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The structure of $Te(OH)_6.Na_3P_3O_9.K_3P_3O_9$.

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Abstract

The structure of this compound, originally described in space group $C2/c$ [Averbuch-Pouchot & Durif (1987). *Acta Cryst.* C**43**, 1653–1655] is properly described as rhombohedral, space group $R\bar{3}c$, with $a = 12{\cdot}355$ (4) Å, $\alpha = 51{\cdot}01$ (2)°, $Z = 2$. (Hexagonal cell: $a = 10{\cdot}640$ (4), $c = 32{\cdot}16$ (2) Å, $Z = 6$.) Revised coordinates are given.

The structure of this compound was originally described as monoclinic, space group $C2/c$, with $a = 18{\cdot}42$ (1), $b = 10{\cdot}644$ (5), $c = 12{\cdot}348$ (8) Å, $\beta = 119{\cdot}76$ (5)°, $Z = 4$. The vectors $[\frac{1}{2},-\frac{1}{2},1]$, $[\frac{1}{2},\frac{1}{2},1]$ and $[0,0,1]$ lead to an effectively rhombohedral cell with $a_r = b_r = 12{\cdot}358$, $c_r = 12{\cdot}348$ Å, $\alpha_r = \beta_r = 51{\cdot}00$, $\gamma_r = 51{\cdot}02$°; the vectors $[0,-1,0]$, $[\frac{1}{2},\frac{1}{2},0]$ and $[1,0,3]$ lead to the corresponding hexagonal cell with $a_h = 10{\cdot}644$, $b_h = 10{\cdot}637$, $c_h = 32{\cdot}158$ Å, $\alpha_h = 89{\cdot}95$, $\beta_h = 90{\cdot}00$, $\gamma_h = 120{\cdot}02$°. The transformations $x_h = x-y-z/3$, $y_h = 2x-2z/3+0{\cdot}5$, $z_h = z/3$, when applied to the values in Table 1 of Averbuch-Pouchot & Durif (1987) and appropriately averaged, lead to the hexagonal coordinates in Table 1. No value in the earlier table needs to be changed by more than 1·0 e.s.d. to achieve the symmetry of $R\bar{3}c$.

Table 1. *Coordinates, space group $R\bar{3}c$; hexagonal setting*

		x	y	z
Te	6(*b*)	0	0	0
K	18(*e*)	0	0·39420 (4)	0·25
P	36(*f*)	0·00629 (4)	0·15923 (4)	0·15905 (1)
Na	18(*e*)	0·19898 (7)	0·19898	0·25
O	36(*f*)	0·1667 (1)	0·0683 (1)	0·03492 (4)
O(*L*)	36(*f*)	0·1374 (1)	0·1315 (1)	0·14581 (4)
O(*E*1)	36(*f*)	0·0138 (1)	0·2712 (1)	0·13027 (4)
O(*E*2)	36(*f*)	0·0066 (1)	0·1776 (1)	0·20471 (4)
H	36(*f*)	0·202 (2)	0·028 (2)	0·0306 (6)

The 'e.s.d.'s', given in parentheses, both for these coordinates and for the cell dimensions given in the *Abstract*, are estimated from the values reported by Averbuch-Pouchot & Durif (1987). Since covariances among the original parameters are not available, uncertainties of the transformed parameters can only be estimated.

There are no significant changes in the interatomic distances reported earlier. However, the change in space group points up the symmetry properties of the compound: the TeO_6 octahedron has crystallographic symmetry $\bar{3}$; the K atoms (as well as the Na atoms) are all equivalent and lie on twofold axes; and the P_3O_9 ring, rather than having 'no internal symmetry', lies on a threefold axis.

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Reference

AVERBUCH-POUCHOT, M. T. & DURIF, A. (1987). *Acta Cryst.* C**43**, 1653–1655.

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$Zr_2Al_3C_{5-x}$ and $Hf_2Al_3C_{5-x}$ described with higher symmetrical space group $P6_3/mmc$.

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Abstract

An analysis of the symmetry elements contained in the structure of $Zr_2Al_3C_{5-x}$ and isotypic $Hf_2Al_3C_{5-x}$ shows that it can be described with space group $P6_3/mmc$ instead of $P31c$ originally proposed by Schuster & Nowotny [*Z. Metallkd.* (1980), **71**, 341–346]. Based on the carbon occupation restriction rule for neighbouring octahedral interstitial sites in close-packed structures the composition for maximum carbon content should be $Zr_2Al_3C_4$.

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Discussion

The crystal structure of $Zr_2Al_3C_{5-x}$ and isotypic $Hf_2Al_3C_{5-x}$ has been determined by Schuster & Nowotny (1980) and described with a hexagonal unit cell ($a = 3{\cdot}3445$, $c = 22{\cdot}23$ Å and $a = 3{\cdot}319$, $c = 22{\cdot}09$ Å, respectively) and space group $P31c$. A misprint in the publication for the y coordinate of one C atom has been noted by the editor of *Structure Reports* (1982). However, a new error slipped into the *Structure Reports* data for the z parameter of Al in 2(*b*)