Second column, equations II(*a*)

The first and third equations should read:

$$yyyyyxxy^- = c_1\, xxxxxxxx^- + c_2\, yyyyy\bar{\bar{y}}^{2}\bar{x}x^- + c_3\, \bar{y}\bar{y}\bar{y}\bar{y}^{5}\bar{x}yyx^-$$

$$yyyyyxxy^- = \tfrac{2}{3}\, xxxxxxxx^- + \tfrac{2}{3}\, yyyyy\bar{\bar{y}}^{2}\bar{x}x^- - \tfrac{1}{3}\, \bar{y}\bar{y}\bar{y}\bar{y}^{5}\bar{x}yyx^-.$$

Second column, equations II(*b*)

The first and third equations should read:

$$yyyyxxxx^- = c_1\, xxxxxxxx^- + c_2\, yyyy\bar{y}\bar{y}^{3}\bar{x}x^- + c_3\, \bar{y}\bar{y}\bar{y}^{4}\bar{x}yyyx^-$$

$$yyyyxxxx^- = \tfrac{1}{3}\, xxxxxxxx^- - \tfrac{2}{3}\, yyyy\bar{y}\bar{y}^{3}\bar{x}x^- + \tfrac{1}{3}\, \bar{y}\bar{y}\bar{y}^{4}\bar{x}yyyx^-.$$

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A simple method for Bravais lattice determination.

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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 (Křivý & 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.

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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

Table 1. *Connections between lattice symmetry and multiplicity of lattice vectors*

MAX and MIN are the maximum and the lowest multiplicities of the vectors for the corresponding point group.

Point group	MAX	MIN	Elements of symmetry containing MIN*	MIN vectors defining the Bravais cell	Lattice type	Identification of the lattice type
$\bar{1}$	2	2	None	The three shortest non-coplanar vectors are **a**, **b** and **c**	*P*	No other possibilities
2/*m*	4	2	Twofold axis (Set M1)† Mirror plane (SetM2)	The shortest vector of SetM1 is **b**; the two shortest vectors with $\beta > 90°$ are **a** and **c**	*P*	**a** and **c** are the shortest vectors not belonging to SetM1
					C	One vector with multiplicity 4 is shorter than **a** and/or **b**
mmm	8	2	Twofold axes	The three shortest vectors with angles $\alpha = \beta = \gamma = 90°$ are **a**, **b** and **c**	*P*	**a**, **b** and **c** are the shortest non-coplanar vectors
					C	As for *C* monoclinic
					F	Each of three vectors with multiplicity 4 is shorter than **a** and/or **b** and/or **c**
					I	One vector with multiplicity 8 is shorter than **a** and/or **b** and/or **c**
$\bar{3}m$	12	2	Threefold axis (SetR1)	*Rhombohedral setting*: the three shortest and equal vectors of SetR2 with angle $\gamma < 120°$ are **a**	*R*	No other possibilities
		6	Mirror planes (SetR2) Twofold axes (SetR3)‡	*Hexagonal setting*: the shortest vector of SetR1 is **c**; the two shortest and equal vectors of SetR3 with angle $\gamma = 120°$ are **a**		
4/*mmm*	16	2	Fourfold axis (SetT1)	The shortest vector of SetT1 is **c**; the two shortest and equal vectors of SetT2 with angle $\gamma = 90°$ are **a**	*P*	**a** is the shortest vector not belonging to SetT1
		4	Twofold axes (SetT2)		*I*	One vector with multiplicity 8 is shorter than **a** and/or **c**
6/*mmm*	24	2	Sixfold axis (SetH1)	The shortest vector of SetH1 is **c**; the two shortest and equal vectors of SetH2 with angle $\gamma = 120°$ are **a**	*P*	No other possibilities
		6	Twofold axes (SetH2)			
*m*3*m*	48	6	Fourfold axes	The three shortest and equal vectors with angles $\alpha = \beta = \gamma = 90°$ are **a**	*P*	**a** is the shortest vector
					I	One vector with multiplicity 8 is shorter than **a**
					F	One vector with multiplicity 12 is shorter than **a**

* If MIN vectors are parallel to both axes and planes, only axes are shown.
† MIN vectors which are parallel to the twofold axis are perpendicular to all the MIN vectors which lie in the mirror plane.
‡ MIN vectors which are parallel to the twofold axes are not coplanar with other MIN vectors showing multiplicity 6.

lower, than that of the atomic structure and, therefore, diffracted intensities should be checked as well, if possible. Angles between vectors can also be helpful as shown in the following examples which illustrate problems connected with accidental higher multiplicity.

(1) A lattice with real symmetry 6/*mmm* shows MAX 48. The suggested *m*3*m* symmetry can be proved false by the presence of angles of 120° between equal MIN vectors. Besides, multiplicity 8 as required by *m*3*m* should not be found.

(2) A lattice with real symmetry $\bar{3}m$ shows MAX 24. The suggested 6/*mmm* symmetry cannot be accepted because the hexagonal cell is non-primitive.

Closeness of independent sets of lattice vectors is clear evidence of pseudo-symmetry; its nature can be easily detected by increasing the tolerance. If that is done by steps, some quantitative evaluation of the deviation from the accepted symmetry can be obtained as well.

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