REMARKS ON CRYSTALLOGRAPHIC NOMENCLATURE

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Abstract

In special cases the lattice (not structure) of a crystal in any system may be indistinguishable from the lattice typical of any higher system. Thus it is formally better to define and name the systems on the basis of symmetry (as groups of classes); for this purpose a set of self-explanatory names and symbols is proposed.

With the great increase of interest in crystallography which has developed since the first world war and the enormous extension of the field beyond its former boundaries, there had been a movement to revise the nomenclature of the science, to clarify and extend it where necessary, and to devise notations suitable for international use. In the largest single department of crystallographic terminology which has come under consideration, namely that which refers to the symmetry groups required in structural crystallography, the need for a good notation has been well met by the system of Hermann-Mauguin. Made generally available in the original *International Tables* (1933) this system has been well tried and generally adopted, and we may expect to find any necessary refinements and corrections to the scheme in the new edition now in preparation.

Less attention has been paid to the nomenclature of morphological crystallography, and it cannot be said that there is a generally accepted terminology for crystal systems, crystal classes, and crystal forms which has the consistency and self-explanatory character of the international notation for point groups and space groups. Those interested mainly in structural crystallography have naturally not been much concerned with the nomenclature of morphology; on the other hand those who have been principally occupied with crystal form have been well aware of certain imperfections in the relevant terminology, which constantly crop up in teaching and research, but they have seemed reluctant to give up established terms and usages which have served their turn despite inherent illogic and inelegance. But for those who see modern crystallography as a logical development of the classical science, the need for some improvements in the nomenclature of the older subject is apparent to bring it in line with the excellent terminology of the newer branch. It is with this in mind that I venture some discussion and proposals regarding the definition and terminology of the crystal systems, crystal classes, and crystal forms.

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Crystal systems

The crystal systems are the broad divisions into which the working crystallographer using the classical methods (reflecting goniometer and polarising microscope) can always place a well-formed crystal. Frequently a morphological study is limited to the determination of the crystal system, the geometrical elements, and a description of the forms; in a structural study the crystal system and lattice dimensions are also first determined, but only as a first step towards finding the space group and the structure. Thus the classical systems have become groups of convenience and their definitions and names have been retained without much critical concern.

Historically, the orthogonal and hexagonal systems were recognized first, and the inclined systems were admitted later, with the suggestion that they are in some ways defective. Without exception the textbooks presented the systems in the historical order, cubic to triclinic; and I can well recall the twinge of sympathy I felt as a student for the triclinic crystal, shown like a scarecrow with axes all awry, bereft of all symmetry except a centre of inversion, and pictured by a wall-eyed stereogram in unhappy contrast to the full fat smiling visage of the cubic holohedry. This historical order of presenting the crystal system, from the most specialized to the most general, is the reverse of universal mathematical procedure, and it has caused much of the unsatisfactory terminology with which we are concerned.

The classical crystal systems, with some alternative names and the usual definitions in terms of lattice dimensions, are as follows:

Cubic (isometric): $a(= b = c)$; $(\alpha = \beta = \gamma = 90°)$.

Hexagonal: $a(= b) \neq c$; $(\alpha = \beta = 90°; \gamma = 120°)$.

Tetragonal (quadratic): $a(= b) \neq c$; $(\alpha = \beta = \gamma = 90°)$.

Orthorhombic (rhombic, rectangular): $a \neq b \neq c$; $(\alpha = \beta = \gamma = 90°)$.

Monoclinic (monosymmetric): $a \neq b \neq c$; $(\gamma = \alpha = 90°)$; $\beta > 90°$.

Triclinic (anorthic): $a \neq b \neq c$; $\alpha \neq \beta \neq \gamma \neq 90°$.

The usual definitions of the crystal systems rest on the metrical properties of the axes or lattice elements (lengths and angles) and, apart from the names hexagonal and tetragonal, which involve symmetry, the commonest system names express essential metrical properties. Thus, cubic (or isometric), monoclinic, and triclinic are entirely suitable names for metrical systems. Some name other than hexagonal would be useful to denote the metrical system based on the two modes of stacking hexagonal nets, but none suggests itself. Rhombohedral is not mentioned here since the rhombohedral lattice is merely a mode of the hexagonal lattice, from the purely metrical point of view. Quadratic is preferable to tetragonal as a metrical system name; and if rectangular could be accepted in place of orthorhombic, to avoid the now inappropriate allusion to the base-centred mode of the lattice, a fairly satisfactory nomenclature for the metrical systems would result. This would read: cubic (isometric and optically isotropic); hexagonal and quadratic (dimetric and optically uniaxial); rectangular, monoclinic, triclinic (trimetric and optically biaxial).

