Synthesis and Magnetic Properties of a New Polymorph of $Cu_2(VO_4)(OH)$ with a Quasi-2D layer Structure

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Supporting Information

Table S1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for $Cu_2(VO_4)(OH)$.

Table S2. Important bond length (Å) and bond angles (°) for $Cu_2(VO_4)$ (OH).

Figure S1. Energy-dispersive X-ray spectroscopy of $Cu_2(VO_4)(OH)$.

Figure S2. Simulated and experimental XRD powder patterns for $Cu_2(VO_4)(OH)$.

Scheme S1. The coordinaton enviroments of Cu(1)-Cu(4) atoms (a-d).

Scheme S2. The coordinaton enviroments of V(1) and V(2) atoms (a, b).

Table S1. Atomic coordinates (x10^4) and equivalent isotropic displacement parameters (Å^2 x10^3) for $Cu_2(VO_4)(OH)$.

	x	y	z	U(eq)
Cu(1)	-2738(1)	3369(1)	9264(1)	16(1)
Cu(2)	-236(1)	6198(1)	8600(1)	7(1)
Cu(3)	2359(1)	8977(1)	7852(1)	7(1)
Cu(4)	4693(1)	6221(1)	8640(1)	7(1)
V(1)	-7723(1)	2778(1)	8448(1)	5(1)
V(2)	7160(1)	9379(1)	9199(1)	5(1)
O(1)	-7813(6)	2081(3)	9475(2)	15(1)
O(2)	-7532(5)	1222(2)	7724(2)	9(1)
O(3)	-10205(4)	3914(4)	8249(2)	9(1)
O(4)	-5381(5)	3939(4)	8319(2)	8(1)

O(5)	-2758(5)	5638(3)	9375(2)	7(1)
O(6)	2289(5)	6722(2)	7855(2)	5(1)
O(7)	4710(5)	8533(4)	8788(2)	12(1)
O(8)	7260(5)	11284(3)	8874(2)	12(1)
O(9)	9448(5)	8451(4)	8783(2)	13(1)
O(10)	7170(5)	9234(3)	10306(2)	12(1)

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Table S2. Important bond length (Å) and bond angles (°) for $Cu_2(VO_4)$ (OH).

Cu(1)-O(8)#1	1.877(2)	Cu(1)-O(1)#2	1.926(3)
Cu(1)-O(5)	1.949(2)	Cu(1)-O(4)	2.190(3)
Cu(1)-O(3)#3	2.207(3)	Cu(2)-O(6)	1.945(3)
Cu(2)-O(9)#4	1.957(3)	Cu(2)-O(5)	1.975(3)
Cu(2)-O(3)#3	2.024(3)	Cu(2)-O(10)#5	2.221(3)
Cu(3)-O(6)	1.930(2)	Cu(3)-O(2)#7	1.932(2)
Cu(3)-O(7)	2.032(3)	Cu(3)-O(3)#6	2.102(3)
Cu(3)-O(9)#4	2.291(3)	Cu(4)-O(6)	1.918(3)
Cu(4)-O(5)#3	1.959(3)	Cu(4)-O(7)	1.991(3)
Cu(4)-O(4)#3	2.012(3)	Cu(4)-O(10)#5	2.229(3)
V(1)-O(1)	1.650(2)	V(1)-O(2)	1.720(2)
V(1)-O(4)	1.742(3)	V(1)-O(3)	1.814(3)
V(2)-O(10)	1.661(3)	V(2)-O(8)	1.702(2)
V(2)-O(9)	1.714(3)	V(2)-O(7)	1.762(3)
O(8)#1-Cu(1)-O(1)#2	96.56(11)	O(8)#1-Cu(1)-O(5)	166.78(10)
O(1)#2-Cu(1)-O(5)	96.64(10)	O(8)#1-Cu(1)-O(4)	90.62(12)
O(1)#2-Cu(1)-O(4)	131.26(14)	O(5)-Cu(1)-O(4)	80.10(12)
O(8)#1-Cu(1)-O(3)#3	89.32(12)	O(1)#2-Cu(1)-O(3)#3	137.08(14)
O(5)-Cu(1)-O(3)#3	81.50(12)	O(4)-Cu(1)-O(3)#3	90.94(10)
O(6)-Cu(2)-O(9)#4	85.95(11)	O(6)-Cu(2)-O(5)	178.73(11)
O(9)#4-Cu(2)-O(5)	94.69(11)	O(6)-Cu(2)-O(3)#3	93.83(11)

