Supplementary Materials: Crystal Chemistry of an Erythrite-Köttigite Solid Solution (Co3–xZnx)(AsO4)2·8H2O

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Table S1. Anisotropic displacement parameters in Co-rich köttigite.

Atom	U(1,1)	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
As	0.0043(2)	0.0114(2)	0.0077(2)	0	0.0008(2)	0
(Zn,Co)1	0.0061(3)	0.0147(3)	0.0098(3)	0	0.0002(2)	0
(Zn,Co)2	0.0086(2)	0.0119(3)	0.0107(3)	0	0.0024(2)	0
O1	0.0051(11)	0.0202(13)	0.0119(12)	0	0.0020(9)	0
O2	0.0103(12)	0.0146(12)	0.0082(11)	0	−0.0022(9)	0
O3	0.0100(8)	0.0127(8)	0.0138(9)	0.0021(7)	0.0037(7)	0.0000(7)
O4	0.0100(9)	0.0179(9)	0.0148(9)	0.0005(7)	0.0024(7)	0.0001(7)
O5	0.0203(10)	0.0177(9)	0.0173(9)	0.0034(8)	0.0040(8)	0.0032(8)

Table S2. Selected bond distances (Å) and angles (°) in Co-rich köttigite.

(Zn,Co)2–(Zn,Co)2^{i}	3.0802(8)	As–O1–(Zn,Co)1	121.38(14)
O2^{ii}–(Zn,Co)2–Zn2^{i}	42.48(5)	As–O2–(Zn,Co)2^{ii}	131.68(6)
O5^{iii} –(Zn,Co)2–Zn2^{i}	135.58(5)	(Zn,Co)2^{ii}–O2–(Zn,Co)2^{iv}	95.04(10)
O3^{iv}– (Zn,Co)2–Zn2^{i}	87.04(5)	As–O3–(Zn,Co)2^{v}	120.08(9)

O3^{vi}–As–O1–(Zn,Co)1	−62.51(7)	O3^{vi}–As–O2–(Zn,Co)2^{iv}	−16.2(2)
O3–As–O1–(Zn,Co)1	62.51(7)	O3–As–O2–Zn2^{iv}	−145.69(15)
O2–As–O1–(Zn,Co)1	180.000(1)	O1–As–O2–Zn2^{iv}	99.08(17)
O3^{vi}–As–O2–(Zn,Co)2^{ii}	145.68(15)	O3^{vi}–As–O3–Zn2^{v}	−34.94(18)
O3–As–O2–(Zn,Co)2^{ii}	16.2(2)	O2–As–O3–Zn2^{v}	91.13(13)
O1–As–O2–(Zn,Co)2^{ii}	−99.08(17)	O1–As–O3–Zn2^{v}	−153.90(11)

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