

## 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  $32$ ,  $3m$ ,  $\bar{3}m$ ,  $4m$ , 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  $mm$ ,  $32$ ,  $3m$ ,  $\bar{3}m$ ,  $4m$ , 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 system | Crystal class |            |        | Space group |        |        |
|----------------|---------------|------------|--------|-------------|--------|--------|
|                | Geometric     | Arithmetic |        |             |        |        |
|                |               | Number     | Symbol | Number      | Symbol |        |
| Oblique        | 1             | 1          | $1p$   | 1           | $p1$   |        |
|                | 2             | 2          | $2p$   | 2           | $p2$   |        |
| Rectangular    | $m$           | 3          | $mp$   | 3           | $pm$   |        |
|                | $2mm$         | 4          | $mc$   | 4           | $pg$   |        |
|                |               | 5          | $2mmp$ | 5           | $cm$   |        |
|                |               | 6          | $2mmc$ | 6           | $p2mm$ |        |
|                |               |            |        | 7           | $p2mg$ |        |
| 8              | $p2gg$        |            |        |             |        |        |
| 9              | $c2mm$        |            |        |             |        |        |
| Square         | 4             | 7          | $4p$   | 10          | $p4$   |        |
|                | $4mm$         | 8          | $4mmp$ | 11          | $p4mm$ |        |
|                |               | 12         |        | 12          | $p4gm$ |        |
| Hexagonal      | 3             | 9          | $3p$   | 13          | $p3$   |        |
|                | $3m$          | 10         | $3m1p$ | 14          | $p3m1$ |        |
|                |               | 11         | $31mp$ | 15          | $p31m$ |        |
|                |               | 12         | $6p$   | 16          | $p6$   |        |
|                | 6             | $6mm$      | 13     | $6mmp$      | 17     | $p6mm$ |

# 1. CRYSTAL GEOMETRY AND SYMMETRY

## 1.4.1.2. Arithmetic crystal classes in one, two and higher dimensions

In one dimension, there are two geometric crystal classes, 1 and  $m$ , and a single Bravais lattice,  $\bar{1}$ . Two arithmetic crystal classes result,  $\bar{1}$  and  $m\bar{1}$ . In two dimensions, there are ten geometric crystal classes, and two Bravais lattices,  $p$  and  $c$ ; 13 arithmetic

crystal classes result. The two-dimensional geometric and arithmetic crystal classes are listed in Table 1.4.1.1.

The number of arithmetic crystal classes increases rapidly with increasing dimensionality; there are 710 (plus 70 enantiomorphs) in four dimensions (Brown, Bülow, Neubüser, Wondratschek & Zassenhaus, 1978), but those in dimensions higher than three are not needed in this volume.

Table 1.4.2.1. The three-dimensional space groups, arranged by arithmetic crystal class; in a few geometric crystal classes this differs somewhat from the conventional numerical order; see International Tables Volume A, p. 728