However, there have long been misgivings regarding the validity of the metrical systems. Metrical pseudosymmetry (near equality of typically unequal lattice lengths and near approach to 90° or 120° of typically non-rectangular or non-hexagonal lattice angles) is a commonplace, and practising crystallographers are all familiar with cases where such inequalities, if real, are within the limits of goniometric accuracy. Thus we may have a crystal whose form development is typically "monoclinic" while the angle β cannot be distinguished from 90° (datolite); or again a crystal whose structure and optics are hexagonal (rhombohedral), but with a lattice which is exactly "cubic" (shandite). To meet such examples the definitions of the metrical systems are sometimes qualified by the proviso that the typical relations must obtain at all temperatures within the stability range of the phase. At first glance this seems to safeguard the metrical definitions, at least theoretically; but apart from the practical difficulty of making exact measurements at high and low temperatures, the temperature qualification is not adequate in the inclined systems. With change of temperature the β angle of a monoclinic crystal might change from 91° to exactly a right angle; by the metrical definitions the crystal would belong neither to the monoclinic nor to the rectangular system.

The truth is that, despite the names and definitions of the metrical systems, enlightened observers have always assigned crystals to their systems on the basis of symmetry, particularly the highest symmetry common to all the observable properties of the crystal. Some recognition of this fact is seen in the names monosymmetric (for monoclinic), tetragonal, and hexagonal. Would it not be reasonable to recognize clearly that the crystal systems are actually symmetry systems, and to devise a practical nomenclature which expresses this fact?

This has been attempted in the following table which shows the proposed names and symbols for the symmetry systems in relation to the most widely accepted names for the symmetry classes and their Hermann-Mauguin symbols. Below the names of the symmetry systems are given the names of the normally corresponding lattices; these are identical with the metrical system names, except that the rhombohedral lattice is recognized as distinct from the hexagonal lattice. It is emphasized that in any symmetry system the metrical relations or lattice may in special cases be indistinguishable from those typical of any higher symmetry system. As implied in the table the symmetry systems are defined simply as groups of crystal classes which are also grouped as usual into the centrosymmetrical Laue symmetries. The new names are in line with the current names, trigonal, tetragonal, and hexagonal, and they are in keeping with the principles of the international notation for the crystal classes. The symbols for the symmetry systems are the appropriate numerals, written in parentheses to distinguish them from the similar class symbols. A word of explanation will suffice for each of the symmetry systems.

Monogonal (1) is proposed for the system which comprises the classes characterized by a 1-fold rotation axis (no symmetry) or a 1-fold rotation-inversion axis (centre of symmetry).

Digonal (2) describes the system which includes the classes with a single 2-fold rotation axis or a single 2-fold rotation-inversion axis (mirror plane).

Tri-digonal (222) refers to the system of classes with three non-equivalent 2-fold axes, two of which may be 2-fold rotation-inversion axes (mirror planes).

Trigonal (3) is already used for the system of classes with a single 3-fold rotation axis or a single 3-fold rotation-inversion axis, in which the lattice may be rhombohedral or hexagonal.

Tetragonal (4) is likewise used for the system of classes characterized by a single 4-fold rotation axis or 4-fold rotation-inversion axis.

Hexagonal (6) is also used in the restricted sense of the system of classes with a 6-fold rotation axis or a 6-fold rotation-inversion axis, in which the lattice is always hexagonal.

Tetra-trigonal 4(3) is finally the logical name for the system of classes which have four equivalent 3-fold rotation axes or 3-fold rotation-inversion axes.

Triclinic, monoclinic, orthorhombic (or rectangular), tetragonal (or quadratic), hexagonal, rhombohedral, and cubic are of course still suitable names for the simple lattices; and in developing crystal morphology from the lattice, it is convenient also to use these same names for lattice systems, which are identical with the metrical systems except for hexagonal and rhombohedral, which denote distinct lattice systems but only one metrical system. If, in formal treatment, it is then shown that

Symmetry Systems		Symmetry Classes	
Monogonal (Triclinic)	**(1)**	Pedial	1
		Pinakoidal	$\bar{1}$
Digonal (Monoclinic)	**(2)**	Domatic	m (= $\bar{2}$)
		Sphenoidal	2
		Rhombic prismatic	$2/m$
Tri-digonal (Rectangular)	**(222)**	Rhombic pyramidal	$mm2$ (= $\bar{2}\bar{2}2$)
		Rhombic disphenoidal	222
		Rhombic dipyramidal	$2/m\ 2/m\ 2/m$
Trigonal (Rhombohedral or hexagonal)	**(3)**	Trigonal pyramidal	3
		Rhombohedral	$\bar{3}$
		Ditrigonal pyramidal	$3m$
		Trigonal trapezohedral	32
		Ditrigonal scalenohedral	$\bar{3}\ 2/m$
Tetragonal (Quadratic)	**(4)**	Tetragonal disphenoidal	$\bar{4}$
		Tetragonal pyramidal	4
		Tetragonal dipyramidal	$4/m$
		Tetragonal scalenohedral	$\bar{4}2m$
		Ditetragonal pyramidal	$4mm$
		Tetragonal trapezohedral	422
		Ditetragonal dipyramidal	$4/m\ 2/m\ 2/m$
Hexagonal (Hexagonal)	**(6)**	Trigonal dipyramidal	$\bar{6}$
		Hexagonal pyramidal	6
		Hexagonal dipyramidal	$6/m$
		Ditrigonal dipyramidal	$\bar{6}m2$
		Dihexagonal pyramidal	$6mm$
		Hexagonal trapezohedral	622
		Dihexagonal dipyramidal	$6/m\ 2/m\ 2/m$
Tetra-trigonal (Cubic)	**4(3)**	Tetartoidal	23
		Diploidal	$2/m\ \bar{3}$
		Hextetrahedral	$\bar{4}3m$
		Gyroidal	432
		Hexoctahedral	$4/m\ \bar{3}\ 2/m$

the lattice systems or the metrical systems are better replaced by symmetry systems with suitable names, the desired clarification of the nomenclature for the crystal systems will have been achieved.

