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The structure of $Te(OH)_6.Na_3P_3O_9.K_3P_3O_9$. By RICHARD E. MARSH, *Arthur Amos Noyes Laboratory of Chemical Physics,* California Institute of Technology, Pasadena, CA* 91125, *USA*

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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 $a = 12\cdot355$ (4) Å, $\alpha = 51\cdot01$ (2)°, $Z = 2$. (Hexagonal cell: $a = 10\cdot640$ (4), $c = 32\cdot16$ (2) Å, $Z = 6$.) Revised coordinates are given.

The structure of this compound was originally described as monoclinic, space group $C2/c$, with $a = 18\cdot42$ (1), $b = 10\cdot644$ (5), $c = 12\cdot348$ (8) Å, $\beta = 119\cdot76$ (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 $a_r = b_r = 12\cdot358$, $c_r = 12\cdot348$ Å, $\alpha_r = \beta_r = 51\cdot00$, $\gamma_r = 51\cdot02°$; the vectors $[0,-1,0]$, $[\frac{1}{2},\frac{1}{2},0]$ and $[1,0,3]$ lead to the corresponding hexagonal cell with $a_h = 10\cdot644$, $b_h = 10\cdot637$, $c_h = 32\cdot158$ Å, $\alpha_h = 89\cdot95$, $\beta_h = 90\cdot00$, $\gamma_h = 120\cdot02°$. The transformations $x_h = x-y-z/3$, $y_h = 2x-2z/3+0\cdot5$, $z_h = z/3$, 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 $R\bar{3}c$.

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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.

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 $P6_3/mmc$. By E. PARTHÉ and B. CHABOT, *Laboratoire de Cristallographie aux Rayons X, Université de Genève,* 24, *Quai Ernest-Ansermet, CH-*1211 *Genève* 4, *Switzerland*

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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 $Zr_2Al_3C_4$.

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 ($a = 3\cdot3445$, $c = 22\cdot23$ Å and $a = 3\cdot319$, $c = 22\cdot09$ 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*)

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Table 1. *Corrected structure data of* $Zr_2Al_3C_{5-x}$ *described with incorrect space group* $P31c$ (*No.* 159)

		x	y	z
Zr(1)	in 2 (*b*)	$\frac{1}{3}$	$\frac{2}{3}$	0·1912
(2)	in 2 (*b*)	$\frac{1}{3}$	$\frac{2}{3}$	0·8088
Al(1)	in 2 (*a*)	0	0	0·0900
(2)	in 2 (*a*)	0	0	0·4100
(3)	in 2 (*b*)	$\frac{1}{3}$	$\frac{2}{3}$	0·5
C(1)	in 2 (*a*)	0	0	0·25
(2)	in 2 (*b*)	$\frac{1}{3}$	$\frac{2}{3}$	0·0450
(3)	in 2 (*b*)	$\frac{1}{3}$	$\frac{2}{3}$	0·6339
(4)	in 2 (*b*)	$\frac{1}{3}$	$\frac{2}{3}$	0·3661
(5)	in 2 (*b*)	$\frac{1}{3}$	$\frac{2}{3}$	0·9550

Table 2. *Standardized data of* $Zr_2Al_3C_{5-x}$ *in the correct space group* $P6_3/mmc$ (*No.* 194)

Site C(2) is probably only half occupied. Composition is then $Zr_2Al_3C_4$.

		x	y	z
C(1)	in 4 (*f*)	$\frac{1}{3}$	$\frac{2}{3}$	0·1161
Zr	in 4 (*f*)	$\frac{1}{3}$	$\frac{2}{3}$	0·5588
C(2)	in 4 (*f*)	$\frac{1}{3}$	$\frac{2}{3}$	0·7050
Al(1)	in 4 (*e*)	0	0	0·1600
Al(2)	in 2 (*c*)	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$
C(3)	in 2 (*a*)	0	0	0

which should be $\frac{1}{2}$ instead of 0. The corrected data for $Zr_2Al_3C_{5-x}$ described with space group $P31c$ are given in Table 1.

The standardization of the data listed in Table 1 with the *STRUCTURE TIDY* program (Gelato & Parthé, 1987) leads to two identical solutions for settings $-x, -y, -z$ and $-x, -y, +z$, which is an indication that the polar space group used is a subgroup of the correct one. A brief inspection of the z coordinates of the atoms indicates that there are pairs of numerical values which add up to $\frac{1}{2}$ or 1. Searching the structure for overlooked symmetry elements we find that the atom arrangement can be described with space group $P6_3/mmc$. A representation of the structure in this space group (Table 2) needs an origin shift of $00\frac{1}{4}$ of the original data and the grouping of the original atom coordinates as follows: Zr(1) and Zr(2)→Zr, Al(1) and Al(2)→Al(1), Al(3)→Al(2), C(3) and C(4)→C(1), C(2) and C(5)→C(2) and C(1)→C(3). No error limits for the adjustable atom coordinates were given in the original paper. Since corresponding numerical values for the two structure descriptions agree with each other up to the last decimal place we feel that the true space group of $Zr_2Al_3C_{5-x}$ is $P6_3/mmc$.

While this study was in progress the *MISSYM* program by Le Page (1987) to find overlooked symmetry elements became available to us. The computer results indicate in addition to the symmetry elements contained in $P31c$ the following new ones: 6_3, -1 and three extra mirror planes perpendicular to the basal plane. This corresponds in the final analysis to space group $P6_3/mmc$.

It was stated by Schuster & Nowotny (1980) that carbon voids are to be expected because of carbon–carbon repulsion. According to the restriction rule for the occupation of neighbouring octahedral interstices (Parthé & Yvon, 1970) it can be assumed that the C(2) position in 4(*f*) is only half occupied by C atoms. The composition for maximum C content is then $Zr_2Al_3C_4$.

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The equivalent isotropic displacement factor. By REINHARD X. FISCHER and EKKEHART TILLMANNS,

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Abstract

A check of recent articles in *Acta Crystallographica* Section C shows that some confusion exists about the definition of the equivalent isotropic displacement factor U_{eq}. A common error is the use of the non-orthogonalized tensor U for the calculation of U_{eq} in non-orthogonal crystal systems. In addition, a number of cases have been found where a_i^* is confused with a_i or B with β, or where the wrong factors are used to relate U_{ij} or β_{ij} to B_{ij} or *vice versa.* U_{eq}'s for the different crystal systems are derived from the general expression $U_{eq} = \frac{1}{3}\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$.

Introduction

Since anisotropic displacement factors* are to be deposited the equivalent isotropic displacement factors are published together with the atomic coordinates. Browsing through the structure papers in *Acta Crystallographica* one can find some fifty different definitions for U_{eq} or B_{eq}, many of which are definitely wrong. Consequently, the Commission on Journals (1986) recommended use of the definitions given by

* We follow here the recommendation by Brock (1984) and use the expression 'displacement factor' instead of 'temperature factor'.

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