International Tables for Crystallography (2006). Vol. C, Table 9.8.3.4, pp. 920–921.



Table 9.8.3.3. (3 + 1)-*Dimensional point groups and arithmetic crystal classes (cont.)*

| System | Point group $K_E$ | Point group $K_s$ | External Bravais class | Arithmetic crystal class(es) |
|---|---|---|---|---|
| Trigonal (*cont.*) | $3m$ | $(3m, 11)$ | $\bar{3}mR$ | $3mR(00\gamma)$ |
| | | | $6/mmmP$ | $3m1P(00\gamma), 31mP(00\gamma), 31mP(\frac{1}{3}\frac{1}{3}\gamma)$ |
| | $\bar{3}m$ | $(\bar{3}m, \bar{1}1)$ | $\bar{3}mR$ | $\bar{3}mR(00\gamma)$ |
| | | | $6/mmmP$ | $\bar{3}1mP(00\gamma), \bar{3}1mP(\frac{1}{3}\frac{1}{3}\gamma), \bar{3}m1P(00\gamma)$ |
| Hexagonal | $6$ | $(6, 1)$ | $6/mmmP$ | $6P(00\gamma)$ |
| | $\bar{6}$ | $(\bar{6}, \bar{1})$ | $6/mmmP$ | $\bar{6}P(00\gamma)$ |
| | $6/m$ | $(6/m, 1\bar{1})$ | $6/mmmP$ | $6/mP(00\gamma)$ |
| | $622$ | $(622, 1\bar{1}\bar{1})$ | $6/mmmP$ | $622P(00\gamma)$ |
| | $6mm$ | $(6mm, 111)$ | $6/mmmP$ | $6mmP(00\gamma)$ |
| | $\bar{6}m2$ | $(\bar{6}m2, \bar{1}1\bar{1})$ | $6/mmmP$ | $\bar{6}m2P(00\gamma)$ |
| | $\bar{6}2m$ | $(\bar{6}2m, \bar{1}\bar{1}1)$ | $6/mmmP$ | $\bar{6}2mP(00\gamma)$ |
| | $6/mmm$ | $(6/mmm, 1\bar{1}11)$ | $6/mmmP$ | $6/mmmP(00\gamma)$ |

Written in components, the non-primitive translation $\upsilon_s$ associated with the point-group element $(R, R_I)$ is $(\mathbf{v}, \upsilon_I)$, where $\upsilon_I$ can be written as $\delta - \mathbf{q}\cdot\mathbf{v}$. In accordance with (9.8.1.12), $\delta$ is defined as $\upsilon_4$. The origin-invariant part $\upsilon_s^o$ of $\upsilon_s$ is

$$\upsilon_s^o = (\mathbf{v}^o, \upsilon_I^o) = \frac{1}{n}\sum_{m=1}^{n}(R^m\mathbf{v}, R_I^m\upsilon_I) = (\mathbf{v}^o, \tau - \mathbf{q}\cdot\mathbf{v}^o), \quad (9.8.3.6)$$

where

$$\tau = \upsilon_4^o = \upsilon_I^o + \mathbf{q}\cdot\mathbf{v}^o.$$

The internal transformation $R_I(R) = \varepsilon(R) = \varepsilon$ is either $+1$ or $-1$. When $\varepsilon = -1$ it follows from (9.8.3.6) that $\upsilon_I^o = 0$. For $\varepsilon = +1$, one has $\upsilon_I^o = \upsilon_I$. Because in that case

$$\mathbf{q}\cdot\mathbf{v}^o = \frac{1}{n}\sum_{m=1}^{n}\mathbf{q}\cdot R^m\mathbf{v} = \mathbf{q}^i\cdot\mathbf{v}, \quad (9.8.3.7)$$

it follows that

$$\tau = \upsilon_I + \mathbf{q}\cdot\mathbf{v}^o = \delta - \mathbf{q}\cdot\mathbf{v} + \mathbf{q}\cdot\mathbf{v}^o = \delta - \mathbf{q}^r\cdot\mathbf{v}. \quad (9.8.3.8)$$

For $R_s$ of order $n$, $R_s^n$ is the identity and the associated translation is a lattice translation. The ensuing values for $\tau$ are $0, \frac{1}{2}, \pm\frac{1}{3}, \pm\frac{1}{4}$ or $\pm\frac{1}{6}$ (modulo integers). This remains true also in the case of a centred basis. The symbol of the (3 + 1)-dimensional space-group element is determined by the invariant part of its three-dimensional translation and $\tau$. Again, that information can be given in terms of either a one-line or a two-line symbol.

