

attempted that do not suffer from the inherent drift of free molecular dynamics calculations (Kuriyan & Brünger, work in progress).

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## An Alternative Convention for Solving the Ambiguity Problem of (3+1) Superspace Group Symbols

BY V. PETŘÍČEK

*Institute of Physics, Czechoslovak Academy of Sciences, Na Slovance 2, 180 40 Praha 8, Czechoslovakia*

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#### Abstract

An alternative convention is proposed for solving the ambiguity problem of (3+1) superspace group symbols described by Yamamoto, Janssen, Janner & de Wolff [*Acta Cryst.* (1985), **A41**, 528-530] based on the requirement that the condition for equivalence of modulation vectors to be independent on a selection of basis vectors is satisfied.

The ambiguity of (3+1) superspace group symbols was discussed by Yamamoto, Janssen, Janner & de Wolff (1985) (hereafter referred to as I) and their solution consists of making a specific choice of

symbols for basic space groups summarized in their Table 2.

In order to make clearer our alternative solution we will present below a simple derivation of transformation properties of a supersymmetry operator in (3+d) superspace for the case of replacing modulation vectors.

A translational periodicity in (3+d) superspace is characterized by a lattice  $\Lambda$  spanned by  $\mathbf{b}_1, \dots, \mathbf{b}_{3+d}$  (de Wolff, 1974; Janner, Janssen & de Wolff, 1983):

$$\mathbf{b}_i = \mathbf{a}_i - \sum_{j=1}^d \mathbf{e}_j \sigma_{ji} \quad (i = 1, 2, 3) \quad (1)$$

$$\mathbf{b}_{i+3} = \mathbf{e}_i \quad (i = 1, \dots, d)$$

where  $\mathbf{e}_i$  are additional vectors perpendicular to an external space  $V_E$  and  $\sigma_{ji}$  are components of modulation vectors with respect to  $\mathbf{a}_1^*$ ,  $\mathbf{a}_2^*$  and  $\mathbf{a}_3^*$ . The matrix  $\boldsymbol{\sigma}$  can be decomposed (see Janner & Janssen, 1979) into

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}_r + \boldsymbol{\sigma}_i. \quad (2)$$

A matrix form of supersymmetry operator with respect to the base (1) is

$$\begin{pmatrix} \Gamma_E & \mathbf{0} \\ \Gamma_M & \Gamma_I \end{pmatrix} \begin{pmatrix} \mathbf{r}_E \\ \mathbf{r}_I \end{pmatrix} + \begin{pmatrix} \mathbf{s}_E \\ \mathbf{s}_I \end{pmatrix} = \begin{pmatrix} \mathbf{r}'_E \\ \mathbf{r}'_I \end{pmatrix} \quad (3)$$

where  $\Gamma_E$ ,  $\Gamma_M$  and  $\Gamma_I$  are  $3 \times 3$ ,  $d \times 3$  and  $d \times d$  matrices, respectively and  $\mathbf{s}_E$  and  $\mathbf{s}_I$  are  $3 \times 1$  and  $d \times 1$  matrices, respectively.  $\Gamma_M$  can be written as

$$\Gamma_M = \boldsymbol{\sigma}_r \Gamma_E - \Gamma_I \boldsymbol{\sigma}_r. \quad (4)$$

Instead of  $\mathbf{s}_I$  the more convenient parameter

$$\boldsymbol{\tau} = \mathbf{s}_I - \boldsymbol{\sigma}_r \mathbf{s}_E \quad (5)$$

is used for characterizing the translational part in an internal space  $V_I$ .

The change  $\boldsymbol{\sigma}^\Delta$  of modulation vectors defined by the equation

$$\boldsymbol{\sigma}' = \boldsymbol{\sigma} + \boldsymbol{\sigma}^\Delta \quad (6)$$

can be split into two parts in the same way as for  $\boldsymbol{\sigma}$  [see (2)]:

$$\boldsymbol{\sigma}^\Delta = \boldsymbol{\sigma}_r^\Delta + \boldsymbol{\sigma}_i^\Delta. \quad (7)$$

