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Strong spin frustration from isolated triangular Cu(II) trimers in $SrCu(OH)_3Cl$ with a novel cuprate layer

Teng-Teng Zhu[a], Wei Sun[a], Ya-Xi Huang[a], Zhi-Mei Sun[b], Yuanming Pan[c], Leon Balents[d], and Jin-Xiao Mi[a,*]

[a]Fujian Provincial Key Laboratory of Advanced Materials, Department of Materials Science and Engineering, College of Materials, Xiamen University, Xiamen 361005, Fujian Province, People's Republic of China

[b]School of Materials Science and Engineering, Beihang University, Beijing 100191, People's Republic of China

[c]Department of Geological Sciences, University of Saskatchewan, 114 Science Place, Saskatoon, Canada SK S7N 5E2

[d]Kavli Institute for Theoretical Physics, University of California, Santa Barbara, California 93106, USA

* Corresponding author. Phone: +86-13696905136, Fax: +86-592-2183937, E-mail: jxmi@xmu.edu.cn

Table S1. Anisotropic atomic displacement parameters (Å^2) of $SrCu(OH)_3Cl$

atoms	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr(1)	0.0067 (5)	0.0092 (4)	0.0090 (4)	0.000	0.000	−0.0006 (4)
Sr(2)	0.0054 (3)	0.0103 (3)	0.0096 (3)	−0.0005 (2)	0.0001 (3)	0.0004 (3)
Cu(1)	0.0046 (6)	0.0099 (5)	0.0102 (6)	0.000	0.000	0.0014 (6)
Cu(2)	0.0050 (4)	0.0081 (4)	0.0106 (4)	0.0007 (3)	0.0011 (4)	0.0017 (4)
Cl(1)	0.0076 (13)	0.0177 (13)	0.0181 (14)	0.000	0.000	−0.0026 (10)
Cl(2)	0.0119 (9)	0.0097 (8)	0.0167 (9)	−0.0010 (7)	0.0032 (8)	−0.0019 (7)
O(1)	0.005 (3)	0.011 (3)	0.008 (2)	−0.002 (2)	0.000 (2)	0.001 (2)
O(2)	0.006 (4)	0.011 (4)	0.014 (4)	0.000	0.000	0.000 (4)
O(3)	0.007 (3)	0.009 (2)	0.014 (3)	0.001 (2)	0.005 (2)	0.000 (2)
O(4)	0.006 (2)	0.009 (2)	0.015 (3)	0.000 (2)	−0.001 (3)	0.005 (3)
O(5)	0.008 (3)	0.008 (2)	0.014 (3)	−0.003 (2)	−0.002 (2)	0.003 (2)

Table S2. Geometric parameters (Å, °) of $SrCu(OH)_3Cl$

Atom — atom	Distance	Atom — atom	Distance
Sr(1)—O(4)	2.499 (6)	Sr(2)—Cl(2)^{v}	2.998 (2)
Sr(1)—O(4)^{i}	2.499 (6)	Sr(2)—Cl(1)^{iv}	3.0102 (13)
Sr(1)—O(1)^{i}	2.542 (6)	Sr(2)—Cl(2)^{iii}	3.019 (2)
Sr(1)—O(1)	2.542 (6)	Cu(1)—O(4)^{vii}	1.940 (6)
Sr(1)—O(5)	2.568 (5)	Cu(1)—O(4)^{viii}	1.940 (6)
Sr(1)—O(5)^{i}	2.568 (5)	Cu(1)—O(1)	1.957 (5)
Sr(1)—O(2)	2.668 (7)	Cu(1)—O(1)^{i}	1.958 (5)
Sr(2)—O(3)^{iii}	2.512 (6)	Cu(2)—O(5)^{ix}	1.950 (5)
Sr(2)—O(4)	2.518 (5)	Cu(2)—O(3)	1.959 (5)
Sr(2)—O(3)^{iv}	2.558 (6)	Cu(2)—O(2)	1.959 (5)
Sr(2)—O(5)	2.632 (5)	Cu(2)—O(1)	1.974 (5)

