

Collimators are specified by the subscript 0 (source–monochromator), 1 (monochromator–sample), 2 (sample–analyzer) and 3 (analyzer–detector). For a double-axis spectrometer  $\alpha_3 = \beta_3 \rightarrow \infty$  in the above expressions giving

$$\alpha_A = \alpha_2 \quad \beta_A = \beta_2. \quad (5c)$$

The following points should be noted.

(a)  $f_h$  is independent of  $\theta_s$  and can be absorbed into other constants. However, it gives a simple expression for the loss of intensity due to horizontal collimation.

(b) If  $4\eta_v^2 > (\beta_M^2 + \beta_A^2)$  there will necessarily be a cross over from a small- $Q$  region where

$$f_v \simeq 1, \quad L \sim \frac{1}{\sin \theta_s}$$

to a large- $Q$  region where

$$f_v = \frac{[\beta_M^2 + \beta_A^2]^{1/2}}{2\eta_v \sin \theta_s}, \quad L \sim \frac{[\beta_M^2 + \beta_A^2]^{1/2}}{2\eta_v (\sin \theta_s)^2}.$$

*Acta Cryst.* (1983). **A39**, 594

**Statistical geometry. I. A self-consistent approach to the crystallographic inversion problem based on information theory: Erratum.** By STEPHEN W. WILKINS, *CSIRO, Division of Chemical physics, PO Box 160, Clayton, Victoria, Australia 3168 and Institut Laue–Langevin, BP156 Centre de Tri, Grenoble Cedex 38042 France*, JOSEPH N. VARGHESE, *CSIRO, Division of Protein Chemistry, Royal Parade, Parkville, Victoria, Australia 3052* and MOGENS S. LEHMANN, *Institut Laue–Langevin, BP156 Centre de Tri, Grenoble Cedex 38042, France*

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#### Abstract

As a result of a printer's error, the first line of § 4.6 (page 56) of Wilkins, Varghese & Lehmann [*Acta Cryst.* (1983), **A39**, 47–60] is in error. The first sentence of that section

should read: 'In order to give an illustration of the way in which the SGM may be used, ...'.

All information is given in the *Abstract*.

*Acta Cryst.* (1983). **A39**, 594–595

**Tensor properties and rotational symmetry of crystals. III. Use of symmetrized components in group 3(3<sub>2</sub>). Erratum.** By F. G. FUMI and C. RIPAMONTI, *Istituto di Scienze Fisiche, Università di Genova, Italy and GNSM-CNR, Unità di Genova, Italy*

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#### Abstract

In Fumi & Ripamonti [*Acta Cryst.* (1983), **A39**, 245–251], there are errors on page 249 in equation II(b) for the even-parity  $c^+$  subtensor and II(a) and (b) for the even-parity  $c^-$  subtensor.

The correct equations are given.

Several misprints are present on page 249 of Fumi & Ripamonti (1983):

First column, equations II(b)

The first and third equations should read:

$$\begin{aligned} yyyyyx^+ &= c_1 \overset{15}{j\bar{j}j\bar{j}x\bar{x}x^+} + c_2 \overset{20}{j\bar{j}j\bar{x}\bar{x}yx^+} \\ yyyyyx^+ &= \frac{1}{3} \overset{15}{j\bar{j}j\bar{j}x\bar{x}x^+} - \frac{1}{3} \overset{20}{j\bar{j}j\bar{x}\bar{x}yx^+}. \end{aligned}$$

Second column, equations II(a)

The first and third equations should read:

$$\begin{aligned} yyyxyxxx^- &= c_1 xxxxxxxx^- + c_2 yyyyy\bar{y}\bar{x}x^- + c_3 \bar{y}\bar{y}\bar{y}\bar{x}yxyx^- \\ yyyxyxxx^- &= \frac{1}{3} xxxxxxxx^- - \frac{2}{3} yyyyy\bar{y}\bar{x}x^- + \frac{1}{3} \bar{y}\bar{y}\bar{y}\bar{x}yxyx^- \end{aligned}$$

Second column, equations II(b)

The first and third equations should read:

$$\begin{aligned} yyyxyxxx^- &= c_1 xxxxxxxx^- + c_2 yyyyy\bar{y}\bar{x}x^- + c_3 \bar{y}\bar{y}\bar{y}\bar{x}yxyx^- \\ yyyxyxxx^- &= \frac{1}{3} xxxxxxxx^- - \frac{2}{3} yyyyy\bar{y}\bar{x}x^- + \frac{1}{3} \bar{y}\bar{y}\bar{y}\bar{x}yxyx^- \end{aligned}$$

#### Reference

FUMI, F. G. & RIPAMONTI, C. (1983). *Acta Cryst.* **A39**, 245–251.

