Electronic Supplementary Information

β-Vesignieite $BaCu_3V_2O_8(OH)_2$: A Structurally Perfect S = 1/2 Kagomé Antiferromagnet

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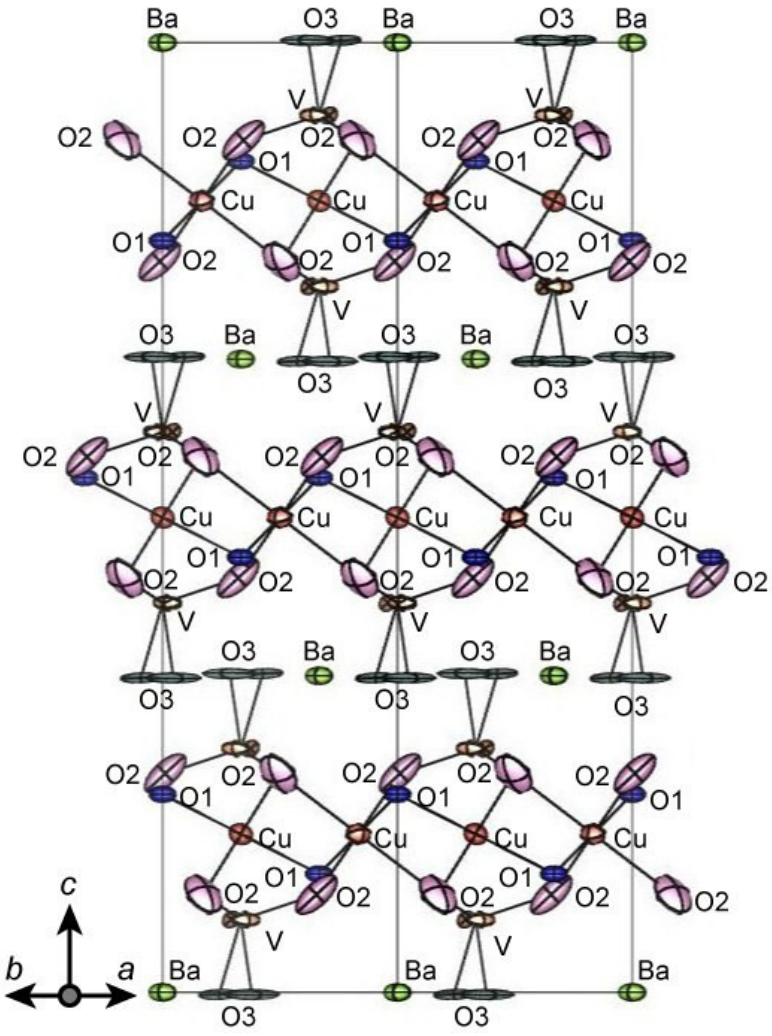

Figure S1. Crystal structure of β-vesignieite, $BaCu_3V_2O_8(OH)_2$ with thermal ellipsoids at 80% for legibility. The hydrogen atoms are not shown.

Table S1. Details of X-ray diffraction data collection and refinement results of *β*-vesignieite.

compound	$BaCu_3V_2O_8(OH)_2$
color/shape	lightgreen/hexagonal plate
formula weight (g mol^{-1})	591.9
space group	*R*-3*m*
Temperature (K)	293
a	5.9295(10)
b	5.9295(10)
c	20.790(4)
volume	633.0(2)
Z	3
density(calc.) (g m^{-3})	4.6562
absorption coefficient (mm^{-1})	14.178
radiation	Mo Kα (0.71069 Å)
crystal dimension(mm)	0.06(diagonal)×0.02
reflections collected	2806
independent reflections	535
reflections with $I > 2$sigma	424
range of *h*,*k*,*l*	*h*:−10/9, *k*:0/10, *l*:−37/37
F(000)	813
goodness of fit	1.69
$R_{obs}(F)$	0.0217
$wR_{all}(F^2)$	0.0337
D*r*(max)/D*r*(min) (e $Å^{-3}$)	2.05/−1.36