| Crystal system | Crystal class        |            |                      | Space group |              |
|----------------|----------------------|------------|----------------------|-------------|--------------|
|                | Geometric            | Arithmetic |                      | Number      | Symbol       |
|                |                      | Number     | Symbol               |             |              |
| Triclinic      | $\bar{1}$            | 1          | $\bar{1}P$           | 1           | $P\bar{1}$   |
|                |                      | 2          | $\bar{1}P$           | 2           | $P\bar{1}$   |
| Monoclinic     | 2                    | 3          | $2P$                 | 3           | $P2$         |
|                |                      | 4          | $2C$                 | 4           | $P2_1$       |
|                |                      | 5          | $mP$                 | 5           | $C2$         |
|                |                      | 6          | $mC$                 | 6           | $Pm$         |
|                | $m$                  | 7          |                      | 7           | $Pc$         |
|                |                      | 8          |                      | 8           | $Cm$         |
|                |                      | 9          |                      | 9           | $Cc$         |
|                |                      | 10         | $2/mP$               | 10          | $P2/m$       |
| $2/m$          | 11                   |            | 11                   | $P2_1/m$    |              |
|                | 13                   |            | 13                   | $P2/c$      |              |
|                | 14                   |            | 14                   | $P2_1/c$    |              |
|                | 12                   | $2/mC$     | 12                   | $C2/m$      |              |
| 15             |                      | 15         | $C2/c$               |             |              |
| Orthorhombic   | 222                  | 9          | $222P$               | 16          | $P222$       |
|                |                      |            |                      | 17          | $P222_1$     |
|                |                      |            |                      | 18          | $P2_12_12$   |
|                |                      | 10         | $222C$               | 19          | $P2_12_12_1$ |
|                |                      |            |                      | 20          | $C222_1$     |
|                |                      |            |                      | 21          | $C222$       |
|                |                      | 11         | $222F$               | 22          | $F222$       |
|                |                      |            |                      | 23          | $I222$       |
|                |                      |            |                      | 24          | $I2_12_12_1$ |
|                | $mm$                 | 13         | $mm2P$               | 25          | $Pmn2$       |
|                |                      |            |                      | 26          | $Pmc2_1$     |
|                |                      |            |                      | 27          | $Pcc2$       |
|                |                      |            |                      | 28          | $Pma2$       |
|                |                      |            |                      | 29          | $Pca2_1$     |
|                | 14                   | $mm2C$     | 30                   | $Pnc2$      |              |
|                |                      |            | 31                   | $Pmn2_1$    |              |
|                |                      |            | 32                   | $Pba2$      |              |
| 33             |                      |            | $Pna2_1$             |             |              |
| 34             |                      |            | $Pnn2$               |             |              |
| 35             |                      |            | $Cmm2$               |             |              |
| 36             |                      |            | $Cmc2_1$             |             |              |
| 37             |                      |            | $Ccc2$               |             |              |
| 15             | $2mmC$<br>( $Amm2$ ) | 38         | $C2mm$<br>( $Amm2$ ) |             |              |
|                |                      | 39         | $C2me$<br>( $Aem2$ ) |             |              |
|                |                      | 40         | $C2cm$<br>( $Ama2$ ) |             |              |
| 16             | $mm2F$               | 41         | $C2ce$<br>( $Aea2$ ) |             |              |
|                |                      | 42         | $Fmm2$               |             |              |
|                |                      | 43         | $Fdd2$               |             |              |
| 17             | $mm2I$               | 44         | $Imm2$               |             |              |
|                |                      | 45         | $Iba2$               |             |              |
|                |                      | 46         | $Ima2$               |             |              |

