

following relations for those cases:

$$Q^{1/2} = 1/d = (Na^{*2} + l^2c^{*2})^{1/2}.$$

The term l^2c^{*2} is neglected for the cubic system. N is $h^2 + k^2 + l^2$ for cubic, $h^2 + k^2$ for tetragonal and $h^2 + hk + k^2$ for trigonal and hexagonal systems, respectively. Since indices h , k and l are integers, different combinations of h , k and l give the same values for N and give rise to superposition of Debye-Scherrer lines (e.g. 333 and 511 reflections for the cubic lattice). For evaluation of the Patterson function we should exclude Debye-Scherrer lines that are superpositions of lines caused by such metrical characteristics of the reciprocal lattice.

Determination of Laue classes from diffraction data of polycrystalline materials is thus possible and it is now feasible to study crystal structures of those

materials with the same process applied to single crystals.

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SHORT COMMUNICATIONS

Acta Cryst. (1995). **A51**, 91–92

Comment on *Enantiomorphism and multiple-beam X-ray diffraction* by Roberto Colella (1994). By HANS BURZLAFF, JOACHIM LANGE and HELMUTH ZIMMERMANN, *Institut für Angewandte Physik, Lehrstuhl für Kristallographie der Universität Erlangen-Nürnberg, Bismarckstrasse 10, D-91054 Erlangen, Germany*

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Abstract

For the transition of the structure factors of benzil (B) to benzil (A), Colella [*Acta Cryst.* (1994), **A50**, 55–57] employs the relation

$$F_A(h, k, l) = F_B(-h-k, k, -l), \quad (1)$$

i.e., in matrix notation,

$$\begin{aligned} (h, k, l)_A &= H_A \\ &= H_B \begin{pmatrix} -1 & 0 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \\ &= H_B A \\ &= (-h-k, k, -l). \end{aligned} \quad (2)$$

This relation is wrong since $\det(A) = 1$. It is *not* a mapping onto an enantiomorph; for the change of handedness, $\det(A)$ must be -1 . Moreover, matrix A is an element of the related point group 321. Thus, the result is symmetrically equivalent to the starting set of structure factors. As a consequence, all arguments presented on the basis of (1) are invalid.

To avoid confusion, it is convenient to give some further explanations with respect to the problem.

Enantiomorphic objects are defined by their symmetry; their symmetry operations are only proper rotations R , i.e. $\det(R) = 1$. The transition from one enantiomorph to the other is described by a pair of matrices (A , S). The application of (A , S) acts on the coordinates by

$$X = (A, S)^{-1} X = A^{-1}(X - S) \quad (3)$$

and on the symmetry operations by

$$\begin{aligned} (R, T) &= (A, S)(R, T)(A, S)^{-1} \\ &= \{ARA^{-1}, AT + [(E-A)RA^{-1}]S\}. \end{aligned} \quad (4)$$

For the mapping (A , S), $\det(A)$ must be equal to -1 (see above). The simplest matrix of this type is the matrix for a center of inversion. It can be separated from any improper rotation. With this center of symmetry, the transformation relations can be simplified significantly:

$$X_j = S - X_j; \quad R_k = R_k; \quad T_k = (E - R_k)S - T_k. \quad (5)$$

Here, j counts the atoms in the unit cell and k the symmetry operations of the space group. Inserting these expressions into the structure-factor equation, we get the structure factor F of the enantiomorph:

$$F(H) = F(-H) \exp(2\pi iHS) \quad (6a)$$

or

$$|F(H)| = |F(-H)| \quad \text{and} \quad \varphi(H) = -\varphi(H) + 2\pi HS, \quad (6b)$$

i.e., if the center of symmetry does not coincide with the origin of the structure, the structure factors are affected by a phase shift of $\exp(2\pi iHS)$. Since the basis is fixed, $H = (h, k, l)$ does not change. The structure factors, however, differ with respect to the enantiomorphic pairs.

The space groups of enantiomorphic structures are merohedral space groups that give rise to ambiguities with respect to handedness (Hahn & Klapper, 1992). To resolve these ambiguities, a suitable property, derivable from X-ray diffraction data, is needed (Burzlaff & Hümmner, 1988). This property can be expressed by a set of structure-factor moduli affected by anomalous dispersion or by a set of suitable triplet phases, as is shown below.

Before discussion of the triplets, it is convenient to discuss the implications connected with space groups of enantiomorphic structures and their normalizers. For enantiomorphic structures, two cases may be distinguished:

(i) The space group of an enantiomorphic structure is mapped onto itself, *i.e.* it does not 'feel' the enantiomorphic property. All space groups of this type have a normalizer (Euclidean or affine) that has a center of symmetry. Thus, it is convenient to use a center of symmetry of the normalizer for the mapping of the enantiomorphs onto each other (see above).

(ii) The space group of an enantiomorphic structure is mapped onto another so-called *enantiomorphic space group*. In this case, the normalizers are noncentrosymmetric groups. Inspection of the eleven pairs of enantiomorphic space groups, however, shows that they can be mapped onto each other by a center of symmetry placed in the origin, if the standard setting of *International Tables for Crystallography* (1992) is used.

Restrictions and special relations for structure-factor phases of enantiomorphic structures due to symmetry are treated explicitly by Koch (1986) (see also Koch & Fischer, 1992).

After this discussion, it can easily be seen that suitable triplet phases resolve the enantiomorphic ambiguity. By (6b), the following relations hold for any triplet $H, K, -K-H$ with its triplet phase $\Phi(H, K) = \varphi(H) + \varphi(K) + \varphi(-K-H)$:

$$\begin{aligned} \Phi(H, K) &= \varphi(H) + \varphi(K) + \varphi(-K-H) \\ &= -\varphi(H) - \varphi(K) - \varphi(-K-H) \\ &\quad + 2\pi[H + K - (K + H)]S \\ &= -\Phi(H, K); \end{aligned} \quad (7)$$

thus, the experimental observation of $\Phi(H, K)$ is equivalent to a determination of absolute structure. As was shown by Hümmner, Weckert & Bondza (1989) for benzil, suitable triplets can be found.

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The use of the non-negativity criterion and histogram matching as figures of merit in direct methods of phase determination. By CORNELIA SMYKALLA and PAUL T. BEURSKENS, *Crystallography Laboratory, University of Nijmegen, Toernooiveld 1, 6525 ED Nijmegen, The Netherlands*

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Abstract

Two figures of merit for the selection of correct phase sets from a number of possible or trial phase sets are defined: (1) based on the criterion that significantly negative points should be sparse in electron-density maps; and (2) based on comparison of electron-density histograms with the theoretically expected histogram [Lunin (1993). *Acta Cryst.* **D49**, 90–99]. It is shown that both figures of merit are useful for judging random phase sets and useless for phase sets that originate from direct-methods procedures such as symbolic addition or tangent refinement.

Introduction

The first equation employed for direct phase determination, the inequality of Harker & Kasper (1948), is based on the non-negativity criterion: the electron-density function

must be zero or positive everywhere. The most important equations used in direct-methods procedures, however, are the triple-phase relationship and the tangent formula. They were derived from statistical considerations (*e.g.* Hauptman & Karle, 1953) and related to the Sayre (1952) equation, and are based on atomicity: the electron-density function consists of peaks (at discrete points) in otherwise almost empty space. We investigated the use of these two basic principles, non-negativity and atomicity, as figures of merit for trial phase sets, especially when a large number of phase sets has been generated.

The non-negativity criterion

The non-negativity criterion is not as powerful as atomicity (for a discussion regarding this topic, see Navaza & Navaza, 1992) but as it is not explicitly used in most