The transformed base  $\mathbf{b}'_i$  ( $i = 1, \dots, 3+d$ ) is related to the original one by

$$\begin{aligned} \mathbf{b}'_i &= \mathbf{b}_i - \sum_{j=1}^d \mathbf{b}_{j+3} \sigma_{ji}^\Delta \quad (i = 1, 2, 3) \\ \mathbf{b}'_{i+3} &= \mathbf{b}_{i+3} \quad (i = 1, \dots, d), \end{aligned} \quad (8)$$

and similarly for diffraction indices  $\mathbf{H} = (\mathbf{H}_E, \mathbf{H}_I)$ :

$$\begin{aligned} \mathbf{H}'_E &= \mathbf{H}_E - \mathbf{H}_I \boldsymbol{\sigma}^\Delta \\ \mathbf{H}'_I &= \mathbf{H}_I. \end{aligned} \quad (9)$$

The supersymmetry operator can be written with respect to the base (8) and the following transformation holds:

$$\begin{aligned} \Gamma'_E &= \Gamma_E \\ \Gamma'_I &= \Gamma_I \\ \Gamma'_M &= \Gamma_M + \boldsymbol{\sigma}_r^\Delta \Gamma_E - \Gamma_I \boldsymbol{\sigma}_r^\Delta \\ &= \boldsymbol{\sigma}'_r - \Gamma'_I \boldsymbol{\sigma}'_r \\ \mathbf{s}'_E &= \mathbf{s}_E \\ \mathbf{s}'_I &= \mathbf{s}_I + \boldsymbol{\sigma}^\Delta \mathbf{s}_E \\ \boldsymbol{\tau}' &= \boldsymbol{\tau} + \boldsymbol{\sigma}_i^\Delta \mathbf{s}_E. \end{aligned} \quad (10)$$

These transformation properties were derived without any restrictions on possible changes of modulation

vectors. But we are interested in such transformations when one set of modulation vectors is replaced by an equivalent one.

The transformation law (10) was derived for general  $(3+d)$  superspace. For the  $(3+1)$  superspace which we are interested in it can be simplified by replacing the matrices  $\boldsymbol{\sigma}$  by modulation vectors  $\mathbf{q}$  and matrix multiplications (such as  $\boldsymbol{\sigma} \cdot \mathbf{s}_E$ ) by a scalar product ( $\mathbf{q} \cdot \mathbf{s}_E$ ).

Two modulation vectors  $\mathbf{q}$  and  $\mathbf{q}'$  are called equivalent if the difference (or sum)  $\mathbf{q}$  is a reciprocal-lattice vector of a basic lattice (de Wolff, Janssen & Janner, 1981). A problem can arise when a basic lattice is centred. In order to make the term equivalence of modulation vectors independent of basis selection (primitive basic vectors or centred ones) we have to reduce possible differences  $\mathbf{q}$  from reciprocal-lattice vectors that really exist which means that we have to use the extinction rules following from the use of a centred cell.

In I the case

$$P^I \begin{matrix} 2c \\ 111 \\ 111 \end{matrix} b$$

was used to show an ambiguity of certain symbols. But the vectors  $\mathbf{q} = \gamma \mathbf{c}^*$  and  $\mathbf{q}' = (1 - \gamma) \mathbf{c}^*$  can be called equivalent in the primitive orthorhombic lattice but not in an  $I$ -centred one if the proposed equivalence rule is accepted. There are several ways to replace  $\mathbf{q}$ , by  $\mathbf{q}' = (1 - \gamma) \mathbf{c}^*$  but it is always necessary to change  $\mathbf{q}_r$  also. The simplest of them are  $\mathbf{q}' = \mathbf{a}^* + (1 - \gamma) \mathbf{c}^*$  and  $\mathbf{q}' = \mathbf{b}^* + (1 - \gamma) \mathbf{c}^*$  with corresponding symbols

$$L^I \begin{matrix} 2c \\ 111 \\ 111 \end{matrix} b \quad \text{and} \quad M^I \begin{matrix} 2c \\ 111 \\ 111 \end{matrix} b,$$

respectively. On the other hand, use of the equivalence principle without respecting extinction rules following from the use of a centred cell leads to the possibility of transforming the Bravais classes

$$L^C \begin{matrix} m \\ 111 \\ 111 \end{matrix} m \quad \text{and} \quad L^F \begin{matrix} m \\ 111 \\ 111 \end{matrix} m$$

to

$$P^C \begin{matrix} m \\ 111 \\ 111 \end{matrix} m \quad \text{and} \quad P^F \begin{matrix} m \\ 111 \\ 111 \end{matrix} m,$$

respectively, by using  $\mathbf{q}' = \mathbf{q} + \mathbf{a}^*$ . This transformation (9) leads to extinction rules  $h + k + m = 2n$  and  $h + k + m = 2n_1$ ,  $h + l + m = 2n_2$ ,  $k + l = 2n_3$ , respectively. These extinction rules are the only way to distinguish these symbols from ordinary ones.