In the one-line symbol, one finds: the symbol according to *International Tables for Crystallography*, Volume A, for the space group generated by the elements $\{R|\mathbf{v}\}$, in parentheses the components of the modulation vector $\mathbf{q}$ followed by the values of $\tau$, one for each generator appearing in the three-dimensional space-group symbol. A letter symbolizes the value of $\tau$ according to

$$\begin{array}{llllll} \tau & 0 & \frac{1}{2} & \pm\frac{1}{3} & \pm\frac{1}{4} & \pm\frac{1}{6} \\ \text{symbol} & 0 & s & t & q & h \end{array}. \quad (9.8.3.9)$$

As an example, consider the superspace group

$$P2_1/m(\alpha\beta 0)0s.$$

The external components $\{R|\mathbf{v}\}$ of the elements of this group form the three-dimensional space group $P2_1/m$. The modulation wavevector is $\alpha\mathbf{a}^* + \beta\mathbf{b}^*$ with respect to a conventional basis of the monoclinic lattice with unique axis $\mathbf{c}$. Therefore, the point group is $(2/m, 1\bar{1})$. The point-group element $(2, \bar{1})$ has associated a non-primitive translation with invariant part $(\frac{1}{2}\mathbf{c}, 0) = (00\frac{1}{2}0)$ and the point-group generator $(m, 1)$ one with $(\mathbf{0}, \frac{1}{2}) = (000\frac{1}{2})$.

Table 9.8.3.4(*a*). (2 + 1)-*Dimensional superspace groups*

The number labelling the superspace group is denoted by *n.m*, where *n* is the number attached to the two-dimensional basic space group and *m* numbers the various superspace groups having the same basic space group. The symbol of the basic space group, the symbol for the three-dimensional point group, the number of the three-dimensional Bravais class to which the superspace group belongs (Table 9.8.3.1*a*) and the superspace-group symbol are also given.

| No. | Basic space group | Point group $K_s$ | Bravais class No. | Group symbol |
|---|---|---|---|---|
| **Oblique** | | | | |
| 1.1 | $p1$ | $(1, 1)$ | 1 | $p1(\alpha\beta)$ |
| 2.1 | $p2$ | $(2, \bar{1})$ | 1 | $p2(\alpha\beta)$ |
| **Rectangular** | | | | |
| 3.1 | $pm$ | $(m, 1)$ | 2 | $pm1(0\beta)$ |
| 3.2 | | | 2 | $pm1(0\beta)s0$ |
| 3.3 | | | 3 | $pm1(\frac{1}{2}\beta)$ |
| 3.4 | | $(m, \bar{1})$ | 2 | $p1m(0\beta)$ |
| 3.5 | | | 3 | $p1m(\frac{1}{2}\beta)$ |
| 4.1 | $pg$ | $(m, 1)$ | 2 | $pg1(0\beta)$ |
| 4.2 | | | 3 | $pg1(\frac{1}{2}\beta)$ |
| 4.3 | | $(m, \bar{1})$ | 2 | $p1g(0\beta)$ |
| 5.1 | $cm$ | $(m, 1)$ | 4 | $cm1(0\beta)$ |
| 5.2 | | | 4 | $cm1(0\beta)s0$ |
| 5.3 | | $(m, \bar{1})$ | 4 | $c1m(0\beta)$ |
| 6.1 | $pmm$ | $(mm, 1\bar{1})$ | 2 | $pmm(0\beta)$ |
| 6.2 | | | 2 | $pmm(0\beta)s0$ |
| 6.3 | | | 3 | $pmm(\frac{1}{2}\beta)$ |
| 7.1 | $pmg$ | $(mm, 1\bar{1})$ | 2 | $pmg(0\beta)$ |
| 7.2 | | | 2 | $pgm(0\beta)$ |
| 7.3 | | | 3 | $pgm(\frac{1}{2}\beta)$ |
| 8.1 | $pgg$ | $(mm, 1\bar{1})$ | 2 | $pgg(0\beta)$ |
| 9.1 | $cmm$ | $(mm, 1\bar{1})$ | 4 | $cmm(0\beta)$ |
| 9.2 | | | 4 | $cmm(0\beta)s0$ |

Table 9.8.3.4(*b*). (2 + 2)-*Dimensional superspace groups*

The number labelling the superspace group is denoted by *n.m*, where *n* is the number attached to the two-dimensional basic space group and *m* numbers the various superspace groups having the same basic space group. The symbol of the basic space group, the symbol for the four-dimensional point group, the number of the four-dimensional Bravais class to which the superspace group belongs (Table 9.8.3.1*b*) and the superspace-group symbol are also given.

