Introducing this in ($A5$) and using ($A1$), we have

$$a_r^2=\{(N-2)b_r^2\}\Big/\Big\{(N-1)\Big(\sum_m b_m-2b_r+v_r\Big)\Big\}. \quad (A6)$$

Equation ($A6$) is used to obtain a numerical solution. If we set first all v_r to zero, approximate values $a'_r \geq a_r$ are calculated. These serve to obtain approximate values v'_r which are introduced in ($A6$) to obtain improved estimates of a_r. If $(\sum_m b_m-2b_r)/b_r>0{\cdot}01$, about five iterations are sufficient to reach convergence at the 0·1% level, *i.e.* $|(a'_r-a_r)/a'_r|<0{\cdot}001$ and $[b_m(\text{calc.})-b_m]/b_m<0{\cdot}001$.

An explicit solution is easily calculated for the special case where all b_m except one are equal:

$b_1, b_2=b_3=\ldots=b_N$:

$$\left.\begin{aligned} a_1^2&=\{(N-2)b_1^2\}/\{(N-1)^2b_2-(N-1)b_1\}\\ a_2^2&=a_3^2=\ldots=a_N^2\\ &=\{(N-1)b_2-b_1\}/\{(N-1)(N-2)\}. \end{aligned}\right\} \quad (A7)$$

References

BERNARDINELLI, G. & FLACK, H. D. (1985). *Acta Cryst.* **A41**, 500-511.

MILLEDGE, H. J., MENDELSSOHN, M. J., O'BRIEN, C. M. & WEBB, G. I. (1985). *Structure and Statistics in Crystallography*, edited by A. J. C. WILSON, pp. 197-211. Guilderland, NY: Adenine.

ROLLETT, J. S., MCKINLAY, T. G. & HAIGH, N. P. (1976). *Crystallographic Computing Techniques*, edited by F. R. AHMED, pp. 417-419. Copenhagen: Munksgaard.

STEWART, J. M., KRUGER, G. J., AMMON, H. L., DICKINSON, C. W. & HALL, S. R. (1972). The *XRAY*72 system. Tech. Rep. TR-192. Computer Science Center, Univ. of Maryland, College Park, Maryland, USA.

STEWART, J. M., MACHIN, P. A., DICKINSON, C. W., AMMON, H. L., HECK, H. & FLACK, H. D. (1976). The *XRAY* system - version of 1976. Tech. Rep. TR-446. Computer Science Center, Univ. of Maryland, College Park, Maryland, USA.

WASER, J. (1974). *Acta Cryst.* **A30**, 261-264.

WATKIN, D. J., CARRUTHERS, J. R. & BETTERIDGE, P. W. (1985). *CRYSTALS User Guide.* Chemical Crystallography Lab., Univ. of Oxford, England.

WERK, M. L., CHAPUIS, G. & PERRET, R. (1987). *Z. Kristallogr.* **178**, 215.

Acta Cryst. (1988). **A44**, 506-508

On the Ambiguities in Merohedral Crystal Structures

BY HANS BURZLAFF AND KURT HÜMMER

Lehrstuhl für Kristallographie, Institut für Angewandte Physik, Bismarckstrasse 10, 8520 *Erlangen, Federal Republic of Germany*

(*Received* 8 *December* 1987; *accepted* 8 *March* 1988)

Dedicated to Professor Dr Th. Hahn on the occasion of his 60*th birthday*

Abstract

The ambiguities in merohedral crystal classes are discussed from the group-theoretical point of view. A classification of merohedral point groups and the extension of these terms to space groups and crystal structures is proposed. Similarities and differences for special types of merohedries are discussed.

1. Introduction

Recently Jones (1986) discussed ambiguities and their resolution in non-centrosymmetric crystal classes. He subdivides the non-centrosymmetric point groups into chiral, polar and roto-inversional subclasses, the last one containing only non-centrosymmetric point groups with roto-inversions $\bar{4}$ and $\bar{6}$. The ambiguities are resolved for the chiral subclass by determination of the absolute configurations, for the polar subclass by fixing the polar direction, and for the roto-inversional subclass by the assignment of absolute axes.