Atom –atom–atom	Angle	Atom –atom–atom	Angle
O(4)—Sr(1)—O(4)^{i}	67.7 (3)	O(4)—Sr(2)—Cl(1)^{iv}	74.22 (13)
O(4)—Sr(1)—O(1)^{i}	143.92 (18)	O(3)^{iv}—Sr(2)—Cl(1)^{iv}	76.93 (13)
O(4)^{i}—Sr(1)—O(1)^{i}	103.15 (18)	O(5)—Sr(2)—Cl(1)^{iv}	84.18 (13)
O(4)—Sr(1)—O(1)	103.15 (18)	Cl(2)^{v}—Sr(2)—Cl(1)^{iv}	99.98 (7)
O(4)^{i}—Sr(1)—O(1)	143.92 (18)	O(3)^{iii}—Sr(2)—Cl(2)^{iii}	78.72 (13)
O(1)^{i}—Sr(1)—O(1)	62.8 (2)	O(4)—Sr(2)—Cl(2)^{iii}	81.34 (13)
O(4)—Sr(1)—O(5)	78.13 (16)	O(3)^{iv}—Sr(2)—Cl(2)^{iii}	72.63 (13)
O(4)^{i}—Sr(1)—O(5)	127.24 (18)	O(5)—Sr(2)—Cl(2)^{iii}	144.88 (12)
O(1)^{i}—Sr(1)—O(5)	127.13 (17)	Cl(2)^{v}—Sr(2)—Cl(2)^{iii}	124.88 (4)
O(1)—Sr(1)—O(5)	81.07 (17)	Cl(1)^{iv}—Sr(2)—Cl(2)^{iii}	115.67 (7)
O(4)—Sr(1)—O(5)^{i}	127.24 (18)	O(4)^{vii}—Cu(1)—O(4)^{viii}	91.7 (3)
O(4)^{i}—Sr(1)—O(5)^{i}	78.13 (16)	O(4)^{vii}—Cu(1)—O(1)	172.2 (3)
O(1)^{i}—Sr(1)—O(5)^{i}	81.07 (17)	O(4)^{viii}—Cu(1)—O(1)	91.1 (2)
O(1)—Sr(1)—O(5)^{i}	127.13 (17)	O(4)^{vii}—Cu(1)—O(1)^{i}	91.1 (2)
O(5)—Sr(1)—O(5)^{i}	93.4 (2)	O(4)^{viii}—Cu(1)—O(1)^{i}	172.2 (3)
O(4)—Sr(1)—O(2)	83.28 (19)	O(1)—Cu(1)—O(1)^{i}	85.2 (3)
O(4)^{i}—Sr(1)—O(2)	83.28 (19)	O(5)^{ix}—Cu(2)—O(3)	92.5 (2)
O(1)^{i}—Sr(1)—O(2)	60.7 (2)	O(5)^{ix}—Cu(2)—O(2)	91.4 (3)
O(1)—Sr(1)—O(2)	60.72 (19)	O(3)—Cu(2)—O(2)	174.3 (3)
O(5)—Sr(1)—O(2)	132.04 (13)	O(5)^{ix}—Cu(2)—O(1)	174.5 (2)
O(5)^{i}—Sr(1)—O(2)	132.04 (13)	O(3)—Cu(2)—O(1)	92.1 (2)
O(3)^{iii}—Sr(2)—O(4)	104.56 (18)	O(2)—Cu(2)—O(1)	84.1 (3)
O(3)^{iii}—Sr(2)—O(3)^{iv}	114.00 (10)	Cu(1)—O(1)—Cu(2)	119.4 (3)
O(4)—Sr(2)—O(3)^{iv}	127.08 (19)	Cu(1)—O(1)—H(1)	117 (7)
O(3)^{iii}—Sr(2)—O(5)	80.77 (18)	Cu(2)—O(1)—H(1)	102 (6)
O(4)—Sr(2)—O(5)	76.62 (18)	Cu(2)—O(2)—Cu(2)^{i}	112.6 (4)
O(3)^{iv}—Sr(2)—O(5)	142.31 (16)	Cu(2)—O(2)—H(2)	106 (5)

O(3)^{iii}—Sr(2)—Cl(2)^{v}	73.62 (13)	Cu(2)^{i}—O(2)—H2	106 (5)
O(4)—Sr(2)—Cl(2)^{v}	151.39 (15)	Cu(2)—O(3)—H3	110 (7)
O(3)^{iv}—Sr(2)—Cl(2)^{v}	76.63 (13)	Cu(1)^{ii}—O(4)—H4	102 (7)
O(5)—Sr(2)—Cl(2)^{v}	74.92 (12)	Cu(2)^{v}—O(5)—H5	106 (8)
O(3)^{iii}—Sr(2)—Cl(1)^{iv}	164.73 (14)		

