### 3. DETERMINATION OF SPACE GROUPS

Table 3.1.4.1. *Reflection conditions, diffraction symbols and possible space groups*

#### TRICLINIC. Laue class 1

<table>
<thead>
<tr>
<th>Reflection conditions</th>
<th>Extinction symbol</th>
<th>Point group</th>
</tr>
</thead>
<tbody>
<tr>
<td>None</td>
<td>$P-$</td>
<td>$P1(1)$</td>
</tr>
</tbody>
</table>

**MONOCLINIC, Laue class 2/m**

<table>
<thead>
<tr>
<th>Unique axis $b$</th>
<th>Reflection conditions</th>
<th>Laue class 1 2/m 1</th>
<th>Extinction symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>$hk0$</td>
<td>$hkl$</td>
<td>$00l$</td>
<td>$0k0$</td>
</tr>
<tr>
<td>$hk0$</td>
<td>$00l$</td>
<td>$0k0$</td>
<td>$0k0$</td>
</tr>
</tbody>
</table>

| $h + k$          | $h$                  | $k$               | $P1$             | $P11$ (3)     | $P1m1$ (6)   | $P1$ (2/m 1 (10) |
| $h + k$          | $h$                  | $k$               | $P11$            | $P11$ (3)     | $P1m1$ (6)   | $P1$ (2/m 1 (10) |
| $h + k$          | $l$                  | $k$               | $P11$            | $P11$ (3)     | $P1m1$ (6)   | $P1$ (2/m 1 (10) |
| $h + k$          | $h$                  | $l$               | $P11$            | $P11$ (3)     | $P1m1$ (6)   | $P1$ (2/m 1 (10) |
| $h + k$          | $l$                  | $h$               | $P11$            | $P11$ (3)     | $P1m1$ (6)   | $P1$ (2/m 1 (10) |

**Unique axis $c$**

<table>
<thead>
<tr>
<th>Reflection conditions</th>
<th>Laue class 1 2/m</th>
<th>Extinction symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>$hk0$</td>
<td>$hk0$</td>
<td>$0k0$</td>
</tr>
</tbody>
</table>

| $h + k$          | $h$               | $k$              | $P11$            | $P11$ (3)     | $P1m1$ (6)   | $P1$ (2/m 1 (10) |
| $h + k$          | $h$               | $l$              | $P11$            | $P11$ (3)     | $P1m1$ (6)   | $P1$ (2/m 1 (10) |
| $h + k$          | $l$               | $k$              | $P11$            | $P11$ (3)     | $P1m1$ (6)   | $P1$ (2/m 1 (10) |
| $h + k$          | $h$               | $k$              | $P11$            | $P11$ (3)     | $P1m1$ (6)   | $P1$ (2/m 1 (10) |

### 3.1.5. Diffraction symbols and possible space groups

Table 3.1.4.1 contains 219 extinction symbols which, when combined with the Laue classes, lead to 242 different diffraction symbols. If, however, for the monoclinic and orthorhombic systems specified conditions. For further discussions and references, see Perez-Mato & Iglesias (1977).
## 3.1. SPACE-GROUP DETERMINATION AND DIFFRACTION SYMBOLS

### Table 3.1.4.1. Reflection conditions, diffraction symbols and possible space groups (cont.)

**ORTHORHOMBIC, Laue class 2/m (cont.)**

<table>
<thead>
<tr>
<th>Reflection conditions</th>
<th>Extinction symbol</th>
<th>2</th>
<th>m</th>
<th>2/m</th>
</tr>
</thead>
<tbody>
<tr>
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<td>$hk0$</td>
<td>$00l$</td>
<td>$h00$</td>
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<tr>
<td>$hkl$</td>
<td>$0kl$</td>
<td>$hk0$</td>
<td>$00l$</td>
<td>$h00$</td>
</tr>
<tr>
<td>$h+k$</td>
<td>$k$</td>
<td>$h$</td>
<td>$P_{--}$</td>
<td>$P_{21nm}$ (31)</td>
</tr>
<tr>
<td>$h+k$</td>
<td>$k$</td>
<td>$l$</td>
<td>$P_{--}$</td>
<td>$P_{21nm}$ (31)</td>
</tr>
<tr>
<td>$h+k$</td>
<td>$l$</td>
<td>$h$</td>
<td>$P_{--}$</td>
<td>$P_{21nm}$ (31)</td>
</tr>
<tr>
<td>$h+k$</td>
<td>$k$</td>
<td>$k$</td>
<td>$P_{--}$</td>
<td>$P_{21nm}$ (31)</td>
</tr>
<tr>
<td>$h+k$</td>
<td>$k$</td>
<td>$l$</td>
<td>$P_{--}$</td>
<td>$P_{21nm}$ (31)</td>
</tr>
<tr>
<td>$h+k$</td>
<td>$l$</td>
<td>$h$</td>
<td>$P_{--}$</td>
<td>$P_{21nm}$ (31)</td>
</tr>
</tbody>
</table>

