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Table 1.4.3.1. *Arithmetic crystal classes classified by the number of space groups that they contain*

Number of space groups in the class	Symbols of the arithmetic crystal classes					
1	1*P*	$\bar{1}P$				
	2*C*					
	222*F*					
	$\bar{4}P$	$\bar{4}I$				
	3*R*	$\bar{3}P$	$\bar{3}R$	32*R*		
	$\bar{6}P$					
	23*F*					
2	2*P*	*mP*	*mC*	2/*mC*		
	222*C*	222*I*	*mm*2*F*	*mmmF*		
	4*I*	4/*mI*	422*I*	$\bar{4}m2I$	$\bar{4}2mI$	
	3*P**	312*P**	321*P**	3*m*1*P*	31*mP*	3*mR*
	$\bar{3}1mP$	$\bar{3}m1P$	$\bar{3}mR$			
	6/*mP*	$\bar{6}m2P$	$\bar{6}2mP$			
	23*P*	23*I*	$m\bar{3}F$	$m\bar{3}I$	432*F*	432*I*
	$\bar{4}3mP$	$\bar{4}3mF$	$\bar{4}3mI$	$m\bar{3}mI$		
3	*mm*2*C*	*mm*2*I*				
	3*P*†	312*P*†	321*P*†			
	4*P**					
	$m\bar{3}P$	432*P**				
4	2/*mP*					
	222*P*	2*mmC*	(= *mm*2*A*)	*mmmI*		
	4*P*†	4/*mP*	4*mmI*	$\bar{4}2mP$	$\bar{4}m2P$	4/*mmmI*
	6*P**	622*P**	6*mmP*	6/*mmmP*		
	432*P*†	$m\bar{3}mP$	$m\bar{3}mF$			
6	*mmmC*					
	422*P**					
	6*P*†	622*P*†				
8	422*P*†	4*mmP*				
10	*mm*2*P*					
16	*mmmP*					
	4/*mmmP*					

* Enantiomorphs combined. † Enantiomorphs distinguished.

1.4.2. Classification of space groups

Arithmetic crystal classes may be used to classify space groups on a scale somewhat finer than that given by the geometric crystal classes. Space groups are members of the same arithmetic crystal class if they belong to the same geometric crystal class, have the same Bravais lattice, and (when relevant) have the same orientation of the lattice relative to the point group. Each one-dimensional arithmetic crystal class contains a single space group, symbolized by *p*1 and *pm*, respectively. Most two-dimensional arithmetic crystal classes contain only a single space group; only 2*mmp* has as many as three.

The space groups belonging to each geometric and arithmetic crystal class in two and three dimensions are indicated in Tables 1.4.1.1 and 1.4.2.1, and some statistics for the three-dimensional classes are given in Table 1.4.3.1. 12 three-dimensional classes contain only a single space group, whereas two contain 16 each. Certain arithmetic crystal classes (3*P*, 312*P*, 321*P*, 422*P*, 6*P*, 622*P*, 432*P*) contain enantiomorphous pairs of space groups, so that the number of members of these classes depends on whether the enantiomorphs are combined or distinguished. Such classes occur twice in Table 1.4.3.1, marked with $*$ or †, respectively.

The space groups in Table 1.4.2.1 are listed in the order of the arithmetic crystal class to which they belong. It will be noticed that arrangement according to the conventional space-group numbering would separate members of the same arithmetic crystal class in the geometric classes 2/*m*, 3*m*, 23, $m\bar{3}$, 432, and $\bar{4}3m$. This point is discussed in detail in Volume A of *International Tables*, p. 728. The symbols of five space groups [*C*2*me* (*Aem*2), *C*2*ce* (*Aea*2), *Cmce*, *Cmme*, *Ccce*] have been conformed to those recommended in the fourth, revised edition of Volume A of *International Tables*.

