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Symmetry restrictions on the components of the second-order tensors in the cubic crystal system: Correction of an error in *International Tables for X-ray Crystallography* (1974). By C. SCHERINGER, *Mineralogisches Institut der Universität Marburg, D 3550 Marburg, Federal Republic of Germany*

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Abstract

In the symmetry restrictions on the components of the second-order tensors, as given in *International Tables for X-ray Crystallography* [(1974) Vol. IV. Birmingham: Kynoch Press], the signs have to be changed. The corrections refer to the special positions with site symmetry $\bar{3}m, 3m, 32, \bar{3}, 3$ in the cubic crystal system (entries B7 and B8 in Table 5.5B of *International Tables for X-ray Crystallography*, 1974. Vol. IV. Birmingham: Kynoch Press).

In *International Tables for X-ray Crystallography* (1974), entries B7 and B8 in Table 5.5B, the signs for the off-diagonal components of the second order (thermal vibration) tensors have to be changed. For entries B7 and B8 the sequence of the off-diagonal components should be $-D, D, -D$ and $-D, -D, D$ respectively. Thus, there are always two minus signs in the D notation of the second-order tensors for the three point group generators $3[1, 1, \bar{1}], 3[1, \bar{1}, 1], 3[\bar{1}, 1, 1]$. We note that the signs of the off-diagonal components for these three generators were also incorrectly given by Peterse & Palm (1966). In Fig. 1 of these authors, entry point 18, the off-diagonal components are given with only one minus sign.

Method of calculation: we choose a Cartesian coordinate system with the x axis in the direction of one of the cubic threefold axes (body diagonal). In this coordinate system the symmetry restrictions for the site symmetries $\bar{3}m, 3m, 32, \bar{3}, 3$ are known, and the second-order tensor has the general form

$$\mathbf{B} = \begin{pmatrix} B & & \\ & C & \\ & & C \end{pmatrix}. \quad (1)$$

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We now transform the components of \mathbf{B} to a Cartesian coordinate system with axes parallel to the cubic crystal axes, letting the rotation of the base vectors be defined by $\mathbf{a}_{\text{cryst}} = \mathbf{G}\mathbf{a}$, where the base vectors \mathbf{a} refer to our initial Cartesian coordinate system. \mathbf{G} is orthogonal, i.e. $\mathbf{G}^{-1} = \mathbf{G}^T$, and is slightly different for the four symmetry-equivalent body diagonals. We obtain

$$\mathbf{B}_{\text{cryst}} = \mathbf{G}\mathbf{B}\mathbf{G}^T, \quad (2)$$

(Scheringer, 1966). With the notation of *International Tables for X-ray Crystallography* (1974), and for the generator $3[\bar{1}, 1, 1]$, for example, the evaluation of (2) yields

$$\mathbf{B}_{\text{cryst}} = \begin{pmatrix} A & -D & -D \\ -D & A & D \\ -D & D & A \end{pmatrix}, \quad (3)$$

where

$$A = \frac{1}{3}(B + 2C), \quad D = \frac{1}{3}(B - C), \quad (4a)$$

and further

$$B = A + 2D, \quad C = A - D. \quad (4b)$$

For an isotropic tensor $A = B (= C), D = 0$, as it should be.

References

- International Tables for X-ray Crystallography* (1974). Vol. IV. Birmingham: Kynoch Press.
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