1.4. ARITHMETIC CRYSTAL CLASSES AND SYMMORPHIC SPACE GROUPS

Table 1.4.2.1. *Three-dimensional space groups (cont.)*

| Crystal system                   | Crystal class                  |                    | Space group                    |                                |                    |                         |                                     |                       |                    |    |                                |
|----------------------------------|--------------------------------|--------------------|--------------------------------|--------------------------------|--------------------|-------------------------|-------------------------------------|-----------------------|--------------------|----|--------------------------------|
|                                  | Geometric                      | Arithmetic         |                                | Number                         | Symbol             |                         |                                     |                       |                    |    |                                |
|                                  |                                | Number             | Symbol                         |                                |                    |                         |                                     |                       |                    |    |                                |
| Orthorhombic<br>( <i>cont.</i> ) | <i>mmm</i>                     | 18                 | <i>mmmP</i>                    | 47                             | <i>Pmmm</i>        |                         |                                     |                       |                    |    |                                |
|                                  |                                |                    |                                | 48                             | <i>Pnnn</i>        |                         |                                     |                       |                    |    |                                |
|                                  |                                |                    |                                | 49                             | <i>Pccm</i>        |                         |                                     |                       |                    |    |                                |
|                                  |                                |                    |                                | 50                             | <i>Pban</i>        |                         |                                     |                       |                    |    |                                |
|                                  |                                |                    |                                | 51                             | <i>Pmma</i>        |                         |                                     |                       |                    |    |                                |
|                                  |                                |                    |                                | 52                             | <i>Pnna</i>        |                         |                                     |                       |                    |    |                                |
|                                  |                                |                    |                                | 53                             | <i>Pmna</i>        |                         |                                     |                       |                    |    |                                |
|                                  |                                |                    |                                | 54                             | <i>Pcca</i>        |                         |                                     |                       |                    |    |                                |
|                                  |                                |                    |                                | 55                             | <i>Pbam</i>        |                         |                                     |                       |                    |    |                                |
|                                  |                                |                    |                                | 56                             | <i>Pccn</i>        |                         |                                     |                       |                    |    |                                |
|                                  |                                |                    |                                | 57                             | <i>Pbcm</i>        |                         |                                     |                       |                    |    |                                |
|                                  |                                |                    |                                | 58                             | <i>Pnnm</i>        |                         |                                     |                       |                    |    |                                |
|                                  |                                |                    |                                | 59                             | <i>Pmnm</i>        |                         |                                     |                       |                    |    |                                |
|                                  |                                |                    |                                | 60                             | <i>Pbcn</i>        |                         |                                     |                       |                    |    |                                |
|                                  |                                |                    |                                | 61                             | <i>Pbca</i>        |                         |                                     |                       |                    |    |                                |
|                                  |                                |                    |                                | 62                             | <i>Pnma</i>        |                         |                                     |                       |                    |    |                                |
|                                  |                                |                    |                                | 19                             | <i>mmmC</i>        | 63                      | <i>Cmcm</i>                         |                       |                    |    |                                |
|                                  |                                |                    |                                |                                |                    | 64                      | <i>Cmce</i>                         |                       |                    |    |                                |
|                                  | 65                             | <i>Cmmm</i>        |                                |                                |                    |                         |                                     |                       |                    |    |                                |
|                                  | 20                             | <i>mmmF</i>        | 66                             | <i>Cccm</i>                    |                    |                         |                                     |                       |                    |    |                                |
|                                  |                                |                    | 67                             | <i>Cmme</i>                    |                    |                         |                                     |                       |                    |    |                                |
| 21                               | <i>mmmI</i>                    | 68                 | <i>Ccce</i>                    |                                |                    |                         |                                     |                       |                    |    |                                |
|                                  |                                | 69                 | <i>Fmmm</i>                    |                                |                    |                         |                                     |                       |                    |    |                                |
| Tetragonal                       | 4                              | 22                 | <i>4P</i>                      | 70                             | <i>Fddd</i>        |                         |                                     |                       |                    |    |                                |
|                                  |                                |                    |                                | 71                             | <i>Immm</i>        |                         |                                     |                       |                    |    |                                |
|                                  |                                |                    |                                | 72                             | <i>Ibam</i>        |                         |                                     |                       |                    |    |                                |
|                                  |                                |                    |                                | 73                             | <i>Ibca</i>        |                         |                                     |                       |                    |    |                                |
|                                  |                                |                    |                                | 74                             | <i>Imma</i>        |                         |                                     |                       |                    |    |                                |
|                                  |                                |                    |                                | 4                              | 23                 | <i>4I</i>               | 75                                  | <i>P4</i>             |                    |    |                                |
|                                  |                                |                    |                                |                                |                    |                         | 76                                  | <i>P4<sub>1</sub></i> |                    |    |                                |
