Short Communications

About the Space Group of $\text{H}_3\text{Mo}_{12}\text{PO}_{40}(\text{H}_2\text{O})_{29-31}$; a Discussion

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Recently Strandberg¹ has reported the structure of a hydrated dodecamolybdophosphoric acid. He reports a tetragonal cell with $a = 16.473(5)$ and $c = 23.336(7)$ Å, space group $I4_1/amd$, whereas for the analogous tungsto compound, $\text{H}_3\text{W}_{12}\text{PO}_{40}(\text{H}_2\text{O})_{29}$, 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 $42m$ (i.e. P in 0, 0, 0). By this transformation the space group symbol changes from $I4_1/amd$ into $F4_1/ddm$, which better shows its subgroup relation to $Fd3m$. The transformed lattice constants become about equal: $a_F = a_1 2^{1/2} = 23.296(7) \approx c = 23.336(7)$ (average = 23.31 Å). Furthermore the coordinates achieve the form xxx or xxx and are about identical for the atoms paired in Table 1. The last fact is the essential proof for the cubic structure of $\text{H}_3\text{Mo}_{12}\text{PO}_{40}(\text{H}_2\text{O})_{29-31}$. The averaged coordinates compare well with those of $\text{H}_3\text{PW}_{12}\text{O}_{40}(\text{H}_2\text{O})_{29}$ ³ (see Table 1).

As for the triclinic $\text{H}_3\text{Mo}_{12}\text{PO}_{40}(\text{H}_2\text{O})_{13-14}$ the pseudo-symmetry of the polyanion is reduced to 23 instead of $43m$,³ 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 $F_{hkl} = F_{\bar{h}\bar{k}\bar{l}}$ does not hold. For the about isomorphous tungsto-compound $\text{NaH}_3\text{W}_{12}\text{PO}_{40}(\text{H}_2\text{O})_{12-14}$, however, the pseudo-symmetry remains $43m$.⁴

1. Strandberg, R. *Acta Chem. Scand. A* 29 (1975) 359.
2. Noe-Spirlet, M.-R., Brown, G. M., Busing, W. R. and Levy, H. A. *Acta Crystallogr. A* 31 S80 (Amsterdam meeting).

Table 1. Transformed atomic coordinates for $\text{H}_3\text{PMo}_{12}\text{O}_{40}(\text{H}_2\text{O})_{29-31}$ (original data from Strandberg, 1975) compared with those of $\text{H}_3\text{PW}_{12}\text{O}_{40}(\text{H}_2\text{O})_{29}$ (absolute coordinates from Noe-Spirlet *et al.* 1975).

Atom	$\text{H}_3\text{PMo}_{12}\text{O}_{40}(\text{H}_2\text{O})_{29-31}$ $F4_1/ddm$			$Fd3m(a = 23.31)$ $x=y$ z			$\text{H}_3\text{PW}_{12}\text{O}_{40}(\text{H}_2\text{O})_{29}$ $Fd3m(a = 23.272(5))$ Atom $x=y$ z		
	x	y	z	x	y	z	x	y	z
P	0	0	0	0	0	0	P	0	0
Mo1	0.00430	0.10805	0.10807	0.10806	0.00431	0	W	0.10803	0.00400
Mo2	0.10807	0.10807	0.00432	0.0382	0.0382	0.0382	O(1)	0.03794	0.03794
OP(11'2)	0.0382	0.0382	0.0382	0.0488	0.0488	0.0488	O(2)	0.04873	-0.12736
O(11')	0.0488	0.0488	-0.1279						
O(12)	0.12775	0.04865	-0.0489						
O(11'')	0.0640	-0.0640	-0.1441						
O(12)	0.1442	-0.0639	-0.0639	0.0639	0.1442	0.1442	O(3)	0.06342	0.14369
O(1)	0.1581	0.0079	-0.1582	0.1582	-0.0078	-0.0078	O(4)	0.15873	-0.00765
O(2)	0.15835	0.15835	-0.0077	0.250	-0.0011	-0.0011	not reported		
Aq1	-0.250	0.250	0.0010	≡(0					
Aq2	0.0011	0.250	-0.250						

3. d'Amour, H. and Allmann, R. *Z. Kristallogr. In press.*
4. Allmann, R. and d'Amour, H. *Z. Kristallogr. 141* (1975) 161.

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