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**A new mineral: $PbHPO_4$, the phosphate analogue of schultenite**

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The first natural occurrence of $PbHPO_4$, the phosphate analogue of schultenite ($PbHAsO_4$), is reported from the famous Clara mine, central Black Forest, Germany. Both $PbHPO_4$ and $PbHAsO_4$ are well-known and widely studied synthetic ferroelectrics. The new unnamed mineral, found in August 2004, forms lancet-shaped (bladed on (010)) colourless transparent crystals up to a length of 0.2 mm. The blades often show subparallel or clustered intergrowths. Natural $PbHPO_4$ is closely associated with plumbogummite (containing minor As), mimetite (chemically pure), duftite and barite.

A single-crystal structure determination (Mo-$K\alpha$ X-radiation, CCD area detector, $R(F)$ = 2.7 %) showed the new mineral to be monoclinic, space group $P2/c$ (no. 13), with $a$ = 4.694(1), $b$ = 6.661(1), $c$ = 5.790(1) Å, $\beta$ = 97.05(3)°, $V$ = 179.67(6) Å$^3$, and $Z$ = 2. According to the refinement, natural $PbHPO_4$ is slightly As-bearing and has the structural formula $Pb[(P_{0.93}As_{0.07})O_3OH]$; this was confirmed by subsequent SEM-EDS analyses, and is also reflected by the unit-cell parameters which are slightly larger than that of pure synthetic $PbHPO_4$ ($V$ = 178.56 Å$^3$).

The crystal structure is in good agreement with that reported for synthetic $PbHPO_4$ (*cf.* ICSD 29553). It is based on an interrupted three-dimensional framework of $(P,As)O_3OH$ tetrahedra (<(P,As)-O> = 1.549 Å) connected to approximately [4+2]-coordinated Pb atoms (Pb-O = 2.359(4) (2x), 2.492(4) (2x) and 2.860(5) (2x) Å). Hydrogen atoms could not be located, but there is a very short H bond (O...O = 2.47 Å) between two $(P,As)O_3OH$ tetrahedra related by a centre of symmetry. Slabs composed of $(P,As)O_3OH$ and irregular $PbO_6$ polyhedra are stacked parallel to (010) and interconnected via the very strong H bonds.

A refinement in space group $Pc$ (the symmetry of the paraelectric low-temperature phase) gave $R(F)$ = 3.0 % and indicated that the centrosymmetric space group is more probable, but that it is basically impossible to distinguish between the two space groups on the basis of X-ray diffraction data (the atomic arrangement in $Pc$ is characterised by a strong $P2/c$ pseudosymmetry, and the paraelectric-ferroelectric phase transition is caused by a very small rearrangement of the hydrogen-bonding system). This also confirms literature reports. It is believed that the minor As-for-P substitution in the new mineral disorders the hydrogen-bonding system to some extent and indirectly stabilises the higher symmetry.