**MONOCLINIC, Laue class 2/m 1 1**

<table>
<thead>
<tr>
<th>Reflection conditions</th>
<th>Laue class 2/m 1 1</th>
</tr>
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<tbody>
<tr>
<td>$hkl$</td>
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<tr>
<td>$h0l$</td>
<td>$hkl$</td>
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<tr>
<td>$k0l$</td>
<td>$khl$</td>
</tr>
<tr>
<td>$0kl$</td>
<td>$0kl$</td>
</tr>
</tbody>
</table>

In this table, the symbol $e$ in the space-group symbol represents the two glide planes given between parentheses in the corresponding extinction symbol. Only for one of the two cases does a bold printed symbol correspond with the standard symbol.

### Reflection conditions

<table>
<thead>
<tr>
<th>Reflection conditions</th>
<th>Extinction symbol</th>
<th>Point group</th>
</tr>
</thead>
<tbody>
<tr>
<td>$hkl$</td>
<td>$0kl$</td>
<td>$hk0$</td>
</tr>
<tr>
<td>$h+k$</td>
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<td>$h+k$</td>
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<td>$k$</td>
<td>$l$</td>
</tr>
<tr>
<td>$h+k$</td>
<td>$l$</td>
<td>$h$</td>
</tr>
</tbody>
</table>

**ORTHORHOMBIC, Laue class mmm (2/m 2/m 2/m)**

<table>
<thead>
<tr>
<th>Reflection conditions</th>
<th>Extinction symbol</th>
<th>Point group</th>
</tr>
</thead>
<tbody>
<tr>
<td>$hkl$</td>
<td>$0kl$</td>
<td>$hk0$</td>
</tr>
<tr>
<td>$h+k$</td>
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<td>$h+k$</td>
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<td>$k$</td>
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<td>$h+k$</td>
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<td>$l$</td>
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<tr>
<td>$h+k$</td>
<td>$l$</td>
<td>$h$</td>
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</table>

In this table, the symbol $e$ in the space-group symbol represents the two glide planes given between parentheses in the corresponding extinction symbol. Only for one of the two cases does a bold printed symbol correspond with the standard symbol.
### 3. Determination of Space Groups

**Table 3.1.4.1. Reflection conditions, diffraction symbols and possible space groups (cont.)**

ORTHORHOMBIC, Laue class mmm (2/m 2/m 2/m) (cont.)

<table>
<thead>
<tr>
<th>Reflection conditions</th>
<th>Laue class mmm (2/m 2/m 2/m)</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>Point group</td>
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<tr>
<td></td>
<td>mm2</td>
</tr>
<tr>
<td></td>
<td>m2m</td>
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<tr>
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<td>mmm</td>
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<tr>
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<td>222</td>
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<td><strong>hk0</strong></td>
<td><strong>0kl</strong></td>
</tr>
<tr>
<td>hkl</td>
<td>0kl</td>
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<td>h + l</td>
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<td>k + l</td>
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</table>
### 3.1. SPACE-GROUP DETERMINATION AND DIFFRACTION SYMBOLS

#### Table 3.1.4.1. Reflection conditions, diffraction symbols and possible space groups (cont.)

<table>
<thead>
<tr>
<th>Reflection conditions</th>
<th>Laue class mmm (2/m 2/m 2/m) (cont.)</th>
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<tbody>
<tr>
<td>hkl</td>
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<td>k+l</td>
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<td>h+l</td>
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<tr>
<td>h+k+l</td>
<td>h+k+l</td>
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### 3. DETERMINATION OF SPACE GROUPS

#### 3.1.4.1. Reflection conditions, diffraction symbols and possible space groups (cont.)

**ORTHORHOMBIC**, Laue class mmm (2/m 2/m 2/m) (cont.)

<table>
<thead>
<tr>
<th>Reflection conditions</th>
<th>Laue class mmm (2/m 2/m 2/m)</th>
<th>Point group</th>
</tr>
</thead>
<tbody>
<tr>
<td>hkl</td>
<td>0kl</td>
<td></td>
</tr>
<tr>
<td></td>
<td>h0l</td>
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</tr>
<tr>
<td></td>
<td>hkl</td>
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</tr>
<tr>
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</tr>
<tr>
<td></td>
<td>0k0</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0l0</td>
<td></td>
</tr>
</tbody>
</table>

