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Nomenclature for Crystal Families, Bravais-Lattice Types and Arithmetic Classes

Report of the International Union of Crystallography *Ad-Hoc* Committee on the Nomenclature of Symmetry*

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Abstract

Standard symbols representing crystal families, two- and three-dimensional Bravais-lattice types and arithmetic classes are recommended for use by the IUCr. The six crystal families are designated by lower-case letters. The family letter in the symbol of each of the 14 lattice types is followed by an upper-case letter to distinguish different lattice types within the family. Arithmetic classes are indicated by modified symbols of the corresponding symmorphic space groups.

Crystal families

Six lower-case letters, which originate from words denoting the shape of commonly used unit cells, are recommended as the standard designation of *crystal families* (Table 1). A 'crystal family' is a well defined and unambiguous concept in crystallography [*International Tables for Crystallography* (1983), sections 2.1 and 8.2.6]. Comparing the classification into crystal families with existing classifications into 'crystal systems', it is noted that they coincide except for the hexagonal family in three dimensions, which contains all 'hexagonal', 'trigonal' and 'rhombohedral' space groups. Although this set is often regarded as a single 'crystal system' in the American and Russian literature, other widespread usage divides it into two different systems. Therefore, association of the lower-

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Table 1. *Standard symbols for the crystal families*

Symbol	Two-dimensional crystal family	Three-dimensional crystal family
a	—	Triclinic (anorthic)
m	Oblique	Monoclinic
o	Rectangular	Orthorhombic
t	Square	Tetragonal
h	Hexagonal	Hexagonal
c	—	Cubic

case letters with crystal systems (instead of families) is apt to cause confusion and is not recommended by the *Ad-hoc* Committee.

Adoption of these symbols yields a clear interpretation of the lattice symbols, see below. Direct applications are not envisaged but future use is likely, since the ambiguity of the term 'crystal system' (see above) has so far prevented the general acceptance of a suitable nomenclature for this scale of classification. No such difficulty exists with the term 'crystal families'.

Bravais-lattice types

Symbols for designating Bravais-lattice types independently of any description by a particular unit cell with labelled axes are presented in Table 2. The initial lower-case letter characterizes the crystal family (see above) to which the Bravais-lattice type belongs. The second letter designates the type of centring. These symbols are identical with those listed in *International Tables for Crystallography* (1983) and used in the 60-year index to *Structure Reports* (1976),* with the exception of *mS* and *oS*, which replace *mC* and *oC*.

The letter *C* in the monoclinic and orthorhombic Bravais-lattice-type symbols is ambiguous since *C* is closely associated with one of the common setting and/or unit-cell choices for the lattice, namely *A*, *C* or *I* centring for the monoclinic family and *A*, *B* or *C* centring for the orthorhombic family. The *Ad-Hoc* Committee has chosen the latter *S*, derived from 'side-face centred' (*i.e. seitenflächenzentriert*), to replace *C*. This letter, which is also used to designate similarly centred four-dimensional lattices (Wondratschek, Bülow & Neubüser, 1971), is clearly appropriate for *oS*-type lattices. In the case of *mS*-type lattices, the letter *S* evokes neither an *A*- nor a *C*-centred in preference to an *I*-centred unit cell: the symbol for the monoclinic centred lattice remains *mS* regardless of the basis actually used.

A similar comment applies to the symbol *hR*, which designates the rhombohedral lattice regardless of whether that lattice is described (using rhombohedral coordinates) by a primitive rhombohedral unit cell or (using hexagonal coordinates) by a hexagonal unit cell.

Table 2. *Standard symbols for the Bravais lattice types*

Symbol	Two-dimensional lattice type	Symbol	Three-dimensional lattice type
mp	Oblique	*aP*	Triclinic
op	Rectangular primitive	*mP*	Monoclinic primitive
oc	Rectangular centred	*mS*	Monoclinic centred
tp	Square	*oP*	Orthorhombic primitive
hp	Hexagonal	*oS*	Orthorhombic single-face centred
		oI	Orthorhombic body-centred
		oF	Orthorhombic all faces centred
		tP	Tetragonal primitive
		tI	Tetragonal body-centred
		hP	Hexagonal primitive
		hR	Rhombohedral
		cP	Cubic primitive
		cI	Cubic body-centred
		cF	Cubic face-centred

Arithmetic classes

The *Ad-Hoc* Committee recommends that an *arithmetic class* be designated by the modified symbol of the symmorphic space group contained in that class. The modification consists of interchanging the lattice letter and the point-group symbol. For example, instead of $P\bar{6}2m$, write $\bar{6}2mP$ for the arithmetic class.

An arithmetic class is a class of space groups. Two space groups belong to the same arithmetic class if the following procedure leads to identical results for both:

(*a*) In the Hermann–Mauguin symbol replace screw axes by rotation axes and glide planes by mirror planes.