Crystal classes

These are mentioned here only as a preparation for the subsequent remarks on the naming of crystal forms. The structural crystallographer has little need for class names, since the determination of the point group is but a second step toward the determination of the space group, and he commonly uses the class symbol which often serves also in morphological crystallography. However the determination of the crystal class from external form may be the main objective of a morphological study and consequently a set of appropriate names is naturally desirable.

Only two distinctly different principles have been employed in naming the classes: (1) the principle of subdividing the systems into holohedral or holosymmetric classes and merohedral or merosymmetric classes; (2) the principle of naming the classes after their general forms. The second of these principles is now widely accepted as the most useful, since it directly recalls the morphological characteristics of the classes, and the names given in the table are also in general use. In adopting this nomenclature we must of course adhere to the definitions of the forms after which the classes are named. These definitions are well known and need not all be repeated here.

Crystal forms

Finally I venture to comment on some terms which are still widely used to describe certain forms in the trimetric systems, even though the usage is in sharp conflict with the formal nomenclature on which the class names are based. The form names involved in this conflicting usage are principally pinakoid, dome, prism, and pyramid. In the present day nomenclature these and other forms or types of forms are defined as geometrical figures without reference to their attitude in space. A pinakoid (πίναξ, a board) is a pair of equivalent parallel planes; a dome (*domus*, a house [roof]) is a pair of non-parallel planes symmetrical to a mirror plane; a prism is a closed set of equivalent planes parallel to a common axis; and a pyramid is a closed set of equivalent planes equally inclined to a common axis. In the older usage these same terms have somewhat different meanings and certain restrictions of attitude are implied. Thus pinakoid is restricted to the pairs of axial planes, $\{100\}$, $\{010\}$, $\{001\}$; dome is used for any form of the type $\{0kl\}$ or $\{h0l\}$; prism is used for any form of the type $\{hk0\}$ and prism zone means vertical zone; and pyramid is used for any form of the type $\{hkl\}$. In the orthorhombic system (the old system names are suitable here) this gives {100}, front- or macropinakoid (parallel to the conventionally longer horizontal axis; {010}, side- or brachypinakoid (parallel to the conventionally shorter horizontal axis); {001}, basal pinakoid; {0*kl*}, brachydome [rhombic prism]; {*h*0*l*}, macrodome [rhombic prism]; {*hk*0}, prism [vertical rhombic prism]; {*hkl*}, pyramid [rhombic dipyramid]. Even stronger divergence of meaning results when the older usage is adapted from the orthorhombic system to the more general monoclinic and triclinic systems. In the monoclinic the older nomenclature gives {100}, front- or orthopinakoid (parallel to the ortho-axis [010]); {010}, side- or clinopinakoid (parallel to the clino-axis [100]); {001}, basal pinakoid; {0*kl*}, clinodome [rhombic prism]; {*h*0*l*}, orthodome or hemi-orthodome [pinakoid]; {*hk*0}, prism [rhombic prism]; {*hkl*} pyramid or hemi-pyramid [rhombic prism]. In the triclinic the older nomenclature gets into still deeper trouble. Again {100}, {010}, {001}, are the only forms called pinakoids, although all forms in the holohedral class are pinakoids. {0*kl*} and {*h*0*l*} are called hemidomes, {*hk*0} are hemiprisms, and {*hkl*} would become tetarto-pyramids, if the scheme were carried through.

This discordant nomenclature has long been current in crystallographic laboratories and in descriptive morphological writing and it has been given a new lease of life in F. C. Phillips' *Crystallography* (1946), where it appears with careful apologies in a treatment which substantially accepts the modern nomenclature. Actually the older nomenclature cannot be reconciled with the newer system, nor can it be developed into a consistent scheme of form names and class names which could replace the present system. The undesirable usage can be avoided in two ways. One can describe crystal forms by their strict names followed by the appropriate indices {*hkl*} to show the attitude of the form, when desired. This is the simplest and probably the best solution. Another way would be to devise a consistent and self-explanatory scheme of qualifiers as prefixes or affixes to the strict form names to denote the attitude. Such a scheme would best be worked out in consultation with a number of experienced morphologists.

Acknowledgment. Probably none of the proposals made in the foregoing notes is wholly new in principle, but for the sake of brevity they are offered here, as they were written, with almost no reference to authorities. I wish, however, specifically to acknowledge the incentive to discuss the crystal systems which I received from a preliminary unpublished table of symmetry devised by C. D. West (Cambridge, Massachusetts). In this table Dr. West uses "monogonal" and "digonal" as system names, but with meanings different from those given in this paper.