SHORT COMMUNICATIONS

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The determination of absolute structure. III. An ambiguity table for the non-centrosymmetric crystal classes.*

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Abstract

The general term 'determination of absolute structure' is more precisely defined for each non-centrosymmetric crystal class.

An earlier paper in this series (Jones, 1984*a*) pointed out that there are several ways, depending on the space group involved, of visualizing the ambiguity between a non-centrosymmetric structure and its inverse; this ambiguity is resolved by a successful analysis of anomalous dispersion effects in the typical X-ray experiment (*i.e.* by the determination of 'absolute structure'). It is well known that, if both the crystal class and the chemical species concerned are chiral, the determination of absolute structure is also a determination of absolute configuration. In other non-centrosymmetric crystal classes this is no longer the case and there seems to be some confusion in the literature (especially in higher symmetry classes) as to precisely what is being determined. I present here an 'ambiguity table' (Table 1) detailing the manifestations of non-centrosymmetry that correspond to absolute structures.

The use of the term 'absolute structure' does, however, to some extent obviate the need to describe precisely the particular effects concerned.

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References

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* Part II: Jones (1984*b*).

Table 1. *Resolvable ambiguities in the non-centrosymmetric crystal classes*

Crystal class(es)	Resolvable ambiguity
1, 2, 222, 4, 422, 3, 312/321, 32, 6, 622, 23, 432 (the chiral classes)	Absolute configuration (for chiral species) or conformation (for achiral species); this includes space-group determination for the enantiomorphous pairs*
m	Polar axis (x, z) directions†
*mm*2, 4*mm*, 3*m*1/31*m*, 3*m*,‡ 6*mm*	Polar axis (z) direction†
$\bar{4}$, $\bar{4}2m/\bar{4}m2$	Absolute axis assignment§ (x→y, y→−x)
$\bar{6}$, $\bar{6}m2/\bar{6}2m$	Absolute axis assignment§ (x→−x, y→−y)
$\bar{4}3m$	Absolute axis assignment§ (non-cyclic axis permutation)

* For a detailed definition of molecular chirality, see Cahn, Ingold & Prelog (1966); for comments on absolute conformation, see Jones (1984*a*).

† A polar axis is here defined as a unit-cell axis along which the origin may be arbitrarily placed.

The conventional expression 'determination of polar-axis direction' may be somewhat misleading, since the direction of any one axis (*e.g.* z) cannot be reversed without changing the handedness of the axis system. A better description would be 'determination of the orientation of the structure with respect to the polar axis (axes)'. Thus, in $Pna2_1$ (for example), a change of sign of all z coordinates changes the set of symmetry operators as follows: $(x, y, z;\ \bar{x}, \bar{y}, 0{\cdot}5+z;\ 0{\cdot}5+x, 0{\cdot}5-y, z;\ 0{\cdot}5-x, 0{\cdot}5+y, 0{\cdot}5+z) \rightarrow (x, y, \bar{z};\ \bar{x}, \bar{y}, 0{\cdot}5-z;\ 0{\cdot}5+x, 0{\cdot}5-y, \bar{z};\ 0{\cdot}5-x, 0{\cdot}5+y, 0{\cdot}5-z)$ and an allowed origin shift of 0·5 along z then provides the inverse set of symmetry operators.

‡ Rhombohedral cells on hexagonal axes (on rhombohedral axes the polar axis is [111]).

§ In these classes we must seek some operation that transforms the set of symmetry operators to their inverse. One such suitable operation is found to be the interchange of certain axis directions, *e.g.* x and y in $P\bar{4}2_1c$ (x→y, y→−x): $(x, y, z;\ \bar{x}, \bar{y}, z;\ y, \bar{x}, \bar{z};\ \bar{y}, x, \bar{z};\ 0{\cdot}5-x, 0{\cdot}5+y, 0{\cdot}5-z;\ 0{\cdot}5+x, 0{\cdot}5-y, 0{\cdot}5-z;\ 0{\cdot}5-y, 0{\cdot}5-x, 0{\cdot}5+z;\ 0{\cdot}5+y, 0{\cdot}5+x, 0{\cdot}5+z) \rightarrow (y, \bar{x}, z;\ \bar{y}, x, z;\ \bar{x}, \bar{y}, \bar{z};\ x, y, \bar{z};\ 0{\cdot}5-y, 0{\cdot}5-x, 0{\cdot}5-z;\ 0{\cdot}5+y, 0{\cdot}5+x, 0{\cdot}5-z;\ 0{\cdot}5+x, 0{\cdot}5-y, 0{\cdot}5+z;\ 0{\cdot}5-x, 0{\cdot}5+y, 0{\cdot}5+z)$. We may thus regard the assignment of these axis directions as ambiguous until the absolute structure is determined. The interchange of axes must conform to the following rules: (i) no change of hand of axis system; (ii) no alteration of the sets of lattice symmetry directions (*International Tables for Crystallography*, 1983).

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Program construction for macromolecule atomic model refinement based on the fast Fourier transform and fast differentiation algorithms; *erratum*.

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Abstract

In Lunin & Urzhumtsev [*Acta Cryst.* (1985), A**41**, 327-333] references to Lifshitz (Agarwal, 1981) on pages 327 and 329 should be amended to Lifchitz (Agarwal, 1981).

All information is given in the *Abstract.*

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