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Revision of the symmetry and the crystal structure of čejkaite, $Na_4(UO_2)(CO_3)_3$†

JAKUB PLÁŠIL,[1,*] KARLA FEJFAROVÁ,[1] MICHAL DUŠEK,[1] RADEK ŠKODA,[2] AND JAN ROHLÍČEK[1]

[1]Institute of Physics ASCR, v.v.i., Na Slovance 2, 18221, Praha 8, Czech Republic
[2]Institute of Geological Sciences, Faculty of Science, Masaryk University, Kotlářská 2, CZ-611 37, Brno, Czech Republic

ABSTRACT

The crystal structure of čejkaite, $Na_4(UO_2)(CO_3)_3$, from the type locality, was determined for the first time by single-crystal X-ray diffraction. In contrast to the previously reported pseudohexagonal triclinic symmetry, the current data indicate čejkaite is monoclinic, triply twinned, and belongs to the space group *Cc*. Refined unit-cell parameters are $a = 9.2919(8)$, $b = 16.0991(11)$, $c = 6.4436(3)$ Å, $\beta = 91.404(5)°$, and $V = 963.62(12)$ Å^3. The monoclinic unit cell is also supported by the good fit to the powder diffraction data. The structure of čejkaite consists of uranyl tricarbonate clusters, forming sheets sub-parallel to (001) by sharing edges with (NaΦ) polyhedra. Sheets are interconnected through the uranyl O atoms and columns of (Na1Φ) polyhedra that share their trigonal faces. All Na atoms in the structure are in sixfold coordination . The structure refinement yielded $R_{obs} = 0.0424$ for 1687 observed reflections [$I_{obs} > 3\sigma(I)$] and 0.0538 for all 2016 unique reflections. Refinement and bond-valence analysis of the structure confirmed the previously proposed formula $Na_4(UO_2)(CO_3)_3$, $Z = 4$.

Keywords: Čejkaite, uranyl carbonate, symmetry, crystal structure, single-crystal, twinning, X-ray diffraction