

Deposit Item

Table 3. Experimental data and information on refinement of Fe³⁺-dominant uranian kimzeyite (Table 2, an. 15)

Diffractometer	Bruker APEX II
X-ray radiation	MoK α (0.71073Å)
Temperature	293°(2) K
Monochromator	Graphite
Space group	$Ia\bar{3}d$ (No.230)
a (Å)	12.5965(5)Å
V (Å ³)	1998.71(14) Å ³
Crystal size (μm)	10 \times 20 \times 20
Index range	-16 $< h <$ 15
	-16 $< k <$ 11
	-16 $< l <$ 16
Upper 2 θ limit	56.56°
Reflections collected	6230
Unique reflections	214
Reflections $>4\sigma(F)$	119
Number of parameters	19
$R_{\text{int}}, R_{\sigma}$	6.25 %, 9 %
GooF	0.876
$R_1, F_o > 4\sigma(F)$	2.63 %
R_1 , all data	5.39 %
wR_2 (on F^2)	13.32 %

Table 4. Atomic oordinates, isotropic equivalents (U_{eq}) of displacement factors (Å²), and site scattering (SS) of uranian kimzeyite.

	x	y	z	U_{eq}	$SS (e^-)$ calculated from occupancy	$SS (e^-)$ calculated from EMPA
X	0.125	0	0.25	0.0170(7)	20	20.36
Y	0	0	0	0.0127(5)	40	45.23
Z	0.375	0	0.25	0.0142(7)	20.1(5)	21.55
O	0.0332(2)	0.0508(2)	0.6528(2)	0.026(1)	8	

Table 5. Anisotropic mean-square displacement parameters (Å²) of uranian kimzeyite

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
X	0.0125(11)	0.0192(8)	0.0192(8)	0.0042(7)	0	0
Y	0.0127(5)	0.0127(5)	0.0127(5)	0.0003(2)	0.0003(2)	0.0003(2)
Z	0.0106(11)	0.0160(8)	0.0160(8)	0	0	0
O	0.026(2)	0.026(2)	0.026(2)	-0.0039(16)	0.0006(18)	-0.0038(16)

Table 6. Bond lengths (Å) of uranian kimzeyite

X-O = 2.425(3) \times 4	Y-O = 2.071(4) \times 6
X-O = 2.568(4) \times 4	Z-O = 1.802(4) \times 4