|                                  |                                |                    |                                |                                |                    |                         | 77                                  | <i>P4<sub>2</sub></i> |                    |    |                                |
|                                  |                                |                    |                                |                                |                    |                         | 78                                  | <i>P4<sub>3</sub></i> |                    |    |                                |
|                                  |                                |                    |                                |                                |                    |                         | 79                                  | <i>I4</i>             |                    |    |                                |
|                                  |                                |                    |                                |                                |                    |                         | 80                                  | <i>I4<sub>1</sub></i> |                    |    |                                |
|                                  |                                |                    |                                |                                |                    |                         | 24                                  | <i>4̄</i>             | <i>4̄P</i>         | 81 | <i>P4</i>                      |
|                                  |                                |                    |                                |                                |                    |                         |                                     |                       |                    | 82 | <i>I4</i>                      |
|                                  |                                |                    |                                |                                |                    |                         | 4/ <i>m</i>                         | 26                    | <i>4/<i>mP</i></i> | 83 | <i>P4/<i>m</i></i>             |
|                                  |                                |                    |                                |                                |                    |                         |                                     |                       |                    | 84 | <i>P4<sub>2</sub>/<i>m</i></i> |
| 85                               | <i>P4/<i>n</i></i>             |                    |                                |                                |                    |                         |                                     |                       |                    |    |                                |
| 86                               | <i>P4<sub>2</sub>/<i>n</i></i> |                    |                                |                                |                    |                         |                                     |                       |                    |    |                                |
| 422                              | 27                             | <i>4/<i>mI</i></i> | 87                             | <i>I4/<i>m</i></i>             |                    |                         |                                     |                       |                    |    |                                |
|                                  |                                |                    | 88                             | <i>I4<sub>1</sub>/<i>a</i></i> |                    |                         |                                     |                       |                    |    |                                |
|                                  |                                |                    | 28                             | <i>422P</i>                    | 89                 | <i>P422</i>             |                                     |                       |                    |    |                                |
|                                  |                                |                    |                                |                                | 90                 | <i>P42<sub>1</sub>2</i> |                                     |                       |                    |    |                                |
|                                  |                                |                    | 4 <i>mm</i>                    | 30                             | <i>4<i>mmP</i></i> | 91                      | <i>P4<sub>1</sub>22</i>             |                       |                    |    |                                |
|                                  |                                |                    |                                |                                |                    | 92                      | <i>P4<sub>1</sub>2<sub>1</sub>2</i> |                       |                    |    |                                |
|                                  |                                |                    |                                |                                |                    | 93                      | <i>P4<sub>2</sub>22</i>             |                       |                    |    |                                |
|                                  |                                |                    |                                |                                |                    | 94                      | <i>P4<sub>2</sub>2<sub>1</sub>2</i> |                       |                    |    |                                |
|                                  |                                |                    |                                |                                |                    | 95                      | <i>P4<sub>3</sub>22</i>             |                       |                    |    |                                |
|                                  |                                |                    |                                |                                |                    | 96                      | <i>P4<sub>3</sub>2<sub>1</sub>2</i> |                       |                    |    |                                |
| 97                               | <i>I422</i>                    |                    |                                |                                |                    |                         |                                     |                       |                    |    |                                |
| 98                               | <i>I4<sub>1</sub>22</i>        |                    |                                |                                |                    |                         |                                     |                       |                    |    |                                |
| 31                               | <i>4<i>mmI</i></i>             | 99                 | <i>P4<i>mm</i></i>             |                                |                    |                         |                                     |                       |                    |    |                                |
|                                  |                                | 100                | <i>P4<i>bm</i></i>             |                                |                    |                         |                                     |                       |                    |    |                                |
|                                  |                                | 101                | <i>P4<sub>2</sub><i>cm</i></i> |                                |                    |                         |                                     |                       |                    |    |                                |
| 4 <i>mmI</i>                     | 31                             | <i>4<i>mmI</i></i> | 102                            | <i>P4<sub>2</sub><i>nm</i></i> |                    |                         |                                     |                       |                    |    |                                |
|                                  |                                |                    | 103                            | <i>P4<i>cc</i></i>             |                    |                         |                                     |                       |                    |    |                                |
|                                  |                                |                    | 104                            | <i>P4<i>nc</i></i>             |                    |                         |                                     |                       |                    |    |                                |
|                                  |                                |                    | 105                            | <i>P4<sub>2</sub><i>mc</i></i> |                    |                         |                                     |                       |                    |    |                                |
|                                  |                                |                    | 106                            | <i>P4<sub>2</sub><i>bc</i></i> |                    |                         |                                     |                       |                    |    |                                |
|                                  |                                |                    | 107                            | <i>I4<i>mm</i></i>             |                    |                         |                                     |                       |                    |    |                                |
|                                  |                                |                    | 108                            | <i>I4<i>cm</i></i>             |                    |                         |                                     |                       |                    |    |                                |
|                                  |                                |                    | 109                            | <i>I4<sub>1</sub><i>md</i></i> |                    |                         |                                     |                       |                    |    |                                |
|                                  |                                |                    | 110                            | <i>I4<sub>1</sub><i>cd</i></i> |                    |                         |                                     |                       |                    |    |                                |

