

Acta Cryst. (1990). **A46**, 625

An error in space group $P6_22$ in *International Tables for X-ray Crystallography*. By FUSAO TAKUSAGAWA and SHINTARO MISAKI, *Department of Chemistry, University of Kansas, Lawrence, KS 66045, USA*

(Received 24 August 1989; accepted 6 February 1990)

Abstract

An error in the structure-factor expression for space group $P6_22$ (No. 180) has been found in *International Tables for X-ray Crystallography*, Volume I, 1st through 3rd editions. The minus sign of the second sine function in the B part of the equation for $l=3n \pm 1$ should be a plus sign.

An error in the B part of the equation for $l=3n \pm 1$ for space group $P6_22$ (No. 180) on p. 481 of *International Tables for X-ray Crystallography* (1952, 1965, 1969) has been found. The minus sign of the second sine function

Acta Cryst. (1990). **A46**, 625–626

Determination of the correct reference frame from an atomic coordinate list. By T. O. YEATES, *Department of Molecular Biology, Research Institute of Scripps Clinic, La Jolla, CA 92037, USA*

(Received 26 June 1989; accepted 22 February 1990)

Abstract

A simple method is described for determining the reference coordinate system of a list of atomic coordinates. The reference system is characterized by finding the optimal metric tensor on the basis of the expected bond lengths. The ability to identify the correct frame of reference is important for structures solved in non-orthogonal unit cells.

Atomic coordinates are commonly described with respect to three different reference coordinate systems: (1) basis vectors given by the crystallographic unit-cell axes (coordinates referred to as 'fractional'); (2) basis vectors taken to be 1 Å vectors parallel to the unit-cell axes (coordinates referred to here as 'axial'); and (3) mutually orthogonal 1 Å basis vectors (coordinates referred to as 'orthogonal'). In non-orthogonal unit cells, the 'axial' and 'orthogonal' systems are distinct, but usually cannot be distinguished by inspection of the coordinate list. Since the coordinates of macromolecular structures are frequently converted back and forth between reference frames, uncertainty occasionally arises, especially when receiving coordinates from an external source. The following algebraic analysis is sufficient to resolve any ambiguity.

The coordinate list is used to form a list of interatomic vectors between pairs of atoms that are bonded and whose expected bond length is known. Let x^i be the usual (contravariant) components of an interatomic vector in the given (unknown) coordinate system. The corresponding bond length is given by

$$\|\mathbf{x}\| = \left(\sum_{i=1}^3 \sum_{j=1}^3 \mathbf{G}_{ij} x^i x^j \right)^{1/2} \quad (1)$$

should be a plus sign. The correct equation is

$$B = 4 \{ \sin 2\pi lz \sin \pi h(2x - y) \sin \pi(i - k)y \\ + \sin 2\pi(lz \mp \frac{1}{3}) \sin \pi h(x + y) \sin \pi(i - k)(y - x) \\ + \sin 2\pi(lz \pm \frac{1}{3}) \sin \pi h(x - 2y) \sin \pi(i - k)x \}.$$

Reference

International Tables for X-ray Crystallography (1952, 1965, 1969). Vol. I. Birmingham: Kynoch Press.

where \mathbf{G} , which is to be determined, is the covariant metric tensor for the unknown reference frame.* In more familiar terms of matrices, $\|\mathbf{x}\| = (\mathbf{x}^T \mathbf{G} \mathbf{x})^{1/2}$. If d is the expected bond length (in Å), then the equation

$$\|\mathbf{x}\|^2 = d^2 \quad (2)$$

provides a linear equation in terms of the variables G_{ij} . Since \mathbf{G} may be taken to be symmetric, the equation for the unique components of \mathbf{G} is

$$(x^1)^2 G_{11} + 2x^1 x^2 G_{12} + 2x^1 x^3 G_{13} \\ + (x^2)^2 G_{22} + 2x^2 x^3 G_{23} + (x^3)^2 G_{33} = d^2. \quad (3)$$

Given a large number of interatomic vectors, the G_{ij} can be accurately determined by least squares. The metric tensor obtained is the one which minimizes the sum over the bonds of the squared differences between $\|\mathbf{x}\|^2$ and d^2 . Alternatively, the metric tensor which minimizes the sum of the squared differences between $\|\mathbf{x}\|$ and d may be obtained by iteration.

The reference frame may be described in crystallographic terms ($a, b, c, \alpha, \beta, \gamma$) by equating the values obtained for the G_{ij} with the crystallographic metric tensor (Patterson, 1985; Sands, 1982)

$$\begin{pmatrix} a^2 & ab \cos \gamma & ac \cos \beta \\ ab \cos \gamma & b^2 & bc \cos \alpha \\ ac \cos \beta & bc \cos \alpha & c^2 \end{pmatrix}. \quad (4)$$

If $a = b = c = 1$, and $\alpha = \beta = \gamma = 90^\circ$, then the reference

* In the case of an ordinary Euclidean reference frame, \mathbf{G} is the identity matrix and $\|\mathbf{x}\| = (\mathbf{x}^T \mathbf{x})^{1/2}$.