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 $Zr_2Al_3C_4$.

References

GELATO, L. M. & PARTHÉ, E. (1987). *J. Appl. Cryst.* **20**, 139–143.
LE PAGE, Y. (1987). *J. Appl. Cryst.* **20**, 264–269.
PARTHÉ, E. & YVON, K. (1970). *Acta Cryst.* B**26**, 153–163.
SCHUSTER, J. C. & NOWOTNY, H. (1980). *Z. Metallkd.* **71**, 341–346.
Structure Reports (1982). Vol. 46A, p. 4. Dordrecht: Reidel.

The equivalent isotropic displacement factor.

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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

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

Hamilton (1959) or by Willis & Pryor (1975). Unfortunately, it is not always stated clearly that the eigenvalues of the displacement tensor are derived from the orthogonalized tensor. Willis & Pryor (1975) define $\langle u^2 \rangle = \frac{1}{3}$ trace B, an equation which is often incorrectly applied to non-orthogonalized tensors. Also Prince (1982) does not point out explicitly in his chapter on equivalent isotropic temperature factors that B_{eq} is derived from the orthogonalized tensor. A survey of all articles in *Acta Crystallographica* Section C which have been accepted for publication after the recommendation of the Commission on Journals (1986) still shows many cases of wrongly defined displacement factors. This short note should help to clarify the confusion, which also trapped the present authors on one occasion (Fischer & Tillmanns, 1983).

Common mistakes

Between August 1986 and April 1987 about 160 papers were accepted for publication and have been printed in *Acta Crystallographica* C43, Parts 1–8 where the definition of the equivalent isotropic displacement factors is incorrect. Some of these cases are probably due to typographical errors, where the tensor expression is missing (nine cases), B_{ij} is given instead of β_{ij} (31 cases), or a_i^* is confused with a_i (five cases). A common mistake is simply to take one-third of the trace of the anisotropic displacement tensor, ignoring the fact that the matrix is not orthogonalized (38 cases). There are about 50 papers where off-diagonal elements are included in the calculation but with a wrong derivation. Actually, in most cases this does not change the results significantly, but this does occur when according to the definition given the wrong factors are used to relate U_{ij} or β_{ij} to B_{ij} or *vice versa* (12 cases). There do exist some papers where the equivalent displacement factor is taken not as the arithmetic mean but as the geometric mean, but one still has to note that the tensor has to be orthogonalized, which is ignored in 14 cases.

The correct form of the equivalent isotropic displacement factor

The following definitions are used for the elements of the anisotropic displacement factor:

$$\exp(-2\pi^2\textstyle\sum_i\sum_j U_{ij}h_ih_ja_i^*a_j^*),\ \exp(-\tfrac{1}{4}\sum_i\sum_j B_{ij}h_ih_ja_i^*a_j^*)\ \text{or}$$
$$\exp(-\textstyle\sum_i\sum_j \beta_{ij}h_ih_j).$$

The general expression for the equivalent isotropic displacement factor is

$$U_{eq} = \tfrac{1}{3}\textstyle\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j,$$

or, explicitly written,

$$U_{eq} = \tfrac{1}{3}[U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 \\ + 2U_{12}aba^*b^*\cos\gamma + 2U_{13}aca^*c^*\cos\beta \\ + 2U_{23}bcb^*c^*\cos\alpha].$$

For cubic, tetragonal, and orthorhombic systems this results in

$$U_{eq} = \tfrac{1}{3}(U_{11} + U_{22} + U_{33});$$

for hexagonal and trigonal systems, hexagonal setting:

$$U_{eq} = \tfrac{1}{3}[U_{33} + \tfrac{4}{3}(U_{11} + U_{22} - U_{12})];$$

for trigonal systems, rhombohedral setting:

$$U_{eq} = \tfrac{1}{3}\{(aa^*)^2[U_{11} + U_{22} + U_{33} \\ + 2\cos\alpha(U_{12} + U_{13} + U_{23})]\};$$

for the monoclinic system, setting with unique axis **b**:

$$U_{eq} = \tfrac{1}{3}[U_{22} + 1/\sin^2\beta(U_{11} + U_{33} + 2U_{13}\cos\beta)];$$

for the monoclinic system, setting with unique axis **c**:

$$U_{eq} = \tfrac{1}{3}[U_{33} + 1/\sin^2\gamma(U_{11} + U_{22} + 2U_{12}\cos\gamma)].$$

If the elements are given in B or β the expression becomes

$$U_{eq} = 1/(24\pi^2)\textstyle\sum_i\sum_j B_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j\ \text{or}$$
$$U_{eq} = 1/(6\pi^2)\textstyle\sum_i\sum_j \beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$$

For the derivation of the estimated standard deviation of U_{eq} see Schomaker & Marsh (1983).

References

BROCK, C. P. (1984). *Am. Crystallogr. Assoc. Newsl.* **15**(5), 14.
COMMISSION ON JOURNALS (1986). *Acta Cryst.* C42, 1100.
FISCHER, R. X. & TILLMANNS, E. (1983). *Neues Jahrb. Mineral. Monatsh.* pp. 49–59.
HAMILTON, W. C. (1959). *Acta Cryst.* **12**, 609–610.
PRINCE, E. (1982). *Mathematical Techniques in Crystallography and Materials Science*, p. 65. Berlin: Springer.
SCHOMAKER, V. & MARSH, R. E. (1983). *Acta Cryst.* A39, 819–820.
WILLIS, B. T. M. & PRYOR, A. W. (1975). *Thermal Vibrations in Crystallography*, pp. 101–102. Cambridge Univ. Press.