1. CRYSTAL GEOMETRY AND SYMMETRY

Table 1.4.2.1. *Three-dimensional space groups (cont.)*

| Crystal system        | Crystal class |              |              | Space group  |                |            |
|-----------------------|---------------|--------------|--------------|--------------|----------------|------------|
|                       | Geometric     | Arithmetic   |              |              |                |            |
|                       |               | Number       | Symbol       | Number       | Symbol         |            |
| Tetragonal<br>(cont.) | $\bar{4}m$    | 32           | $\bar{4}2mP$ | 111          | $P\bar{4}2m$   |            |
|                       |               |              |              | 112          | $P\bar{4}2c$   |            |
|                       |               |              |              | 113          | $P\bar{4}2_1m$ |            |
|                       |               |              |              | 114          | $P\bar{4}2_1c$ |            |
|                       |               | 33           | $\bar{4}m2P$ | 115          | $P\bar{4}m2$   |            |
|                       |               |              |              | 116          | $P\bar{4}c2$   |            |
|                       |               |              |              | 117          | $P\bar{4}b2$   |            |
|                       |               |              |              | 118          | $P\bar{4}n2$   |            |
|                       |               |              |              | 119          | $I\bar{4}m2$   |            |
|                       |               |              |              | 120          | $I\bar{4}c2$   |            |
|                       | 34            | $\bar{4}m2I$ | 121          | $I\bar{4}2m$ |                |            |
|                       |               |              | 122          | $I\bar{4}2d$ |                |            |
|                       | $4/mmm$       | 36           | $4/mmmP$     | 123          | $P4/mmm$       |            |
|                       |               |              |              | 124          | $P4/mcc$       |            |
|                       |               |              |              | 125          | $P4/nbm$       |            |
|                       |               |              |              | 126          | $P4/nnc$       |            |
|                       |               |              |              | 127          | $P4/mbm$       |            |
|                       |               |              |              | 128          | $P4/mnc$       |            |
|                       |               |              |              | 129          | $P4/nmm$       |            |
|                       |               |              |              | 130          | $P4/ncc$       |            |
| 131                   |               |              |              | $P4_2/mmc$   |                |            |
| 132                   |               |              |              | $P4_2/mcm$   |                |            |
| 37                    | $4/mmmI$      |              | 133          | $P4_2/nbc$   |                |            |
|                       |               |              | 134          | $P4_2/nnm$   |                |            |
|                       |               |              | 135          | $P4_2/mbc$   |                |            |
|                       |               |              | 136          | $P4_2/mmm$   |                |            |
|                       |               |              | 137          | $P4_2/nmc$   |                |            |
|                       |               |              | 138          | $P4_2/ncm$   |                |            |
|                       |               |              | 139          | $I4/mmm$     |                |            |
|                       |               |              | 140          | $I4/mcm$     |                |            |
|                       |               |              | 141          | $I4_1/amd$   |                |            |
|                       |               |              | 142          | $I4_1/acd$   |                |            |
| Trigonal              | 3             | 38           | $3P$         | 143          | $P3$           |            |
|                       |               |              |              | 144          | $P3_1$         |            |
|                       |               |              |              | 145          | $P3_2$         |            |
|                       | $\bar{3}$     | 39           | $3R$         | $\bar{3}P$   | 146            | $R\bar{3}$ |
|                       |               |              |              |              | 147            | $P\bar{3}$ |
|                       |               |              |              |              | 148            | $R\bar{3}$ |
|                       |               |              |              |              | 149            | $P312$     |
|                       |               |              |              |              | 151            | $P3_112$   |
|                       | 32            | 42           | $312P$       |              | 153            | $P3_212$   |
|                       |               |              |              |              | 150            | $P321$     |
|                       |               |              |              |              | 152            | $P3_121$   |
|                       |               |              |              |              | 154            | $P3_221$   |
|                       |               |              |              |              | 155            | $R32$      |
|                       |               |              |              |              | 156            | $P3m1$     |
|                       |               |              |              |              | 158            | $P3c1$     |
|                       | 3m            | 45           | $3m1P$       |              | 157            | $P31m$     |
|                       |               |              |              |              | 159            | $P31c$     |
| 160                   |               |              |              |              | $R3m$          |            |
| 161                   |               |              |              |              | $R\bar{3}c$    |            |
| 162                   |               |              |              |              | $P\bar{3}1m$   |            |
| $\bar{3}m$            | 48            | $\bar{3}1mP$ |              | 163          | $P\bar{3}1c$   |            |
|                       |               |              |              | 164          | $P\bar{3}m1$   |            |
|                       |               |              |              | 165          | $P\bar{3}c1$   |            |
|                       |               |              |              | 166          | $R\bar{3}m$    |            |
|                       |               |              |              | 167          | $R\bar{3}c$    |            |