O(9)#4-Cu(2)-O(3)#3	171.40(13)	O(5)-Cu(2)-O(3)#3	85.70(11)
O(6)-Cu(2)-O(10)#5	86.86(11)	O(9)#4-Cu(2)-O(10)#5	97.18(12)
O(5)-Cu(2)-O(10)#5	91.97(11)	O(3)#3-Cu(2)-O(10)#5	91.39(11)
O(6)-Cu(2)-O(2)#6	88.12(10)	O(9)#4-Cu(2)-O(2)#6	92.99(11)
O(5)-Cu(2)-O(2)#6	92.94(10)	O(3)#3-Cu(2)-O(2)#6	78.41(10)
O(10)#5-Cu(2)-O(2)#6	168.31(9)	O(6)-Cu(3)-O(2)#7	174.44(10)
O(6)-Cu(3)-O(7)	80.01(12)	O(2)#7-Cu(3)-O(7)	103.30(12)
O(6)-Cu(3)-O(3)#6	87.89(12)	O(2)#7-Cu(3)-O(3)#6	88.23(12)
O(7)-Cu(3)-O(3)#6	165.87(13)	O(6)-Cu(3)-O(9)#4	77.60(11)
O(2)#7-Cu(3)-O(9)#4	106.37(11)	O(7)-Cu(3)-O(9)#4	94.74(11)
O(3)#6-Cu(3)-O(9)#4	89.70(12)	O(6)-Cu(4)-O(5)#3	176.21(10)
O(6)-Cu(4)-O(7)	81.34(10)	O(5)#3-Cu(4)-O(7)	100.76(11)
O(6)-Cu(4)-O(4)#3	93.13(10)	O(5)#3-Cu(4)-O(4)#3	84.49(10)
O(7)-Cu(4)-O(4)#3	172.52(13)	O(6)-Cu(4)-O(10)#5	87.29(11)
O(5)#3-Cu(4)-O(10)#5	95.61(11)	O(7)-Cu(4)-O(10)#5	95.65(11)
O(4)#3-Cu(4)-O(10)#5	89.09(11)	O(1)-V(1)-O(4)	109.66(15)
O(1)-V(1)-O(2)	107.97(12)	O(1)-V(1)-O(3)	108.60(15)
O(2)-V(1)-O(4)	108.52(14)	O(4)-V(1)-O(3)	110.47(11)
O(2)-V(1)-O(3)	111.58(14)	O(10)-V(2)-O(9)	108.93(15)
O(10)-V(2)-O(8)	110.89(12)	O(10)-V(2)-O(7)	108.73(15)
O(8)-V(2)-O(9)	108.16(15)	O(9)-V(2)-O(7)	111.25(13)
O(8)-V(2)-O(7)	108.90(15)		

Symmetry transformations used to generate equivalent atoms:

#1 x-1, y-1, z; #2 x+1/2, -y+1/2, -z+2; #3 x+1, y, z; #4 x-1, y, z; #5 x-1/2, -y+3/2, -z+2; #6 -x-1, y+1/2, -z+3/2; #7 x+1, y+1, z.