Our proposal is to use a  $\mathbf{q}$ -equivalence principle respecting extinction rules following from the use of a centred cell, which means that we propose  $\mathbf{q}$  equivalence to be independent of the base selection. The ambiguity problem is fully solved without using the alternative symbols not only for superspace groups from Table 2 of I but also for the symbols of Bravais classes. From equation (9) it is clear that the centring extinction conditions are not changed by such an equivalent transformation. The proposed  $\mathbf{q}$ -equivalence principle is, moreover, in accordance

with that used in lattice dynamics for defining Brillouin zones.

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## Statistical Descriptors in Crystallography

### Report of the International Union of Crystallography Subcommittee on Statistical Descriptors\*

BY D. SCHWARZENBACH (Chairman), *Institut de Cristallographie, University of Lausanne, BSP Dorigny, CH-1015 Lausanne, Switzerland*, S. C. ABRAHAMS (*ex officio*, IUCr Commission on Crystallographic Nomenclature), *AT&T Bell Laboratories, 600 Mountain Ave, Murray Hill, NJ 07974, USA*, H. D. FLACK, *Laboratoire de Cristallographie aux Rayons X, University of Geneva, 24 Quai Ernest Ansermet, CH-1211 Genève 4, Switzerland*, W. GONSCHOREK, *Institut für Physikalische Chemie der TH Darmstadt, Aussenstelle in KFA/ZFR, Postfach 913, D-5170 Jülich, Federal Republic of Germany*, TH. HAHN (*ex officio*, IUCr Commission on Crystallographic Nomenclature), *Institut für Kristallographie, RWTH, Templergraben 55, D-5100 Aachen, Federal Republic of Germany*, K. HUML (*ex officio*, IUCr Commission on Crystallographic Computing), *Laboratory of X-ray Polymer Structure Analysis, Institute of Macromolecular Chemistry, Czech Academy of Science, 162 06 Praha 6, Czechoslovakia*, R. E. MARSH, *Chemistry Department, California Institute of Technology, Pasadena, CA 91125, USA*, E. PRINCE, *National Bureau of Standards, Reactor Radiation Division, Gaithersburg, MD 20899, USA*, B. E. ROBERTSON, *Department of Physics and Astronomy, University of Regina, Regina, Saskatchewan S4S 0A2, Canada*, J. S. ROLLETT, *Oxford University Computing Laboratory, 8-11 Keble Road, Oxford OX1 3QD, England* AND A. J. C. WILSON (*ex officio*, IUCr Commission on Crystallographic Nomenclature), *University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW, England*

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#### Abstract

The Subcommittee has attempted to elucidate the nature of problems encountered in the definition and use of statistical descriptors as applied to crystallography and to propose procedural improvements. The report contains (a) a dictionary of statistical terms established for use by experimentalists; (b) a description of the statistical basis for refinement procedures; (c) sections dealing with defects in the physical model used for refinement, and with the choice and significance of weighting schemes; and (d) recommendations, some of which may be readily implemented, whilst others may require a long-term effort to bring them into general use.

#### Introduction

A result of several discussions at the XIII International Congress of Crystallography in Hamburg,

1984, particularly those arising at a microsposium devoted to crystallographic statistics, was a renewed recognition of the wide nonuniformity in use and nomenclature of many statistical methods applied to crystallography. The Commission on Crystallographic Nomenclature addressed this problem soon after the Congress had ended and agreed that an attempt should be made to improve the situation. Accordingly, a Subcommittee on Statistical Descriptors in Crystallography was appointed in early 1985 with its terms of reference 'to examine the validity of current statistical approaches used in estimating the variances in crystallographic quantities and to make recommendations for an improved methodology that rests securely on sound modern statistical theory and that can be widely adopted by the crystallographic community'.

Vigorous correspondence within the Subcommittee resulted in a series of draft reports that gradually evolved toward general consensus. An intermediate report was presented orally at an Open Meeting of the Commission during the XIV International Congress of Crystallography in Perth 1987.

Problems arising from the interface between the mathematical theory of probability and statistics and

\* Appointed 27 February 1985 as a Subcommittee of the IUCr Commission on Crystallographic Nomenclature. Following a review by the Chairmen of all relevant IUCr Commissions, the Final Report was accepted on 9 May 1988 by the Commission and on 2 September 1988 by the Executive Committee.