(*b*) Write the ensuing symbol in standard form, *e.g. Cmm*2 for *A*2*mm*.

The result is the (standard) symbol of a symmorphic space group. It follows that the arithmetic class can be represented by the type of symmorphic space groups that it contains.

The arithmetic class is a concept widely used in symmetry classification and in mathematical crystallography. The proposed code not only characterizes the class adequately, but is also recognizable as a code for just this purpose.*

For further discussion of arithmetic classes, see *International Tables for Crystallography* (1983).

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* The first use of this nomenclature was in an example cited by Laves (1966) as chairman of the IUCr Subcommittee on Structure Type Designation. All 14 symbols were published and extensively used by Pearson (1967).

* Note added in proof by the Chairman: The new symbol for classes with symmorphic group symbol *Pm* and *Cm* is identical (*mP*) or very similar (*mC*) to one of the new lattice type symbols given in the preceding section. In view of the context in which the symbols will be used, confusion is not expected to occur.

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Combining Direct Methods with Isomorphous Replacement or Anomalous Scattering Data. III. The Incorporation of Partial Structure Information

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Abstract

The probability formulas given in Parts I and II of this series have been improved by incorporating the information contained in Sim's distribution. Possible applications to the discrimination of the phase ambiguities arising from the single isomorphous replacement technique, the one-wavelength anomalous scattering (OAS) technique or pseudo centrosymmetry in small structures are discussed. With a set of experimental protein OAS data, the efficiency of the improved formula has been shown to be better than that of the older one.

Notation

$\mathbf{H}$ the reciprocal vector, which corresponds to the diffraction index *hkl*

$\mathbf{F}_\mathbf{H}$ the structure factor at the reciprocal-lattice point $\mathbf{H}$

$F_\mathbf{H}$ the modulus of $\mathbf{F}_\mathbf{H}$

$\varphi_\mathbf{H}$ the phase of $\mathbf{F}_\mathbf{H}$

$\mathbf{E}_\mathbf{H}$ the normalized structure factor

$E_\mathbf{H}$ the modulus of $\mathbf{E}_\mathbf{H}$

$\mathbf{F}_{\mathbf{H},A}$ the diffraction contribution calculated from the real-part scattering of the anomalous scatterers, *i.e.*

$$\mathbf{F}_{\mathbf{H},A}=\sum_{A=1}^{N_A}(f_A+\Delta f'_A)\exp[i2\pi\mathbf{H}\,.\,\mathbf{r}_A]$$

$\mathbf{F}''_{\mathbf{H},A}$ the diffraction contribution from the imaginary-part scattering of the anomalous scatterers, *i.e.*

$$\mathbf{F}''_{\mathbf{H},A}=\sum_{A=1}^{N_A} i\Delta f''_A\exp[i2\pi\mathbf{H}.\,\mathbf{r}_A]$$

$\sigma_n=$ $\sum_j Z_j^n$, Z_j is the atomic number of the jth atom in the unit cell, n is an integer equal to 2 or 3

$\sigma_u=$ $\sum_u Z_u^2/\sigma_2$, Z_u is the atomic number of the uth atom, which belongs to the unknown part of the structure

Subscripts:

A the anomalous scattering atoms

R the replacing atoms of an isomorphous pair

N the atoms in the native protein

D the atoms in the heavy-atom derivative of the native protein

p the atoms of the partial structure with known positions in the unit cell

u the atoms of the unknown part in the unit cell

Formulation

A phase doublet can be expressed in the generalized form

$$\varphi_\mathbf{H}=\varphi'_\mathbf{H}\pm|\Delta\varphi_\mathbf{H}|. \quad (1)$$

In the case of single isomorphous replacement (SIR):

$$\varphi'_\mathbf{H}=\varphi_{\mathbf{H},R},$$

where $\varphi_{\mathbf{H},R}$ is the phase calculated from the replacing atoms. If $\varphi_\mathbf{H}$ denotes the phase of a reflection from the native protein, then

$$\Delta\varphi_\mathbf{H}\equiv\Delta\varphi_{\mathbf{H},N}$$
$$=\pm\cos^{-1}[(F^2_{\mathbf{H},D}-F^2_{\mathbf{H},R}-F^2_{\mathbf{H},N})/2F_{\mathbf{H},R}F_{\mathbf{H},N}]. \quad (2)$$

If $\varphi_\mathbf{H}$ denotes that from the heavy-atom derivative, then

$$\Delta\varphi_\mathbf{H}\equiv\Delta\varphi_{\mathbf{H},D}$$
$$=\pm\cos^{-1}[(F^2_{\mathbf{H},D}+F^2_{\mathbf{H},R}-F^2_{\mathbf{H},N})/2F_{\mathbf{H},R}F_{\mathbf{H},D}]. \quad (3)$$

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