Electronic Supplementary Material (ESI) for Dalton Transactions

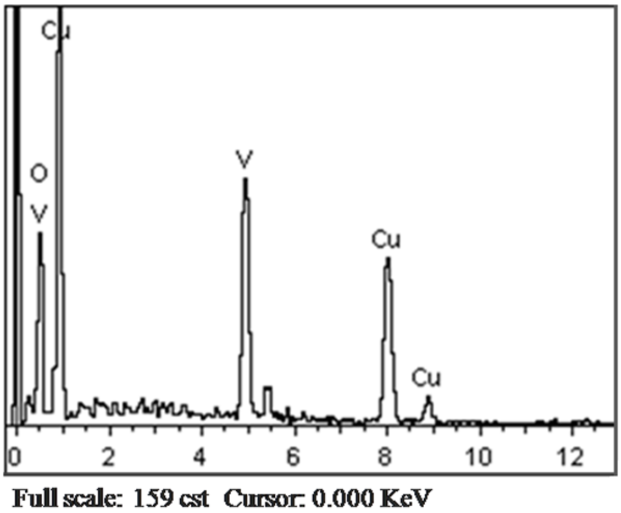


Figure S1. Energy-dispersive X-ray spectroscopy of $Cu_2(VO_4)(OH)$.

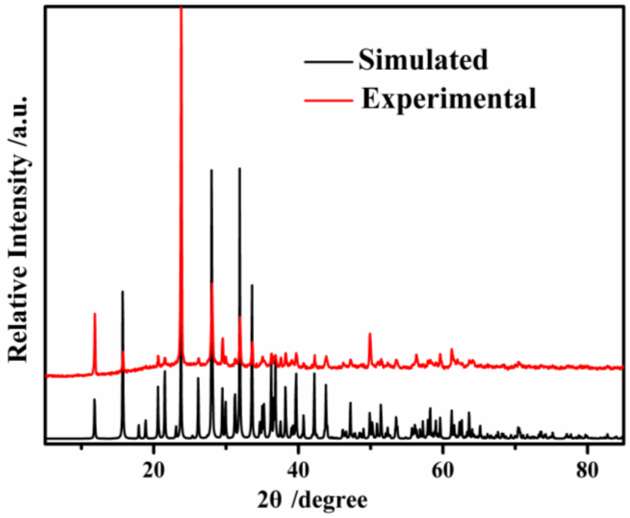
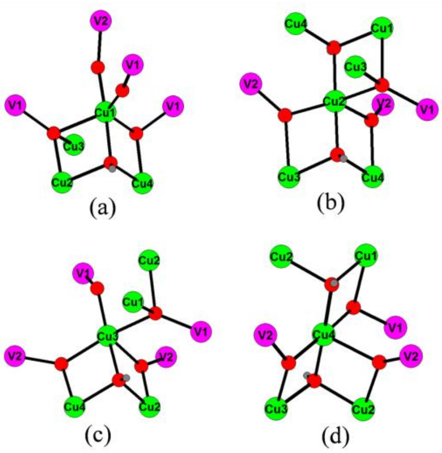
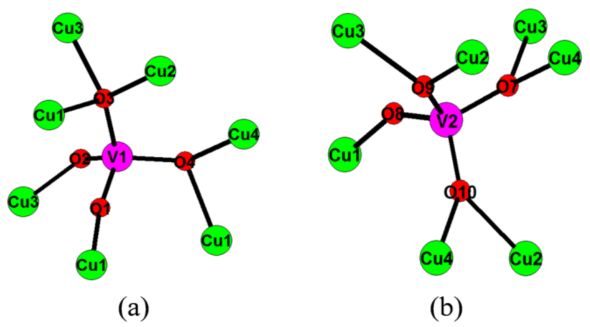


Figure S2. Simulated and experimental XRD powder patterns for $Cu_2(VO_4)(OH)$.



Scheme S1. The coordinaton enviroments of Cu(1)-Cu(4) atoms (a-d).



Scheme S2. The coordinaton enviroments of V(1) and V(2) atoms (a, b).