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

Table S3. Hydrogen-bond geometry (Å, °) of $SrCu(OH)_3Cl$

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O(1)—H(1)···Cl(2)^{x}	0.81 (3)	2.40 (3)	3.210 (6)	175 (8)
O(2)—H(2)···Cl(1)^{ii}	0.82 (3)	2.49 (7)	3.249 (9)	154 (13)
O(3)—H(3)···Cl(2)^{viii}	0.81 (3)	2.95 (8)	3.462 (6)	123 (8)
O(3)—H(3)···Cl(2)^{x}	0.81 (3)	2.80 (6)	3.506 (6)	148 (8)
O(4)—H(4)···Cl(2)	0.81 (3)	2.52 (6)	3.224 (5)	145 (9)
O(5)—H(5)···Cl(2)^{v}	0.81 (3)	2.90 (9)	3.436 (5)	126 (9)
O(5)—H(5)···O(3)^{iii}	0.81 (3)	2.58 (6)	3.334 (8)	155 (11)

Symmetry codes: (ii) $x, y, z+1$; (iii) $-x+3/2, -y+1, z+1/2$; (v) $x, y+1, z$; (viii) $x, y, z-1$; (x) $-x+3/2, -y+1, z-1/2$.

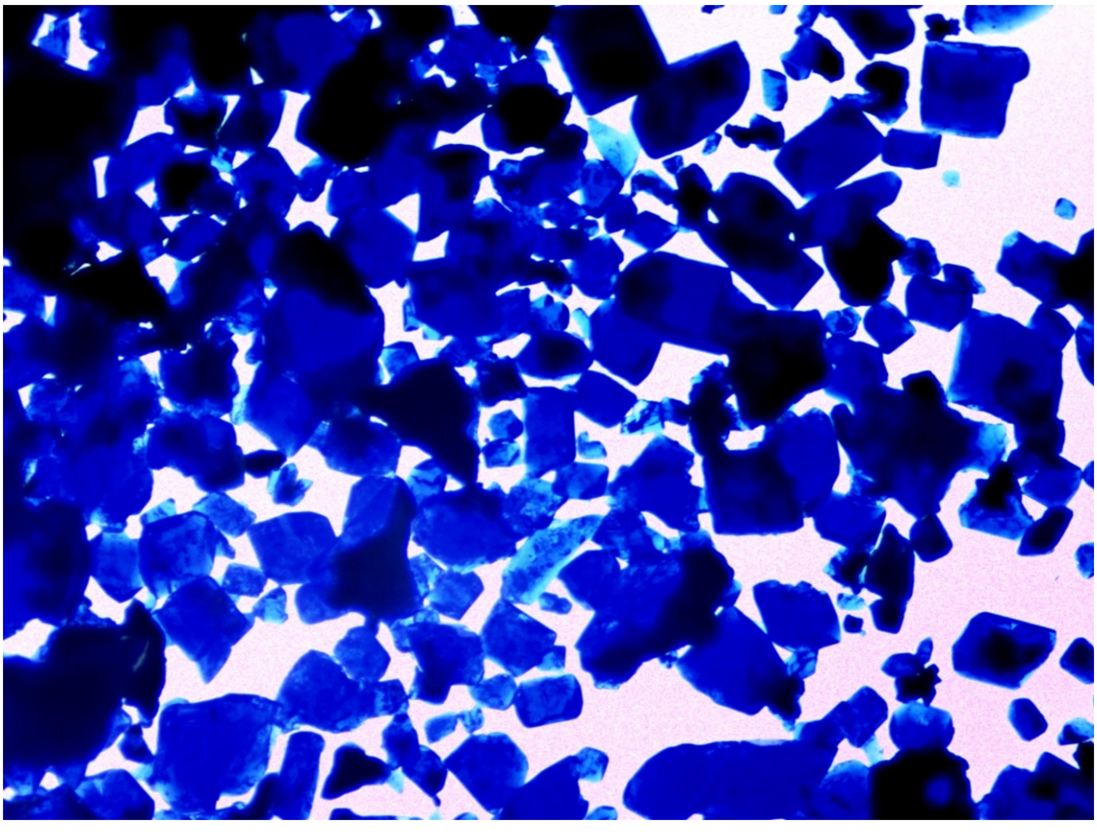

Figure S1. Morphology of $SrCu(OH)_3Cl$ crystals under optical microscope

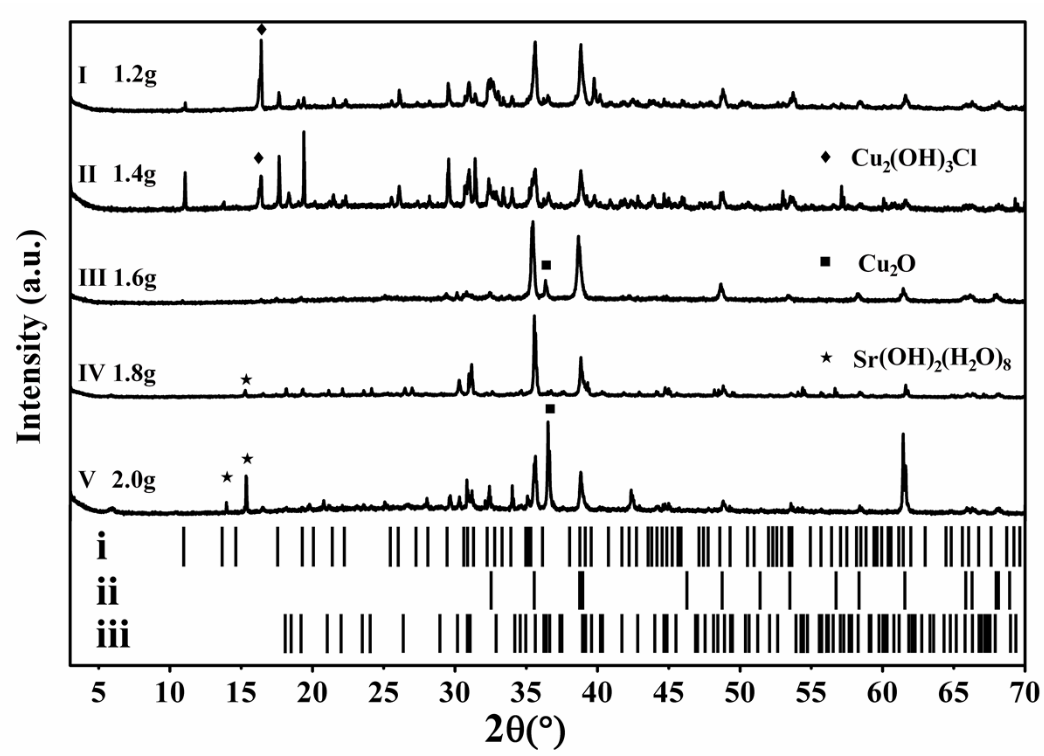

Figure S2. Powder X-ray diffraction patterns of experimental products from variable amounts of $LiOH\cdot H_2O$, while keeping the amounts of $CuCl_2\cdot 2H_2O$ (1.70 g), $LiCl\cdot H_2O$ (1.20 g), $SrCl_2\cdot 6H_2O$ (2.66 g) and H_2O (10 mL), at 513K for 3 days. Bragg bar positions (i), (ii) and (iii) for $SrCu(OH)_3Cl$, CuO and $Sr_2(OH)_2Cu(OH)_4$, respectively.

