1.4. Arithmetic crystal classes and symmorphic space groups

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1.4.1. Arithmetic crystal classes

Arithmetic crystal classes are of great importance in theoretical crystallography, and are treated from that point of view in Volume A of *International Tables for Crystallography* (Hahn, 1995, p. 719). They have, however, at least four applications in practical crystallography:

(1) in the classification of space groups (Section 1.4.2);

(2) in forming symbols for certain space groups in higher dimensions (see Chapter 9.8 and the references cited therein);

(3) in modelling the frequency of occurrence of space groups (see Chapter 9.7 and the references cited therein); and

(4) in establishing 'equivalent origins' (Wondratschek, 1995, p. 719).

The tabulation of arithmetic crystal classes in Volume A is incomplete, and the relation of the notation used in complete tabulations found elsewhere (for example, in Brown, Bülow, Neubüser, Wondratschek & Zassenhaus, 1978) to that of *International Tables* is not immediately obvious. Simple descriptions and complete enumerations of the arithmetic crystal classes in one, two and three dimensions are therefore given here.

1.4.1.1. *Arithmetic crystal classes in three dimensions*

The 32 geometric crystal classes and the 14 Bravais lattices are familiar in three-dimensional crystallography. The three-dimensional arithmetic crystal classes are easily derived in an elementary fashion by enumerating the compatible combinations of geometric crystal class and Bravais lattice; the symbol adopted by the International Union of Crystallography for an arithmetic crystal class is simply the juxtaposition of the symbol for the geometric crystal class and the symbol for the Bravais lattice (de Wolff *et al.*, 1985). For example, in the monoclinic system the geometric crystal classes are 2, m, and $2/m$, and the Bravais lattices are monoclinic P and monoclinic C. The six arithmetic crystal classes in the monoclinic system are thus $2P$, $2C$, mP, mC, $2/mP$, and $2/mC$. In certain cases (loosely, when the geometric crystal class and the Bravais lattice have unique directions that are not necessarily parallel), the crystal class and the lattice can be combined in two different orientations. The simplest example is the combination of the orthorhombic crystal class* mm with the end-centred lattice C. The intersection of the mirror planes of the crystal class defines one unique direction, the C centring of the lattice another. If these directions are placed parallel to one another, the arithmetic class $mm2C$ is obtained; if they are placed perpendicular to one another, a different arithmetic class† $2mmC$ is obtained. The other combinations exhibiting this phenomenon are lattice P with geometric classes 32, $3m$, $\bar{3}m$, $\bar{4}m$, and $\bar{6}m$. By consideration of all possible combinations of geometric class and lattice, one obtains the 73 arithmetic classes listed in Table 1.4.2.1.

* Here and in Chapter 9.7, it is convenient to use the 'short' symbols mm, 32, $3m$, $\bar{3}m$, $\bar{4}m$, and $\bar{6}m$ instead of $mm2$, 321, *etc.*, whenever it is desired to emphasize that no implication about orientation is intended.

† In the arithmetic crystal class $2mmC$, two conventions concerning the nomenclature of axes conflict. The first is that, if only one face of the Bravais lattice is centred, the c axis is chosen perpendicular to that face. The second is that, if there is one axis of symmetry uniquely different from any others, that axis is to be chosen as b in the monoclinic system and as c in the remaining systems. The second convention is usually regarded as the more important, and the 'standard setting' of $2mmC$ is $mm2A$. Both settings are listed in Table 1.4.2.1.

Table 1.4.1.1. *The two-dimensional arithmetic crystal classes*

	Crystal class			Space group	
		Arithmetic			
Crystal system	Geometric	Number	Symbol	Number	Symbol
Oblique	1	1	1*p*	1	*p*1
	2	2	2*p*	2	*p*2
Rectangular	*m*	3	*mp*	3	*pm*
				4	*pg*
		4	*mc*	5	*cm*
	2*mm*	5	2*mmp*	6	*p*2*mm*
				7	*p*2*mg*
				8	*p*2*gg*
		6	2*mmc*	9	*c*2*mm*
Square	4	7	4*p*	10	*p*4
	4*mm*	8	4*mmp*	11	*p*4*mm*
				12	*p*4*gm*
Hexagonal	3	9	3*p*	13	*p*3
	3*m*	10	3*m*1*p*	14	*p*3*m*1
		11	31*mp*	15	*p*31*m*
	6	12	6*p*	16	*p*6
	6*mm*	13	6*mmp*	17	*p*6*mm*

references