and f = 1000 Hz.

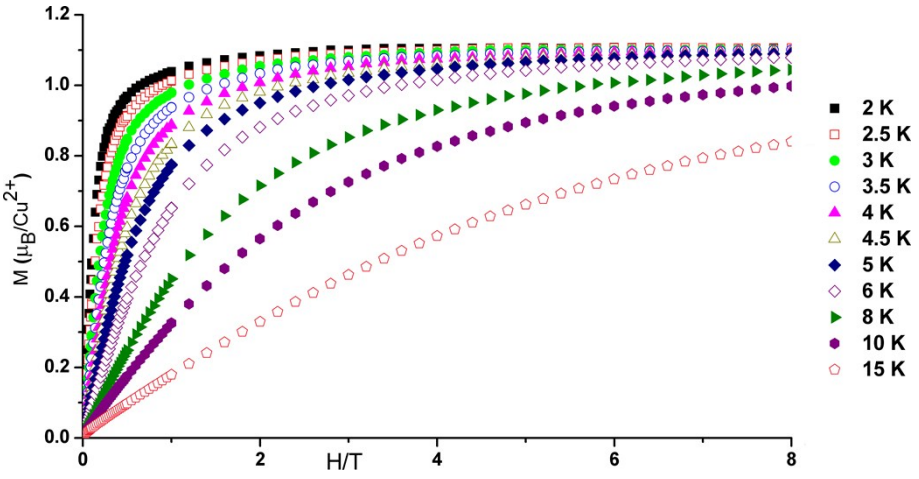

Fig. S9 Isothermal magnetization curves measured at 2, 2.5, 3, 3.5 4, 4.5, 5, 6, 8, 10 and 15 K for compound **2**.

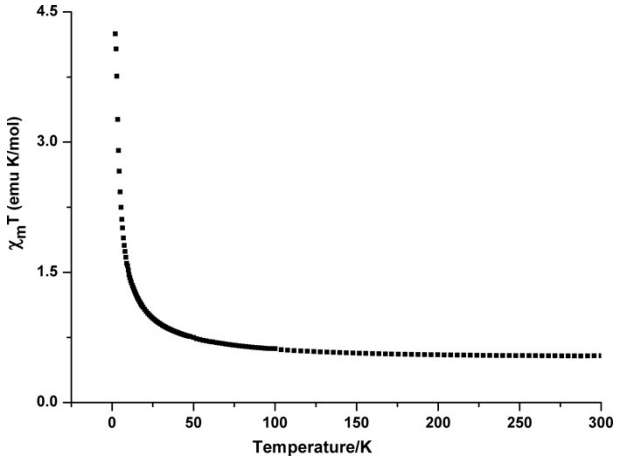

Fig. S10 The $\chi_m T$ vs T curve for compound **2**.

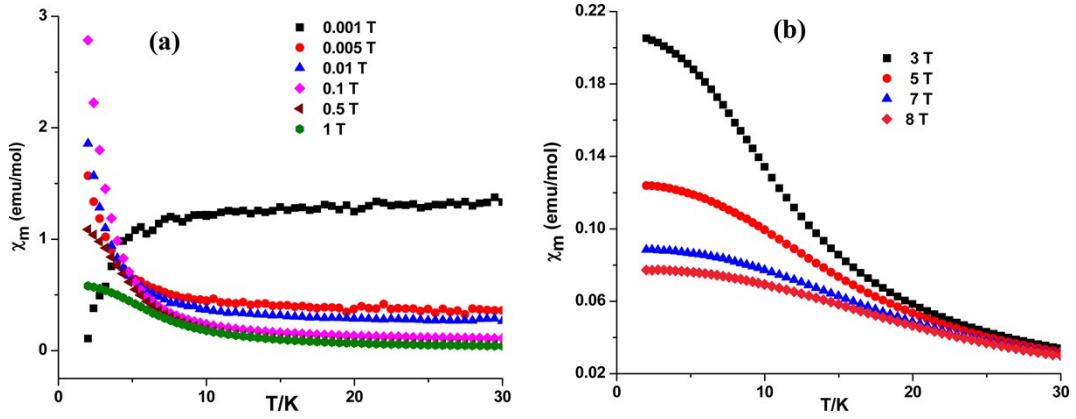

Fig. S11 Magnetic susceptibilities at external fields from 0.001 T to 8 T between 2 and 30 K for compound **2**.