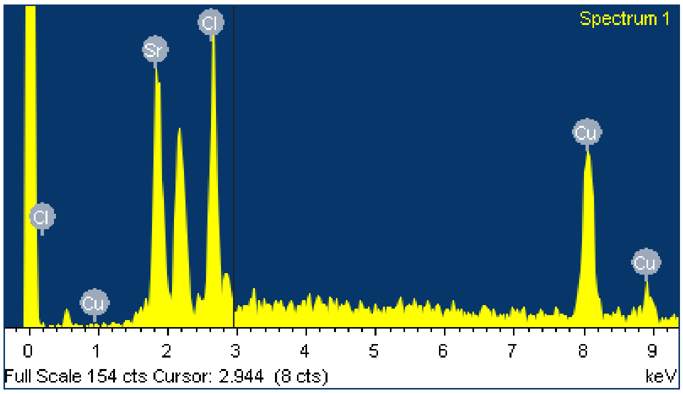

Figure S3. EXD spectrum of $SrCu(OH)_3Cl$

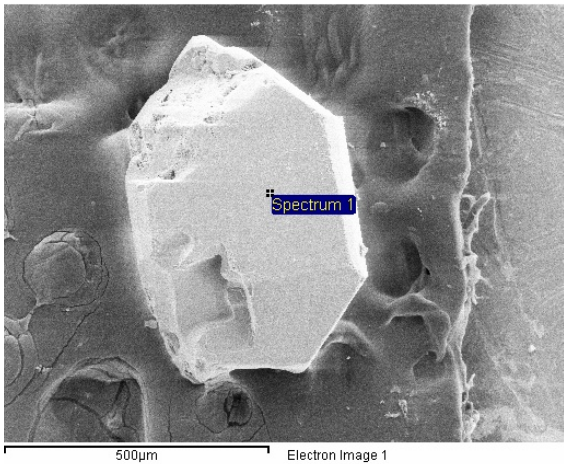

Figure S4. Morphology of a $SrCu(OH)_3Cl$ crystal under scanning electron microscope. Marked spot denotes the position where the EXD spectrum in Figure S3 was measured.

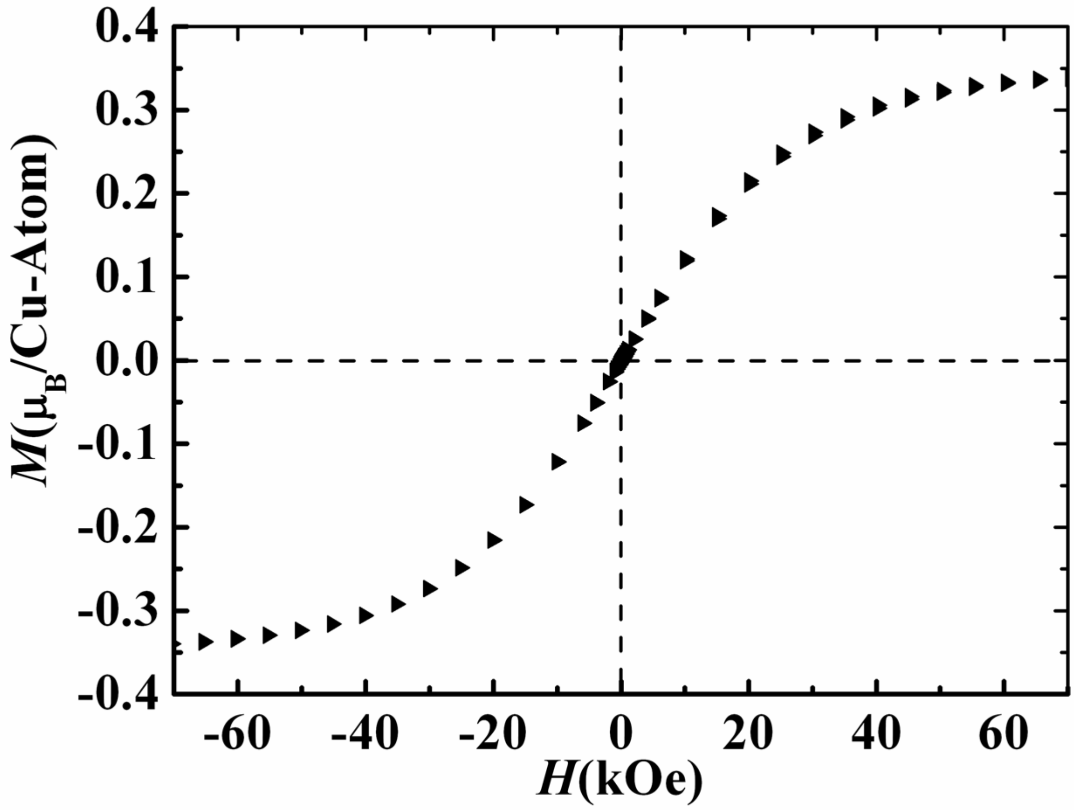

Figure S5. Magnetization-field loop of $SrCu(OH)_3Cl$ at 2 K