| No. | Basic space group | Point group $K_s$ | Bravais classs No. | Group symbol |
|---|---|---|---|---|
| **Oblique** | | | | |
| 1.1 | $p1$ | $(1, 1)$ | 1 | $p1(\alpha\beta, \lambda\mu)$ |
| 2.1 | $p2$ | $(2, 2)$ | 1 | $p2(\alpha\beta, \lambda\mu)$ |
| **Rectangular** | | | | |
| 3.1 | $pm$ | $(m, 1)$ | 2 | $pm1(0\beta, 0\mu)$ |
| 3.2 | | | 2 | $pm1(0\beta, 0\mu)s0, 0$ |
| 3.3 | | | 3 | $pm1(\frac{1}{2}\beta, 0\mu)$ |
| 3.4 | | | 3 | $pm1(\frac{1}{2}\beta, 0\mu)s0, 0$ |
| 3.5 | | $(m, 2)$ | 2 | $p1m(0\beta, 0\mu)$ |
| 3.6 | | | 3 | $p1m(\frac{1}{2}\beta, 0\mu)$ |
| 3.7 | | $(m, m)$ | 4 | $pm1(\alpha 0, 0\mu)$ |
| 3.8 | | | 4 | $pm1(\alpha 0, 0\mu)0s, 0$ |
| 3.9 | | | 5 | $pm1(\alpha\frac{1}{2}, 0\mu)$ |
| 3.10 | | | 5 | $pm1(\alpha\frac{1}{2}, 0\mu)0s, 0$ |
| 3.11 | | | 5 | $p1m(\alpha\frac{1}{2}, 0\mu)$ |
| 3.12 | | | 5 | $p1m(\alpha\frac{1}{2}, 0\mu)0, s0$ |
| 3.13 | | | 6 | $pm1(\alpha\frac{1}{2}, \frac{1}{2}\mu)$ |
| 3.14 | | | 7 | $pm1(\alpha\beta)$ |
| 4.1 | $pg$ | $(m, 1)$ | 2 | $pg1(0\beta, 0\mu)$ |
| 4.2 | | | 3 | $pg1(\frac{1}{2}\beta, 0\mu)$ |
| 4.3 | | $(m, 2)$ | 2 | $p1g(0\beta, 0\mu)$ |
| 4.4 | | $(m, m)$ | 4 | $pg1(\alpha 0, 0\mu)$ |
| 4.5 | | | 7 | $pg1(\alpha\frac{1}{2}, \frac{1}{2}\mu)$ |
| 5.1 | $cm$ | $(m, 1)$ | 8 | $cm1(0\beta, 0\mu)$ |
| 5.2 | | | 8 | $cm1(0\beta, 0\mu)s0, 0$ |
| 5.3 | | $(m, 2)$ | 8 | $c1m(0\beta, 0\mu)$ |
| 5.4 | | $(m, m)$ | 9 | $cm1(\alpha 0, 0\mu)$ |
| 5.5 | | | 9 | $cm1(\alpha 0, 0\mu)0s, 0$ |
| 5.6 | | | 10 | $cm(\alpha\beta)$ |
| 6.1 | $pmm$ | $(mm, 12)$ | 2 | $pmm(0\beta, 0\mu)$ |
| 6.2 | | | 2 | $pmm(0\beta, 0\mu)s0, 0$ |
| 6.3 | | | 3 | $pmm(\frac{1}{2}\beta, 0\mu)$ |
| 6.4 | | | 3 | $pmm(\frac{1}{2}\beta, 0\mu)s0, 0$ |
| 6.5 | | $(mm, mm)$ | 4 | $pmm(\alpha 0, 0\mu)$ |
| 6.6 | | | 4 | $pmm(\alpha 0, 0\mu)0s, 0$ |
| 6.7 | | | 4 | $pmm(\alpha 0, 0\mu)0s, s0$ |
| 6.8 | | | 5 | $pmm(\alpha\frac{1}{2}, 0\mu)$ |
| 6.9 | | | 5 | $pmm(\alpha\frac{1}{2}, 0\mu)0s, 0$ |
| 6.10 | | | 6 | $pmm(\alpha\frac{1}{2}, \frac{1}{2}\mu)$ |
| 6.11 | | | 7 | $pmm(\alpha\beta)$ |
| 7.1 | $pmg$ | $(mm, 12)$ | 2 | $pmg(0\beta, 0\mu)$ |
| 7.2 | | | 2 | $pmg(0\beta, 0\mu)0s, 0$ |
| 7.3 | | | 2 | $pgm(0\beta, 0\mu)$ |
| 7.4 | | | 3 | $pgm(\frac{1}{2}\beta, 0\mu)$ |
| 7.5 | | $(mm, mm)$ | 4 | $pgm(\alpha 0, 0\mu)$ |
| 7.6 | | | 4 | $pgm(\alpha 0, 0\mu)0, s0$ |
| 7.7 | | | 5 | $pmg(\alpha\frac{1}{2}, 0\mu)$ |
| 7.8 | | | 5 | $pmg(\alpha\frac{1}{2}, 0\mu)0s, 0$ |
| 7.9 | | | 7 | $pgm(\alpha\beta)$ |
| 8.1 | $pgg$ | $(mm, 12)$ | 2 | $pgg(0\beta, 0\mu)$ |
| 8.2 | | $(mm, mm)$ | 4 | $pgg(\alpha 0, 0\mu)$ |
| 8.3 | | | 7 | $pgg(\alpha\beta)$ |
| 9.1 | $cmm$ | $(mm, 12)$ | 8 | $cmm(0\beta, 0\mu)$ |
| 9.2 | | | 8 | $cmm(0\beta, 0\mu)0s, 0$ |
| 9.3 | | $(mm, mm)$ | 9 | $cmm(\alpha 0, 0\mu)$ |
| 9.4 | | | 9 | $cmm(\alpha 0, 0\mu)0s, 0$ |
| 9.5 | | | 9 | $cmm(\alpha 0, 0\mu)0s, s0$ |
| 9.6 | | | 10 | $cmm(\alpha\beta)$ |
| **Tetragonal** | | | | |
| 10.1 | $p4$ | $(4, 4)$ | 11 | $p4(\alpha\beta)$ |
| 11.1 | $p4m$ | $(4m, 4m)$ | 12 | $p4m(\alpha 0)$ |
| 11.2 | | | 12 | $p4m(\alpha 0)0, 0s$ |
| 11.3 | | | 13 | $p4m(\alpha\frac{1}{2})$ |
| 11.4 | | $(4\dot{m}, 4\ddot{m})$ | 14 | $p4m(\alpha\alpha)$ |
| 11.5 | | | 14 | $p4m(\alpha\alpha)0, 0s$ |
| 12.1 | $p4g$ | $(4m, 4m)$ | 12 | $p4g(\alpha 0)$ |
| 12.2 | | | 12 | $p4g(\alpha 0)0, 0s$ |
| 12.3 | | $(4\dot{m}, 4\ddot{m})$ | 14 | $p4g(\alpha\alpha)$ |
| 12.4 | | | 14 | $p4g(\alpha\alpha)0, 0s$ |
| **Hexagonal** | | | | |
| 13.1 | $p3$ | $(3, 3)$ | 15 | $p3(\alpha\beta)$ |
| 14.1 | $p3m1$ | $(3m, 3m)$ | 16 | $p3m1(\alpha 0)$ |
| 14.2 | | $(3\dot{m}, 3\ddot{m})$ | 17 | $p3m1(\alpha\alpha)$ |
| 15.1 | $p31m$ | $(3m, 3m)$ | 16 | $p31m(\alpha 0)$ |
| 16.1 | $p6$ | $(6, 6)$ | 15 | $p6(\alpha\beta)$ |
| 17.1 | $p6m$ | $(6m, 6m)$ | 16 | $p6m(\alpha 0)$ |
| 17.2 | | $(6\dot{m}, 6\ddot{m})$ | 17 | $p6m(\alpha\alpha)$ |

