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Krystalová struktura phurcalitu, $Ca_2[(UO_2)_3O_2(PO_4)_2]\cdot 7H_2O$, z Jáchymova

Crystal structure of phurcalite, $Ca_2[(UO_2)_3O_2(PO_4)_2]\cdot 7H_2O$, from Jáchymov

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Abstract

A rare supergene uranyl phosphate mineral, phurcalite, was found on a few specimens originating from the dump material of the Eduard shaft, the Jáchymov ore district, Czech Republic. Phurcalite forms yellow to yellowish-orange perfect prismatic crystals, reaching up to 3 - 4 mm in cavities of vuggy quartz-dominated gangue. Phurcalite was found in the association with walpurgite, uranophane-α, and members of the metatorbernite-metazeunerite series. According to single-crystal X-ray data phurcalite is orthorhombic, space group *Pbca*, with *a* 17.3785(8), *b* 15.9864(6), *c* 13.5477(6) Å, and *V* 3763.8(3) Å^3. Its crystal structure has been refined to *R* = 3.56 % for 3488 unique observed reflections [$I_{obs}>3\sigma(I)$] collected on a Rigaku SuperNova X-ray diffractometer with an Atlas S2 CCD detector and focused Mo*K*α radiation. The results of the structure refinement are in line with the recently published structure refinement of phurcalite from Shinkolobwe (Africa). Nevertheless, in phurcalite from Jáchymov, the substitution of As for P takes place at greater extent. The structural formula obtained for the crystal from Jáchymov is $Ca_2[(UO_2)_3O_2(PO_4)_{1.753}(AsO_4)_{0.247}]\cdot 7H_2O$, Z = 8, $D_{calc.}$ = 4.409 g/cm^3.

Key words: *phurcalite, uranyl phosphate, crystal structure, Jáchymov*

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