

## Deposit Item

Table 3. Experimental data and information on refinement of Fe<sup>3+</sup>-dominant uranian kimzeyite (Table 2, an. 15)

Diffractometer	Bruker APEX II
X-ray radiation	MoK $\alpha$ (0.71073 Å)
Temperature	293°(2) K
Monochromator	Graphite
Space group	<i>Ia</i> $\bar{3}$ <i>d</i> (No.230)
<i>a</i> (Å)	12.5965(5)Å
<i>V</i> (Å <sup>3</sup> )	1998.71(14) Å <sup>3</sup>
Crystal size (μm)	10 × 20 × 20
Index range	-16 < <i>h</i> < 15
	-16 < <i>k</i> < 11
	-16 < <i>l</i> < 16
Upper 2θ limit	56.56°
Reflections collected	6230
Unique reflections	214
Reflections >4σ( <i>F</i> )	119
Number of parameters	19
<i>R</i> <sub>int</sub> , <i>R</i> <sub>σ</sub>	6.25 %, 9 %
GooF	0.876
<i>R</i> <sub>1</sub> , <i>F</i> <sub>o</sub> >4σ( <i>F</i> )	2.63 %
<i>R</i> <sub>1</sub> , all data	5.39 %
w <i>R</i> <sub>2</sub> (on <i>F</i> <sup>2</sup> )	13.32 %

Table 4. Atomic oordinates, isotropic equivalents (*U*<sub>eq</sub>) of displacement factors (Å<sup>2</sup>), and site scattering (SS) of uranian kimzeyite.

	x	y	z	<i>U</i> <sub>eq</sub>	<i>SS</i> ( <i>e</i> <sup>-</sup> ) calculated from occupancy	<i>SS</i> ( <i>e</i> <sup>-</sup> ) 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 (Å<sup>2</sup>) of uranian kimzeyite

	<i>U</i> <sub>11</sub>	<i>U</i> <sub>22</sub>	<i>U</i> <sub>33</sub>	<i>U</i> <sub>23</sub>	<i>U</i> <sub>13</sub>	<i>U</i> <sub>12</sub>
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)×4	Y-O = 2.071(4)×6
X-O = 2.568(4)×4	Z-O = 1.802(4)×4