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Crystal structure of uranyl-oxide mineral wölsendorfite revisited

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Abstract

The crystal structure of the rare supergene Pb^{2+}-containing uranyl-oxide mineral wölsendorfite has been revisited employing the single-crystal X-ray diffraction. The new structure refinement provided deeper insight into the complex structure of this mineral, revealing additional H_2O sites in the interlayer complex and confirming the entrance of the Ca^{2+} into the structure. Studied wölsendorfite is orthorhombic, space group *Cmcm*, with unit cell dimensions *a* = 14.1233(8) Å, *b* = 13.8196(9) Å, *c* = 55.7953(12) Å, *V* = 10890.0(10) Å^3, and *Z* = 8. The structure has been refined to an agreement index (*R*) of 10.74% for 3815 reflections with $I > 3\sigma(I)$ collected using a microfocus X-ray source from the microcrystal. In line with the previous structure determination, the refined structure contains U–O–OH sheets of the wölsendorfite topology and an interstitial complex comprising nine symmetrically unique Pb sites, occupied dominantly by Pb^{2+}. Nevertheless, one of the sites seems to be plausible for hosting Ca^{2+}. Its presence has been successfully modeled by the refinement and further supported by the crystal-chemical considerations. The structural formula of wölsendorfite crystal studied is $Pb_{6.07}Ca_{0.68}[(UO_2)_{14}O_{18}(OH)_5]O_{0.5}(H_2O)_{12.6}$, with $Z = 8$, $D_{calc.} = 6.919$ g·cm^{-3} (including theoretical 30.2 H atoms). The rather complex structure of wölsendorfite makes it the third most complex known uranyl-oxide hydroxy-hydrate mineral.

Keywords: *wölsendorfite, uranyl-oxide, crystal structure, Shinkolobwe, structure complexity, mineral associations*

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