Short Communications

About the Space Group of H₅Mo₁₂PO₄₀(H₂O)₂₉₋₃₁; a Discussion

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Recently Strandberg ¹ has reported the structure of a hydrated dodecamolybdophosphoric acid. He reports a tetragonal cell with a = 16.473(5) Å, space group I₄₁/amd, whereas for the analogous tungsto compound, H₅W₁₂PO₄₀(H₂O)₂₉, Noe-Spirlet et al. ² report a cubic structure with a = 23.272(5) Å, space group Fd₃m. For the title compound we measured a cubic cell too with a = 23.33(1) Å.

Therefore I looked a bit closer at the data reported by Strandberg and it turned out that this structure can be described just as much as a cubic one. This will be shown by applying the transformation matrix $(-\frac{1}{2} - \frac{1}{2} 0 / \frac{1}{2} \frac{1}{2} 0 / 0 0 - 1)$ to the reported coordinates after shifting the origin to 2m (i.e. P in 0, 0, 0). By this transformation the space group symbol changes from I₄₁/amd into F₄₁/ddm, which better shows its subgroup relation to Fd₃m. The transformed lattice constants become about equal: $a = \frac{1}{2}a' = 23.296(7) \approx c = 23.338(7)$ (average = 23.31 Å). Furthermore the coordinates achieve the form $z = 0$ (or $x = y = z$) and are about identical for the atoms paired in Table 1. The last fact is the essential proof for the cubic structure of H₅Mo₁₂PO₄₀(H₂O)₂₉₋₃₁. The averaged coordinates compare well with those of H₅PW₁₀O₄₀(H₂O)₂₉ (see Table 1).

As for the triclinic H₅Mo₁₁PO₄₀(H₂O)₁₃₋₁₄ the pseudo-symmetry of the polyanion is reduced to 23 instead of 43m, we will try to check whether a similar reduction does occur for the 29-hydrate, i.e. whether the space group may be Fd₃ instead of Fd₃m, which means that $F_{134} = F_{341}$ does not hold. For the about isomorphous tungsto-compound Na₅H₅W₁₁PO₄₀(H₂O)₁₃₋₁₄ however, the pseudo-symmetry remains 43m³.


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