Table S2. Structural parameter of both α- (ref. 11) and β-vesignieite.

atom	site	x	y	z	occupation	U_{iso} (Å^2)
			α-vesignieite			
Ba	2c	0	0	0.5	1	1
Cu1	2a	0.5	0.5	0	1	1
Cu2	4e	0.25	0.25	0	1	1
V	4i	0.0898(3)	0.5	0.2697(4)	1	1
O1	4i	0.2080(1)	0	0.1228(13)	1	1
O2	8j	0.4822(10)	0.2411(16)	0.1902(13)	1	1
O3	4i	0.2245(13)	0.5	0.1913(19)	1	1
O4	4i	0.3303(31)	0	0.4941(25)	1	1
H	4i	0.289(26)	0	0.247(35)	1	1.61
			β-vesignieite			
Ba	3a	0	0	0	1	0.01441(10)
Cu	9d	0.333333	0.166667	0.166667	1	0.01258(13)
V	18h	0.35408(18)	0.7082(4)	0.07675(5)	0.3333	0.0116(5)
O1	6c	0.666667	0.333333	0.12530(15)	1	0.0126(7)
O2	18h	0.1726(2)	0.8274(2)	0.10348(12)	1	0.0366(9)
O3	18h	0.6206(7)	0.3794(7)	0.0025(3)	0.3333	0.040(3)
H	18h	0.65(5)	0.33(3)	0.091(3)	0.3333	0.01

Table S3. Anisotropic atomic displacement parameter U_{ij} (Å^2) of both α- (ref. 11) and β-vesignieite.

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
			α-vesignieite			
Ba	0.0041(1)	0.0010(2)	0.0041(2)	0	0.0018(1)	0
Cu1	0.0032(2)	0.0086(6)	0.0051(4)	0	0.0020(2)	0
Cu2	0.0035(2)	0.0068(6)	0.0046(3)	−0.0005(2)	0.0016(2)	−0.0004(3)
V	0.0088(4)	0.0242(9)	0.0038(4)	0	0.0014(3)	0
O1	0.0038(9)	0.0099(23)	0.0048(14)	0	0.0021(10)	0
O2	0.0104(11)	0.0164(24)	0.0182(19)	−0.0039(14)	0.0102(13)	−0.0085(18)
O3	0.0053(12)	0.0174(37)	0.0160(28)	0	−0.0002(5)	0
O4	0.0336(16)	0.0916(50)	0.0074(13)	0	0.0036(10)	0
			β-vesignieite			
Ba	0.01802(13)	0.01802(13)	0.00719(14)	0.00901(6)	0	0
Cu	0.01196(19)	0.01467(16)	0.01022(18)	0.00598(10)	−0.00145(13)	−0.00073(7)
V	0.0183(7)	0.0060(8)	0.0065(3)	0.0030(4)	−0.00050(16)	−0.0010(3)
O1	0.0160(8)	0.0160(8)	0.0057(10)	0.0080(4)	0	0
O2	0.0331(9)	0.0331(9)	0.0381(13)	0.0124(11)	−0.0137(6)	0.0137(6)
O3	0.068(4)	0.068(4)	0.0062(18)	0.050(4)	−0.0004(11)	0.0004(11)

Table S4. Selected bond lengths (Å) and angles (deg.) of both α- (ref. 11) and β-vesignieite.

bond length (Å)		bond angle (deg.)	
α-vesignieite			
Cu1-Cu2	2.9624(5)	Cu1-O1-Cu2	101.8(3)
Cu2-Cu2	2.9555(5)	Cu2-O1-Cu2	101.72(14)
Cu1-O1, O2	1.9131(9), 2.183(8)		
Cu2-O1, O2, O3	1.905(2), 2.174(6), 2.185(6)		
β-vesignieite			
Cu-Cu	2.9648(5)	Cu-O1-Cu	101.40(12)
Cu-O1	1.9156(16)	Cu-O2-Cu	85.56(9)
Cu-O2	2.182(2)		