1.4. ARITHMETIC CRYSTAL CLASSES AND SYMMORPHIC SPACE GROUPS

Table 1.4.2.1. *Three-dimensional space groups (cont.)*

| Crystal system | Crystal class  |  |  | Space group |               |
|----------------|--|--|--|-------------|---------------|
|                | Geometric  | Arithmetic   |  | Number      | Symbol        |
|                |  | Number   | Symbol   |             |               |
| Hexagonal      | 6<br><br>$\bar{6}$<br>$6/m$<br><br>622<br><br>$6mm$<br><br>$\bar{6}m$<br><br>$6/mmm$ | 51<br><br>52<br>53<br><br>54<br><br>55<br><br>56<br>57<br>58   | $6P$<br><br>$\bar{6}P$<br>$6/mP$<br><br>$622P$<br><br>$6mmP$<br><br>$\bar{6}m2P$<br>$\bar{6}2mP$<br>$6/mmmP$   | 168         | $P6$          |
|                |  |  |  | 169         | $P6_1$        |
|                |  |  |  | 170         | $P6_5$        |
|                |  |  |  | 171         | $P6_2$        |
|                |  |  |  | 172         | $P6_4$        |
|                |  |  |  | 173         | $P6_3$        |
|                |  |  |  | 174         | $P6$          |
|                |  |  |  | 175         | $P6/m$        |
|                |  |  |  | 176         | $P6_3/m$      |
|                |  |  |  | 177         | $P622$        |
|                |  |  |  | 178         | $P6_122$      |
|                |  |  |  | 179         | $P6_522$      |
|                |  |  |  | 180         | $P6_222$      |
|                |  |  |  | 181         | $P6_422$      |
|                |  |  |  | 182         | $P6_322$      |
|                |  |  |  | 183         | $P6mm$        |
|                |  |  |  | 184         | $P6cc$        |
|                |  |  |  | 185         | $P6_3cm$      |
|                |  |  |  | 186         | $P6_3mc$      |
| 187            | $P6m2$   |  |  |             |               |
| 188            | $P\bar{6}c2$   |  |  |             |               |
| 189            | $P\bar{6}2m$   |  |  |             |               |
| 190            | $P62c$   |  |  |             |               |
| 191            | $P6/mmm$   |  |  |             |               |
| 192            | $P6/mmc$   |  |  |             |               |
| 193            | $P6_3/mcm$   |  |  |             |               |
| 194            | $P6_3/mmc$   |  |  |             |               |
| Cubic          | 23<br><br>$m\bar{3}$<br><br>432<br><br>$\bar{4}3m$<br><br>$m\bar{3}m$                | 59<br><br>60<br>61<br>62<br><br>63<br>64<br>65<br><br>66<br>67<br>68<br>69<br>70<br>71<br><br>72<br><br>73 | $23P$<br><br>$23F$<br>$23I$<br>$m\bar{3}P$<br><br>$m\bar{3}F$<br>$m\bar{3}I$<br>$432P$<br><br>$432F$<br>$432I$<br>$\bar{4}3mP$<br>$\bar{4}3mF$<br>$\bar{4}3mI$<br>$m\bar{3}mP$<br><br>$m\bar{3}mF$<br><br>$m\bar{3}mI$ | 195         | $P23$         |
|                |  |  |  | 198         | $P2_13$       |
|                |  |  |  | 196         | $F23$         |
|                |  |  |  | 197         | $I23$         |
|                |  |  |  | 199         | $I2_1\bar{3}$ |
|                |  |  |  | 200         | $Pm\bar{3}$   |
|                |  |  |  | 201         | $Pn\bar{3}$   |
|                |  |  |  | 205         | $Pa\bar{3}$   |
|                |  |  |  | 202         | $Fm\bar{3}$   |
|                |  |  |  | 203         | $Fd\bar{3}$   |
|                |  |  |  | 204         | $Im\bar{3}$   |
|                |  |  |  | 206         | $Ia\bar{3}$   |
|                |  |  |  | 207         | $P432$        |
|                |  |  |  | 208         | $P4_232$      |
|                |  |  |  | 213         | $P4_132$      |
|                |  |  |  | 212         | $P4_332$      |
|                |  |  |  | 209         | $F432$        |
|                |  |  |  | 210         | $F4_132$      |
|                |  |  |  | 211         | $I432$        |
|                |  |  |  | 214         | $I4_132$      |
|                |  |  |  | 215         | $P43m$        |
|                |  |  |  | 218         | $P43n$        |
|                |  |  |  | 216         | $F43m$        |
| 219            | $F43c$   |  |  |             |               |
| 217            | $I43m$   |  |  |             |               |
| 220            | $I43d$   |  |  |             |               |
| 221            | $Pm\bar{3}m$   |  |  |             |               |
| 222            | $Pn\bar{3}n$   |  |  |             |               |
| 223            | $Pm\bar{3}n$   |  |  |             |               |
| 224            | $Pn\bar{3}m$   |  |  |             |               |
| 225            | $Fm\bar{3}m$   |  |  |             |               |
| 226            | $Fm\bar{3}c$   |  |  |             |               |
| 227            | $Fd\bar{3}m$   |  |  |             |               |
| 228            | $Fd\bar{3}c$   |  |  |             |               |
| 229            | $Im\bar{3}m$   |  |  |             |               |
| 230            | $Ia\bar{3}d$   |  |  |             |               |