**Reflection conditions**

- **h + k + l**
  - k + l
  - h + l
  - h, k
  - h, k
  - l = -(ab)
  - Imma (74)
  - Imma (74)
  - Imma (74)
  - Imma (74)

- **h + k + l**
  - k + l
  - h, l
  - h, k
  - h, k
  - l = -(ac)-
  - I22m (46)
  - I2c (46)
  - I2c (46)
  - I2c (46)

- **h + k + l**
  - k + l
  - h, l
  - h, k
  - h, k
  - l = cb
  - I2/c (45)
  - I2/c (45)
  - I2/c (45)
  - I2/c (45)

- **h + k + l**
  - k, l
  - h + l
  - h + k
  - h + k
  - Ibc
  - Iba (72)
  - Iba (72)
  - Iba (72)
  - Iba (72)

- **h + k, h + l, k + l**
  - k, l
  - h, l
  - h, k
  - h, k
  - F = --
  - Fmm2 (22)
  - Fmmm (69)
  - Fmmm (69)
  - Fmmm (69)

* Pair of space groups with common point group and symmetry elements but differing in the relative location of these elements.

**TETRAGONAL**, Laue classes 4/m and 4/mmm

<table>
<thead>
<tr>
<th>Reflection conditions</th>
<th>Laue class 4/m (4/m 2/m 2/m)</th>
<th>4/mmm (4/m/m 2/m/m 2/m/m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>hkl</td>
<td>4/m</td>
<td>4/mmm (4/m/m 2/m/m 2/m/m)</td>
</tr>
<tr>
<td></td>
<td>4/mmm (4/m/m 2/m/m 2/m/m)</td>
<td>4/mmm (4/m/m 2/m/m 2/m/m)</td>
</tr>
</tbody>
</table>

**Reflection conditions**

- **hkl**
  - k
  - l
  - k
  - k
  - k
  - k
  - k
  - P = --
  - P4 (75)
  - P4 (75)
  - P4 (75)
  - P4 (75)

- **hkl**
  - 4n
  - k
  - l
  - k
  - P42m (111)
  - P42m (111)
  - P42m (111)
  - P42m (111)

- **hkl**
  - 4n
  - k
  - l
  - k
  - P42c (112)
  - P42c (112)
  - P42c (112)
  - P42c (112)

- **hkl**
  - 4n
  - k
  - l
  - k
  - P4/mmm (131)
  - P4/mmm (131)
  - P4/mmm (131)
  - P4/mmm (131)

- **hkl**
  - 4n
  - k
  - l
  - k
  - P4/mmm (132)
  - P4/mmm (132)
  - P4/mmm (132)
  - P4/mmm (132)

- **hkl**
  - 4n
  - k
  - l
  - k
  - P4/mmm (133)
  - P4/mmm (133)
  - P4/mmm (133)
  - P4/mmm (133)

- **hkl**
  - 4n
  - k
  - l
  - k
  - P4/mmm (134)
  - P4/mmm (134)
  - P4/mmm (134)
  - P4/mmm (134)

- **hkl**
  - 4n
  - k
  - l
  - k
  - P4/mmm (135)
  - P4/mmm (135)
  - P4/mmm (135)
  - P4/mmm (135)

- **hkl**
  - 4n
  - k
  - l
  - k
  - P4/mmm (136)
  - P4/mmm (136)
  - P4/mmm (136)
  - P4/mmm (136)

- **hkl**
  - 4n
  - k
  - l
  - k
  - P4/mmm (137)
  - P4/mmm (137)
  - P4/mmm (137)
  - P4/mmm (137)
3.1. SPACE-GROUP DETERMINATION AND DIFFRACTION SYMBOLS

Table 3.1.4.1. Reflection conditions, diffraction symbols and possible space groups (cont.)

TETRAGONAL, Laue classes 4/m and 4/mmm (cont.)

