SHORT COMMUNICATIONS

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Equivalence of pairs of enantiomorphic space groups in the presence of non-crystallographic symmetry

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Abstract

The 11 pairs of enantiomorphic space groups with screw axes of opposite handedness generally can be distinguished when the asymmetric unit has known chirality. However, when the asymmetric unit has non-crystallographic rotational symmetry of the same fold or a multiple (*in*, where *i* is a positive integer) and the rotation axis is parallel to the screw axis, the screw axis reduces to a pure translational element. Under these circumstances, pairs of enantiomorphic space groups cannot be distinguished.

1. Introduction

Because of Friedel's law, the 11 pairs of enantiomorphic space groups with screw axes of opposite handedness (Vos & Buerger, 1989) cannot be distinguished from the diffraction pattern alone. However, the space group can be unambiguously determined if a good anomalous signal is available (Bijvoet, 1949, 1954; Blundell & Johnson, 1976; Stout & Jensen, 1988). Even in the absence of an anomalous signal, when the absolute configuration of the chemical structure is known, one choice within the enantiomorphic pair generally refines better than the other (Ghosh, O'Donnell, Furey, Robbins & Stout, 1982; Stout, Turley, Sieker & Jensen, 1988; Stout & Jensen, 1988).

We have encountered a case in which the handedness is more difficult to determine, in the course of solving the crystal structure of amphibian M ferritin (Ha, Thiel & Allewell, 1997). Amphibian M ferritin has 432 molecular symmetry and crystallizes in space group $P4_12_12$ or $P4_32_12$. The molecular fourfold rotation axis is parallel to the z axis but displaced by $\sim$9 Å and the molecular twofold axis is parallel to the x axis. Refinement proceeds equally well for both space groups. In this report, we prove that the diffraction patterns are indeed indistinguishable. This ambiguity will apply to all 11 pairs of enantiomorphic space groups when there is a non-crystallographic rotation axis of the same or multiple fold parallel to the crystallographic screw axis, and the screw axis reduces to a pure translation under these conditions. This issue is most likely to arise with macromolecule assemblies such as viruses and multisubunit proteins (Wang & Janin, 1993).

2. Proof and discussion

When identical elements within the unit cell are generated by translation, the packing can be described as the convolution of one structure motif within the asymmetric unit with a packing delta function, which has a value of one at the origin of each motif and zero elsewhere. The Fourier transform of the crystal can then be treated as the product of three independent terms:

$$f(\text{lattice} * \text{packing} * \text{molecule}) = f(\text{lattice}) \times f(\text{packing}) \times f(\text{molecule}). \quad (1)$$

$f(g)$ is the Fourier transform of function g; $g * w$ is the convolution of function g with function w; lattice is a conventional delta function defining a lattice with a value of one at the lattice points; packing is a delta function with a value of one at the origin of every structure motif; molecule is the electron-density distribution of the structure motif.

We will focus on the transform of the packing term. Without losing generality, we will use $P4_1$ (packing function g_1) *vs* $P4_3$ (packing function g_2) as an example. In the case of g_1, suppose that coordinates of the origin of one structure motif are (x, y, z). Then,

$$\begin{aligned} f_{hkl}(g_1) = {} & \exp[2\pi i(hx + ky + lz)] \\ & + \exp[2\pi i(-hx - ky + lz + l/2)] \\ & + \exp[2\pi i(-hy + kx + lz + l/4)] \\ & + \exp[2\pi i(hy - kx + lz + 3l/4)]. \end{aligned} \quad (2)$$

In the case of g_2, the coordinates of the origin of the same structure motif are (x', y', z'). Then,

$$\begin{aligned} F_{hkl}(g_2) = {} & \exp[2\pi i(hx' + ky' + lz')] \\ & + \exp[2\pi i(-hx' - ky' + lz' + l/2)] \\ & + \exp[2\pi i(-hy' + kx' + lz' + 3l/4)] \\ & + \exp[2\pi i(hy' - kx' + lz' + l/4)] \\ = {} & \exp[2\pi i(hx' + ky' + lz')] \\ & + \exp[2\pi i(-hx' - ky' + lz' - l/2)] \\ & + \exp[2\pi i(-hy' + kx' + lz' - l/4)] \\ & + \exp[(2\pi i(hy' - kx' + lz' - 3l/4)] \end{aligned} \quad (3)$$

$$\begin{aligned} F_{h\bar{k}l}(g_2) = {} & \exp[2\pi i(-hx' - ky' - lz')] \\ & + \exp[2\pi i(hx' + ky' - lz' + l/2)] \\ & + \exp[2\pi i(hy' - kx' - lz' + l/4)] \\ & + \exp[2\pi i(-hy' + kx' - lz' + 3l/4)] \\ = {} & \exp[2\pi i(h\bar{x}' + k\bar{y}' + l\bar{z}')] \\ & + \exp[2\pi i(-h\bar{x}' - k\bar{y}' + l\bar{z}' + l/2)] \\ & + \exp[2\pi i(-h\bar{y}' + k\bar{x}' + l\bar{z}' + l/4)] \\ & + \exp[(2\pi i(h\bar{y}' - k\bar{x}' + l\bar{z}' + 3l/4)]. \end{aligned} \quad (4)$$

It is apparent that if $x' = \bar{x}$, $y' = \bar{y}$ and $z' = \bar{z}$

$$f_{\bar{h}\bar{k}\bar{l}}(g_2) = f_{hkl}(g_1). \quad (5)$$

Also, from Friedel's law,

$$|f_{\bar{h}\bar{k}\bar{l}}(g_2)| = |f_{hkl}(g_2)|. \quad (6)$$

Combining (5) and (6), we have $|f_{hkl}(g_1)| = |f_{hkl}(g_2)|$. This conclusion is equally valid for the other ten pairs of enantiomorphic space groups.

When the packing function and structure motif are combined according to (1),

$$\begin{aligned} &|f(\text{lattice} * g_1 * \text{molecule})| \\ &\quad = |f(\text{lattice})| \times |f(g_1)| \times |f(\text{molecule})| \\ &\quad = |f(\text{lattice})| \times |f(g_2)| \times |f(\text{molecule})| \\ &\quad = |f(\text{lattice} * g_2 * \text{molecule})|. \end{aligned}$$

Thus, upon choosing one enantiomorphic space group (g_1) and the origin of the motif at (x, y, z), it is always possible to place the origin of the same structure motif at $(\bar{x}, \bar{y}, \bar{z})$ in the other enantiomorphic space group (g_2) so that the amplitudes of the resulting transform are identical.

Since the non-crystallographic symmetry does not have the stringent constraints imposed by the crystallographic symmetry, it is likely that very accurate data will resolve the ambiguity. Nevertheless, when the non-crystallographic symmetry is close to the conditions discussed above, the differences between enantiomorphic space groups will be small or even undetectable. We would argue that when the data set has moderate resolution and quality, as is likely to be the case for many protein crystals, it is better to acknowledge the ambiguity than to overemphasize the differences.

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