1.4.2.1. *Symmorphic space groups*

The 73 space groups known as 'symmorphic' are in one-to-one correspondence with the arithmetic crystal classes, and their standard 'short' symbols (Bertaut, 1995) are obtained by interchanging the order of the geometric crystal class and the Bravais cell in the symbol for the arithmetic space group. In fact, conventional crystallographic symbolism did not distinguish between arithmetic crystal classes and symmorphic space groups until recently (de Wolff *et al.*, 1985); the symbol of the symmorphic group was used also for the arithmetic class.

This relationship between the symbols, and the equivalent rule-of-thumb *symmorphic space groups are those whose standard (short) symbols do not contain glide planes or screw axes*, reveal nothing fundamental about the nature of symmorphism; they are simply a consequence of the conventions governing the construction of symbols in *International Tables for Crystallography*.*

Although the *standard* symbols of the symmorphic space groups do not contain screw axes or glide planes, this is a result of the manner in which the space-group symbols have been devised. Most symmorphic space groups do in fact contain screw axes and/or glide planes. This is immediately obvious for the symmorphic space groups based on centred cells; $C2$ contains equal numbers of diad rotation axes and diad screw axes, and Cm contains equal numbers of reflection planes and glide planes. This is recognized in the 'extended' space-group symbols (Bertaut, 1995), but these are clumsy and not commonly used; those for $C2$ and Cm are $C1^{2}_{2_1}1$ and $C1^{m}_{a}1$, respectively. In the more symmetric crystal systems, even symmorphic space groups with primitive cells contain screw axes and/or glide planes; $P422$ ($P42^{2}_{2_1}$) contains many diad screw axes and $P4/mmm$ ($P4/m2/m^{2/m}_{2_1/g}$) contains both screw axes and glide planes.

The balance of symmetry elements within the symmorphic space groups is discussed in more detail in Subsection 9.7.1.2.

* Three examples of informative definitions are:

1. The space group corresponding to the zero solution of the Frobenius congruences is called a symmorphic space group (Engel, 1986, p. 155).

2. A space group F is called *symmorphic* if one of its finite subgroups (and therefore an infinity of them) is of an order equal to the order of the point group R_r (Opechowski, 1986, p. 255).

3. A space group is called *symmorphic* if the coset representatives W_j can be chosen in such a way that they leave one common point fixed (Wondratschek, 1995, p. 717).

Even in context, these are pretty opaque.

1.4.3. Effect of dispersion on diffraction symmetry

In the absence of dispersion ('anomalous scattering'), the intensities of the reflections hkl and $\bar{h}\bar{k}\bar{l}$ are equal (Friedel's law), and statements about the symmetry of the weighted reciprocal lattice and quantities derived from it often rest on the tacit or explicit assumption of this law – the condition underlying it being forgotten. In particular, if dispersion is appreciable, the symmetry of the Patterson synthesis and the 'Laue' symmetry are altered.

1.4.3.1. *Symmetry of the Patterson function*

In Volume A of *International Tables*, the symmetry of the Patterson synthesis is derived in two stages. First, any glide planes and screw axes are replaced by mirror planes and the corresponding rotation axes, giving a symmorphic space group (Subsection 1.4.2.1). Second, a centre of symmetry is added. This second step involves the tacit assumption of Friedel's law, and should not be taken if any atomic scattering factors have appreciable imaginary components. In such cases, the symmetry of the Patterson synthesis will not be that of one of the 24 centrosymmetric symmorphic space groups, as given in Volume A, but will be that of the symmorphic space group belonging to the arithmetic crystal class to which the space group of the structure belongs. There are thus 73 possible Patterson symmetries.

An equivalent description of such symmetries, in terms of 73 of the 1651 dichromatic colour groups, has been given by Fischer & Knop (1987); see also Wilson (1993).

1.4.3.2. *'Laue' symmetry*

Similarly, the eleven conventional 'Laue' symmetries [*International Tables for Crystallography* (1995), Volume A, p. 40 and elsewhere] involve the explicit assumption of Friedel's law. If dispersion is appreciable, the 'Laue' symmetry may be that of any of the 32 point groups. The point group, in correct orientation, is obtained by dropping the Bravais-lattice symbol from the symbol of the arithmetic crystal class or of the Patterson symmetry.

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