The usual classification of crystallographic point groups was introduced by Schoenflies (1891) mainly on the basis of subgroup relations; the nomenclature was derived from morphology. The main classes are the lattice point groups, which are called holohedries; point groups which are within a crystal family of subgroups of a holohedry are called merohedries (*cf.* also *International Tables for Crystallography*, 1987). The index of the subgroup is indicated in the name: hemihedry, tetartohedry, ogdohedry for indices 2, 4, 8 respectively. A more subtle distinction subdivides into 'paramorphic, enantiomorphic, hemimorphic' types of merohedries. These expressions, however, are used with different meanings by different authors (*e.g.* Schoenflies, 1891; Niggli, 1919; Burckhardt, 1966; Kleber, 1985). Nevertheless, there was a general consensus that these distinctions derived from

0108-7673/88/040506-03$03.00

Table 1. *Crystallographic point groups and their classification with respect to merohedral subgroup relations*

		Family						
	Index	Cubic	Hexagonal		Tetragonal	Orthorhombic	Monoclinic	Triclinic
Holohedry	1	$m\bar{3}m$	$\frac{6}{m}mm$	$\bar{3}m$	$\frac{4}{m}mm$	mmm	$\frac{2}{m}$	$\bar{1}$
Merohedries								
paramorphic	2	$m\bar{3}$	$\frac{6}{m}$	$\bar{3}$	$\frac{4}{m}$	—	—	—
	4	—	$\bar{3}$	—	—	—	—	—
enantiomorphic	2	432	622	32	422	222	2	1
	4	23	6, 321 (312)	3	4	—	—	—
	8	—	3	—	—	—	—	—
hemimorphic	2	—	$6mm$	$3m$	$4mm$	$mm2$	m	—
	4	—	$3m1$ ($31m$)	—	—	—	—	
roto-inversional	2	$\bar{4}3m$	$\bar{6}m2$ ($\bar{6}2m$)	—	$\bar{4}2m$ ($\bar{4}m2$)	—	—	—
	4		$\bar{6}$		$\bar{4}$			

morphology are also of importance for the physical properties of crystals (Voigt, 1966).

It is the intention of this paper to correlate these terms with properties of the subgroups for the resolution of the ambiguities from a more general point of view. This procedure might include a further application to space groups and crystal structures.

2. Proposal

A point group is called polar if the 'centre of gravity' of the symmetrically equivalent positions does not coincide with the origin:

$$(1/N)\sum_{i=1}^{N} R_i X \neq 0, \quad X = \begin{pmatrix} x \\ y \\ z \end{pmatrix},$$

i.e. the sum of all 3×3 matrices R_i representing the operations does not add up to the zero matrix. For a unique determination of the different types of merohedries the following definitions are introduced. (i) A merohedral subgroup is called 'paramorphic' if it is centrosymmetric (non-holohedral Laue classes). (ii) A merohedral subgroup is called 'enantiomorphic' if it contains only rotations [all $\det(R_i)=+1$]. (iii) A merohedral subgroup is called 'hemimorphic' if it is polar *and* if it contains mirror operations. (iv) A merohedral subgroup is called 'roto-inversional' if it is non-centrosymmetric and if it contains roto-inversions $\bar{4}$ or $\bar{6}$; it is non-polar. The consequences of these definitions for the classification of point groups are given in Table 1.

Roto-inversional subgroups do not allow polar properties such as pyro- or ferroelectricity; they are compatible, however, with piezoelectricity. Hemimorphic subgroups allow polar properties but never chirality.

Enantiomorphic merohedries are specific for chirality; paramorphic merohedries are not compatible with polar, piezoelectric or chiral properties.

3. Discussion

The ambiguities due to a merohedral subgroup are related to a group-theoretical background; they correspond to the number of cosets that are generated by the decomposition of the holohedry with respect to the merohedral subgroup. A geometrical object with the symmetry of the subgroup is mapped by the operations of a coset to another geometrical object. Each operation of the coset produces the same image. All images are equivalent with respect to the holohedry but non-equivalent and thus ambiguous with respect to the subgroup. This means the number of cosets equals the number of different sites of the object with respect to the symmetry of the subgroup, *i.e.* the number of ambiguities. Resolving an ambiguity is equivalent to selecting a specific image of the geometric object. From this point of view all merohedries behave in a similar way.

The non-centrosymmetric merohedries allow the construction of special cosets in a unique way by multiplication of all elements of the subgroup with the centre of inversion $\bar{1}$; thus an enantiomorphic or hemimorphic or roto-inversional coset can be assigned. In the case of a paramorphic merohedry, instead of the centre of inversion another element has to be chosen. It is convenient to employ an element from that *Blickrichtung* that is not used in the merohedric group; this is either a rotation 2 or a mirror *m*.

