MITT.ÖSTERR.MINER.GES. 146 (2001)

THE CRYSTAL STRUCTURE OF WYCHEPROOFITE, A RARE HYDRATED NA-AL-ZR-PHOSPHATE FROM WYCHEPROOF, VICTORIA, AUSTRALIA

by

U. Kolitsch

Institut für Mineralogie und Kristallographie
Geozentrum, Universität Wien, Althanstrasse 14, A-1090 Wien

Wycheproofite is a rare phosphate mineral species known only from pegmatite veins in a granite quarry at Wycheproof, Victoria, Australia. The original description[1] reports the formula $NaAlZr(PO_4)_2(OH)_2 \cdot H_2O$, triclinic symmetry and the preliminary unit-cell parameters a = 10.926(5), b = 10.986(5), c = 12.479(9) Å, α = 71.37(4), β = 77.39(4), γ = 87.54(3)°, V = 1375.9 $Å^3$, determined with the help of electron diffraction. The mineral occurs as compact, finely fibrous masses in small cavities in the pegmatite. The fibrous crystals of the type material are only 5 - 10 µm wide but up to several mm long.[1]

To determine to previously unknown crystal structure of wycheproofite, a single-crystal X-ray study (CCD detector, MoKα radiation) was undertaken, using a tiny, elongate crystal fragment with the dimensions 0.02 x 0.03 x 0.08 mm. It gave a completely revised unit cell, a = 5.263(1), b = 9.251(2), c = 9.480(2) Å, α = 109.49(3), β = 98.57(3), γ = 90.09(3)°, V = 429.60(15) $Å^3$, Z = 2. The crystal structure was solved in space group $P\bar{1}$ (no. 2) to R1 = 4.18 % for 1731 'observed' reflections. It contains zigzag chains of edge-sharing $AlO_2(OH)_4$ octahedra along [100] which are linked via corners to PO_4 tetrahedra. Each corner of the ZrO_6 octahedron is shared with these PO_4 tetrahedra. All mentioned polyhedra are fairly regular and average Al–O, Zr–O and P–O bond lengths are 1.898, 2.063 and 1.529 Å, respectively. A Na site, partially occupied (~ 88 %) and slightly disordered, is located in a void of the resulting three-dimensional framework, and forms a $NaO_3(OH)_2.(H_2O)_{2-x}$ (x ~ 0.7) polyhedron. Three of its O ligands (Ow12 and 2x Ow11) are also only partially occupied and somewhat disordered, in agreement with bond-valence calculations. The originally given formula is therefore an idealised formula. Only very weak hydrogen bonding is present.

Comparisons are drawn to the structures of the few other known natural and synthetic zirconium phosphates (e.g., kosnarite - $KZr_2(PO_4)_3$; selwynite - $NaK(Be,Al)Zr_2(PO_4)_4.2H_2O$; mahlmoodite $FeZr(PO_4)_2.4H_2O$; synthetic $ZrKH(PO_4)_2$ and $Zr_2(NaPO_4)_4.6H_2O$) and related metal phosphates. Common structure features are pointed out.

Dr. Bill Birch, Museum Victoria, Melbourne, is thanked for kindly furnishing the studied sample. The financial support of the Deutsche Forschungsgemeinschaft (DFG) via a Research Fellowship to the author is gratefully acknowledged.

References

[1] BIRCH, W. D., PRING, A., KHARISUN & BEVAN, D. J. M. (1994): Wycheproofite: a new hydrated sodium aluminium zirconium phosphate from Wycheproof, Victoria, Australia and a new occurrence of kosnarite. - Mineral. Mag. 58, 635-39.