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TRICLINIC $PbFe_3(PO_4)_2(OH)_4(H_2O,OH)_2$ AND ITS CRYSTAL STRUCTURE: A NEW PHOSPHATE MINERAL FROM THE TAUNUS, GERMANY

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A new secondary Pb-Fe^{3+}-phosphate mineral has been identified in a single gossan boulder collected in 1986 on the dumps of the Grube Vereinigung, near Eisenbach, about 5 km N of Bad Camberg, Taunus, Hesse, Germany. The new species forms dark yellow, indistinct tabular (pinacoidal) crystals up to 0.5 mm in size that tend to form subparallel to rosette-like intergrowths. The mineral is accompanied by 'limonite' (matrix), kintoreite/corkite and, very rarely, pyromorphite. The chemical formula was derived from a single-crystal structure determination (Mo-$K\alpha$ X-radiation, CCD area detector, $R(F)$ = 5.6 %). The new mineral is triclinic, space group $P\bar{1}$ (no. 2), with a = 5.309(1), b = 7.211(1), c = 7.349(1) Å, α = 87.74(3), β = 86.38(3), γ = 71.40(3)°, V = 266.06(7) Å^3, and Z = 1. Measured X-ray powder diffraction patterns are in good agreement with a calculated pattern. The chemical formula, $PbFe_3(PO_4)_2(OH)_4(H_2O,OH)_2$, was subsequently confirmed by quantitative electron microprobe analyses which also indicated negligible amounts of impurity elements.
The unique crystal structure is based on an interrupted three-dimensional framework of FeO_6 octahedra sharing corners with neighbouring FeO_6 octahedra and PO_4 tetrahedra. The [8]-coordinated Pb atom is located within elliptical [100] channels. The asymmetric unit contains one unique Pb, three Fe, one P, seven O (two of which represent OH groups and one a mixed H_2O/OH ligand with a calculated bond-valence sum of 0.75 valence units) and 3.5 H atoms. The coordination environment of the Pb^{2+} cation can be described as a monoclinically distorted cuboid; the lone electron pair on the cation is not stereochemically active. Average Pb-O, Fe-O and P-O bond lengths are 2.65, 2.02 and 1.53 Å, respectively.
The new mineral may be considered a dimorph of kintoreite, ideally $PbFe_3(PO_4)_2(OH,H_2O)_6$ (PRING et al., 1995; KHARISUN et al., 1997), a member of the alunite supergroup. The structure is, however, only remotely similar to that of kintoreite. The apparent rarity of the new mineral suggests it may be metastable with respect to kintoreite.

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References

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