The complete symmetry included in the use of a crystallographic coordinate system is described by the full lattice symmetry, *i.e.* the holohedry. The additional convention only to use right-handed coordinate systems lowers its symmetry to the enantiomorphic hemihedry. As a consequence enantiomorphic images can be distinguished by the determination of chiral properties because mappings R_i with $\det(R_i)=-1$ must not be applied to the coordinate axes. In contrast to this the hemimorphic, paramorphic and roto-inversional cosets contain mappings with $\det(R_i)=+1$ and $\det(R_i)=-1$ simultaneously. The selection of an image may be regarded as the selection of a right-handed coordinate system compatible with a rotation.

These group-theoretical considerations justify the results of Jones (1986).

4. Practical procedure

In fact the ambiguities are handled by measuring a suitable physical property that specifies the allowed object as far as possible. As crystal structures are usually determined by diffraction experiments it is convenient to use properties derivable from X-ray diffraction data.

In the case of paramorphic merohedries the structure-factor moduli can be used for fixing the ambiguity of the description. The operation R_i (rotation 2 or mirror m) that is used for the construction of the characteristic coset correlates pairs of structure factors. The ratio q of their moduli changes to $1/q$ with the transformation to the other image.

In the case of non-centrosymmetric structures properties must be regarded that are sensitive to structure-factor phases. This can be done by comparing the moduli of Friedel pairs affected by anomalous dispersion or by measuring suitable triplet phases. For enantiomorphic merohedries this means the determination of the absolute configuration (for chiral species) or conformation (for achiral species). For hemimorphic and roto-inversional merohedries this means fixing the ambiguity in the description: The operation $\bar{1}$ correlates the sign of suitable triplet phases or the moduli of suitable Friedel pairs of structure factors; their values change with the transformation to the other image.

As a consequence of these considerations two types of absolute structures can be distinguished. An absolute structure can be determined by experiment in the case of enantiomorphic merohedries because left-handed coordinate systems are excluded. In the case of non-enantiomorphic merohedries an absolute structure is uniquely determined by the selection of one description among different equivalent possibilities. The difference in the two cases corresponds to the special role of chiral properties.

The transfer of these terms to space groups and crystal structures is proposed, because these considerations do not only affect problems of crystal structure determination but also problems in structure description and standardization. The extension on *klassengleiche* subgroup relations will, however, need further discussions.

The authors thank Mr E. Weckert for helpful discussions.

References

BURCKHARDT, J. J. (1966). *Die Bewegungsgruppen der Kristallographie*, p. 90. Basel: Birhäuser.
International Tables for Crystallography (1987). Vol. A, p. 752. Dordrecht: Reidel. (Present distributor Kluwer Academic Publishers, Dordrecht.)
JONES, P. G. (1986). *Acta Cryst.* A**42**, 57.
KLEBER, W. (1985). *Einführung in die Kristallographie*, p. 57. Berlin: VEB Verlag Technik.
NIGGLI, P. (1919). *Geometrische Kristallographie des Diskontinuums*, p. 101. Leipzig: Borntraeger.
SCHOENFLIES, A. (1891). *Kristallsysteme und Kristallstruktur*, pp. 143-147. Leipzig: Teubner.
VOIGT, W. (1986). *Lehrbuch der Kristallphysik*, Table on last page. Stuttgart: Teubner. (Reprint of the first edition, 1910.)

Acta Cryst. (1988). A**44**, 508-516

Penrose Patterns and Related Structures. I. Superstructure and Generalized Penrose Patterns

BY K. N. ISHIHARA

Department of Metal Science and Technology, Kyoto University, Sakyo-ku, Kyoto 606, *Japan*

AND AKIJI YAMAMOTO

National Institute for Research in Inorganic Materials, Sakura-mura, Niihari-gun, Ibaraki 305, *Japan*

(*Received* 27 *October* 1987; *accepted* 11 *March* 1988)

Abstract

The section method is applied to derive the Penrose pattern and related patterns with a ten- or fivefold axis. These are derived from a four-dimensional decagonal crystal or from a five-dimensional icosahedral crystal as a two-dimensional section. The two descriptions correspond to the three- and four-dimensional ones in the usual superstructure and the Penrose pattern can be regarded as the superstructure in the four-dimensional space. The diffraction intensities and symmetries of these patterns are dis-

0108-7673/88/040508-09$03.00