# 1. CRYSTAL GEOMETRY AND SYMMETRY

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                                   | $1P$<br>$2C$<br>$222F$<br>$4P$<br>$3R$<br>$\bar{6}P$<br>$23F$                 | $\bar{1}P$<br><br>$\bar{4}I$<br>$\bar{3}P$  | $\bar{3}R$   | $32R$   |                                      |                         |
| 2                                   | $2P$<br>$222C$<br>$4I$<br>$3P^*$<br>$\bar{3}1mP$<br>$6/mP$<br>$23P$<br>$43mP$ | $mP$<br>$222I$<br>$4/mI$<br>$312P^*$<br>$\bar{3}m1P$<br>$\bar{6}m2P$<br>$23I$<br>$43mF$ | $mC$<br>$mm2F$<br>$422I$<br>$321P^*$<br>$\bar{3}mR$<br>$\bar{6}2mP$<br>$m\bar{3}F$<br>$\bar{4}3mI$ | $2/mC$<br>$mmmF$<br>$4m2I$<br>$3m1P$<br><br>$m\bar{3}I$<br>$m\bar{3}mI$ | $\bar{4}2mI$<br>$31mP$<br><br>$432F$ | $3mR$<br><br><br>$432I$ |
| 3                                   | $mm2C$<br>$3P^\dagger$<br>$4P^*$<br>$m\bar{3}P$                               | $mm2I$<br>$312P^\dagger$<br><br>$432P^*$  | $321P^\dagger$   |   |                                      |                         |
| 4                                   | $2/mP$<br>$222P$<br>$4P^\dagger$<br>$6P^*$<br>$432P^\dagger$                  | $2mmC$<br>$4/mP$<br>$622P^*$<br>$m\bar{3}mP$  | $(= mm2A)$<br>$4mmI$<br>$6mmP$<br>$m\bar{3}mF$   | $mmmI$<br>$42mP$<br>$6/mmmP$  | $\bar{4}m2P$                         | $4/mmmI$                |
| 6                                   | $mmmC$<br>$422P^*$<br>$6P^\dagger$  | $622P^\dagger$  |  |   |                                      |                         |
| 8                                   | $422P^\dagger$  | $4mmP$  |  |   |                                      |                         |
| 10                                  | $mm2P$  |   |  |   |                                      |                         |
| 16                                  | $mmmP$<br>$4/mmmP$  |   |  |   |                                      |                         |

\* 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  $\not{1}$  and  $\not{m}$ , respectively. Most two-dimensional arithmetic crystal classes contain only a single space group; only  $2mmp$  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 ( $3P$ ,  $312P$ ,  $321P$ ,  $422P$ ,  $6P$ ,  $622P$ ,  $432P$ ) 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  $2/m$ ,  $3m$ ,  $23$ ,  $m\bar{3}$ ,  $432$ , and  $43m$ . This point is discussed in detail in Volume A of *International Tables*, p. 728. The symbols of five space groups [ $C2me$  ( $Aem2$ ),  $C2ce$  ( $Aea2$ ),  $Cmce$ ,  $Cmme$ ,  $Ccce$ ] have been conformed to those recommended in the fourth, revised edition of Volume A of *International Tables*.

## 1.4. ARITHMETIC CRYSTAL CLASSES AND SYMMORPHIC SPACE GROUPS

### 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 symmorphisms; 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  $C1_{21}^2 1$  and  $C1_a^m 1$ , respectively. In the more symmetric crystal systems, even symmorphic space groups with primitive cells contain screw axes and/or glide planes;  $P422$  ( $P42_2^2$ ) contains many diad screw axes and  $P4/mmm$  ( $P4/m2/m2_1^2/m2_1/g$ ) contains both screw axes and glide planes.

\*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.

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

### 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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