

**Fe₃(PO₄)₂(OH)₃·5H₂O, A NEW MONOCLINIC FERRIC IRON PHOSPHATE
MINERAL FROM GERMANY: CRYSTAL STRUCTURE, SINGLE-CRYSTAL
RAMAN SPECTRA AND CLOSE RELATION TO WAVELLITE**

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A new monoclinic ferric iron phosphate mineral has been found at the abandoned Grube Mark near Essershausen, Taunus, Hesse, Germany (BLAß, 2002). The mineral forms pale brown-yellow, translucent to transparent, acicular crystals (rarely up to 1.5 mm in length) which are always intergrown to form bundles of subparallel crystals. These are associated with beraunite (reddish "oxiberaunite" variety) and cacoxenite.

All acicular crystals studied were twinned by non-merohedry. The crystal structure has been determined using single-crystal intensity data (MoK α X-radiation, CCD area detector, 293 K) collected from a twin. The model was refined in space group $P2_1/n$ ($a = 9.777(3)$, $b = 7.358(2)$, $c = 17.830(5)$ Å, $\beta = 92.19(4)^\circ$, $V = 1281.7(6)$ Å³, $Z = 4$) to $R1 = 13.3$ % and $wR2_{\text{all}} = 35.3$ % from 2045 'observed' reflections with $F_o > 4 \sigma(F_o)$. The relatively high residuals are due to the twinning and weak intensity data. The chemical formula obtained from the refinement is Fe₃(PO₄)₂(OH)₃·5H₂O, which was confirmed by quantitative electron microprobe analyses. Single-crystal laser-Raman spectra (Renishaw M1000 MicroRaman Imaging System) show, in the region > 1500 cm⁻¹, several bands (s = strong; sh = shoulder) due to OH stretching vibrations (at ~ 3567 , $3412(s)$, $\sim 3197(s)$, ~ 3060 to $\sim 3052(\text{sh})$ cm⁻¹) and H-O-H bending vibrations of water molecules (~ 1625 cm⁻¹).

Chemically, the new mineral is the Fe³⁺-analogue of wavellite (Al₃(PO₄)₂(OH,F)₃·5H₂O, orthorhombic, space group $Pcmm$; ARAKI & ZOLTAI, 1968). Structurally, however, it is not isotypic with wavellite, but crystallises in a monoclinically distorted variant ($P2_1/n$; subgroup of $Pcmm$) of the wavellite structure type. Details of the structure and its hydrogen bonding scheme will be discussed.

The title compound has the same chemical formula as the amorphous species santabarbarite (PRATESI et al., 2003) which forms, however, exclusively on in-situ oxidative alteration of vivianite, Fe²⁺₃(PO₄)₂·8H₂O.

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References

ARAKI, T. & ZOLTAI, T. (1968): Z. Kristallogr., **127**: 21-33.

BLAß, G. (2002): Mineralien-Welt, **13**: 18-43.

PRATESI, G., CIPRIANI, C., GIULI, G. & BIRCH, W.D. (2003): Eur. J. Mineral., **15**: 185-192.