<table>
<thead>
<tr>
<th>Reflection conditions</th>
<th>Extinction symbol</th>
<th>4</th>
<th>4/m</th>
<th>4/mmm</th>
<th>4/m (4/m 2/m 2/m)</th>
<th>4/mmm</th>
</tr>
</thead>
<tbody>
<tr>
<td>hkl</td>
<td>h00</td>
<td>0kl</td>
<td>hkl</td>
<td>0kl</td>
<td>h00</td>
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</tr>
<tr>
<td>h + k + l</td>
<td>k + l + l + l</td>
<td>k</td>
<td></td>
<td></td>
<td>J4 (79)</td>
<td></td>
</tr>
<tr>
<td>h + k + l</td>
<td>k + l + l + l</td>
<td>k</td>
<td></td>
<td></td>
<td>J4 (82)</td>
<td></td>
</tr>
<tr>
<td>h + k + l</td>
<td>k + l + l + l</td>
<td>k</td>
<td></td>
<td></td>
<td>J4/m (87)</td>
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</tr>
<tr>
<td>h + k + l</td>
<td>k + l + l + l</td>
<td>k</td>
<td></td>
<td></td>
<td>J22 (97)</td>
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</tr>
<tr>
<td>h + k + l</td>
<td>k + l + l + l</td>
<td>k</td>
<td></td>
<td></td>
<td>4mn (107)</td>
<td></td>
</tr>
<tr>
<td>h + k + l</td>
<td>k + l + l + l</td>
<td>k</td>
<td></td>
<td></td>
<td>42m (121)</td>
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</tr>
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<td>h + k + l</td>
<td>k + l + l + l</td>
<td>k</td>
<td></td>
<td></td>
<td>4mmm (139)</td>
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</tr>
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<td>h + k + l</td>
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<td>k</td>
<td></td>
<td></td>
<td>J4 (80)</td>
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</tr>
<tr>
<td>h + k + l</td>
<td>k + l + l + l</td>
<td>k</td>
<td></td>
<td></td>
<td>J4/22 (98)</td>
<td></td>
</tr>
<tr>
<td>h + k + l</td>
<td>k + l + l + l</td>
<td>k</td>
<td></td>
<td></td>
<td>J4Nm (109)</td>
<td></td>
</tr>
<tr>
<td>h + k + l</td>
<td>k + l + l + l</td>
<td>k</td>
<td></td>
<td></td>
<td>J4cd (110)</td>
<td></td>
</tr>
<tr>
<td>h + k + l</td>
<td>k + l + l + l</td>
<td>k</td>
<td></td>
<td></td>
<td>J4/a (88)</td>
<td></td>
</tr>
<tr>
<td>h + k + l</td>
<td>k + l + l + l</td>
<td>k</td>
<td></td>
<td></td>
<td>J4/a (141)</td>
<td></td>
</tr>
<tr>
<td>h + k + l</td>
<td>k + l + l + l</td>
<td>k</td>
<td></td>
<td></td>
<td>J4/ac (142)</td>
<td></td>
</tr>
</tbody>
</table>

† Pair of enantiomorphic space groups, cf. Section 3.1.5.
‡ Condition: 2h + l = 4m, l.

(as well as for the R space groups of the trigonal system), the different cell choices and settings of one space group are disregarded, 101 extinction symbols* and 122 diffraction symbols for the 230 space-group types result.

Only in 50 cases does a diffraction symbol uniquely identify just one space group, thus leaving 72 diffraction symbols that correspond to more than one space group. The 50 unique cases can be easily recognized in Table 3.1.4.1 because the line for the possible space groups in the particular Laue class contains just one entry.

The non-uniqueness of the space-group determination has two reasons:

(i) Friedel’s rule, i.e., the effect that, with neglect of anomalous dispersion, the diffraction pattern contains an inversion centre, even if such a centre is not present in the crystal.

Example

A monoclinic crystal (with unique axis b) has the diffraction symbol 1 2/m 1P1c1. Possible space groups are P1c1 (7) without an inversion centre, and P12/c1 (13) with an inversion centre. In both cases, the diffraction pattern has the Laue symmetry 1 2/m 1.

One aspect of Friedel’s rule is that the diffraction patterns are the same for two enantiomorphic space groups. Eleven diffraction symbols each correspond to a pair of enantiomorphic space groups.

In Table 3.1.4.1, such pairs are grouped between braces. Either of the two space groups may be chosen for structure solution. If due to anomalous scattering Friedel’s rule does not hold, at the refinement stage of structure determination it may be possible to determine the absolute structure and consequently the correct space group from the enantiomorphic pair.

(ii) The occurrence of four space groups in two ‘special’ pairs, each pair belonging to the same point group: I222 (23) & I222 (24) and I23 (197) & I23 (199). The two space groups of each pair differ in the location of the symmetry elements with respect to each other. In Table 3.1.4.1, these two special pairs are given in square brackets.

3.1.6. Space-group determination by additional methods

3.1.6.1. Chemical information

In some cases, chemical information determines whether or not the space group is centrosymmetric. For instance, all proteins crystallize in noncentrosymmetric space groups as they are constituted of L-amino acids only. Less certain indications may be obtained by considering the number of molecules per cell and the possible space-group symmetry. For instance, if experiment shows that there are two molecules of formula A2B2 per cell in either space group P212121 or P212121/m and if the molecule A2B2 cannot possibly have either a mirror plane or an inversion centre, then there is a strong indication that the correct space group is P212121/m. Crystallization of A2B2 in P212121/m with random disorder of the molecules cannot be excluded, however. In a similar way, multiplicities of Wyckoff positions and the number of formula units per cell may be used to distinguish between space groups.