*Acta Cryst.* (1983). **A39**, 595–596

**A simple method for Bravais lattice determination.** By GIOVANNI FERRARIS and GABRIELLA IVALDI, *Istituto di Mineralogia, Cristallografia e Geochimica 'G. Spezia', Università di Torino, Via S. Massimo 22, 10123 Torino, Italy*

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#### Abstract

A general procedure for the determination of Bravais lattices, including cases of pseudo-symmetry, is described. The method is based on the multiplicity of the lattice vectors, which may be generated from any experimental primitive cell, and can be easily programmed for a computer.

#### Introduction

At some step in the determination of the lattice geometry, either by powder methods or *via* the automatic orientation of a crystal on a single-crystal diffractometer, a primitive cell is obtained which allows all the reflections to be indexed. The successive determination of some kind of conventional cell (*e.g.* Niggli's reduced cell) and of the lattice symmetry is not easy to automate and, with several available programs, human intervention is sometimes required. Algorithms which at first look for the reduced cell and then deduce the lattice symmetry from a connected matrix (Krivý & Gruber, 1976; Santoro & Mighell, 1970) may fail in special cases because of experimental errors in the cell parameters which can lead to misinterpretation of the equalities and inequalities to be inspected (Clegg, 1981).

To alleviate the above problems, different approaches have been published recently. Clegg (1981) starts from the Niggli reduced cell and, in order to find the correct lattice symmetry, proposes the inspection of a special list of lattice vectors and angles. Himes & Mighell (1982) attack the problem through the enumeration of the different unitary matrices *B* which transform a primitive triplet of non-coplanar vectors into itself (the numbers are 1, 2, 4, 6, 8, 12, and 24 for triclinic, monoclinic, orthorhombic, rhombohedral, tetragonal, hexagonal, and cubic lattices, in that order and excluding centrosymmetry). The method can be easily automated, but the detection of the matrices *B* is by trial and, in principle, could last indefinitely. Besides, the conventional cell must be found in some other way. Le Page (1982) describes an algorithm which is based on the spatial distribution of the twofold axes; this method should be particularly powerful in detecting pseudo-symmetries and possible twin axes.

#### The method

In connection with a computer program for the automatic indexing of powder patterns, we experimented with a simple procedure which, in principle, is able to determine the correct Bravais cell. The method, which first establishes the lattice symmetry and then obtains the conventional cell as a consequence, is based on the following observations.

(i) Lattices with different point-group symmetry have different maximum multiplicity of the lattice vectors (MAX).

(ii) The three vectors defining the Bravais cell are among those with the two lowest multiplicities (MIN).

(iii) Non-primitive lattices show vectors with multiplicities higher than MIN which are shorter than one or more of those defining the Bravais cell.

Table 1 summarizes the connections between multiplicity of lattice vectors on one side and point-group symmetry and lattice type on the other; criteria for discrimination between sets of MIN vectors with the same multiplicity are shown in the footnotes. Starting from any primitive cell of the lattice, a list of lattice vectors is generated up to a prefixed length and then it is sorted, *e.g.* in order of increasing length. If *d* spacings are preferred, it should be remembered that the largest *d*'s do not always correspond to the shortest direct-lattice vectors. Any further step required by Table 1 can be easily programmed on a computer.

#### The pseudo-symmetry

Because of experimental errors, some tolerance connected with the e.s.d.'s of the cell parameters must be allowed while comparing the vectors for the determination of their multiplicity. Unfortunately, as with all other methods, such a tolerance might produce an apparent higher symmetry for the lattice following accidental merging of sets of independent vectors. However, playing on the redundancy of available data and considering all the multiplicities characterizing each point group (not only MIN and MAX), a careful inspection of the list of vectors should lead to the correct identification of the symmetry *within the limits of the admitted tolerance*. Of course, one should keep in mind that the metric symmetry of the lattice can be higher, but not