In the two-line symbol, one finds in the upper line the symbol for the three-dimensional space group, in the bottom line the value of $\tau$ for the case $\varepsilon = +1$ and the symbol '$\bar{1}$' when $\varepsilon = -1$. The rational part of $\mathbf{q}$ is indicated by means of the appropriate prefix. In the case considered, $\mathbf{q}^r = 000$. So the prefix is $P$ and the same superspace group is denoted in a two-line symbol as

$$P^{P2_1/m}_{\bar{1}\;\;s} .$$

In Table 9.8.3.5, the (3 + 1)-dimensional space groups are given by one-line symbols. These are so-called short symbols. Sometimes, a full symbol is required. Then, for the example given above one has $P112_1/m(\alpha\beta 0)000s$ and $P^{P112_1/m}_{11\bar{1}\;\;s}$, respectively. Note that in the short one-line symbol for $\tau = 0$ superspace groups (where the non-primitive translations can be transformed to zero by a choice of the origin) the zeros for the translational part are omitted. Not so, of course, in the full symbol. For example, short symbol $P2_1/m(\alpha\beta 0)$ and full symbol $P112_1/m(\alpha\beta 0)0000$. Table 9.8.3.5 is an adapted version of the tables given by de Wolff, Janssen & Janner (1981) and corrected by Yamamoto, Janssen, Janner & de Wolff (1985).

### 9.8.3.3.2. *Reflection conditions*

The indexing of diffraction vectors is a matter of choice of basis. When the basis chosen is not a primitive one, the indices have to satisfy certain conditions known as *centring conditions*. This holds for the main reflections (centring in ordinary space) as well as for satellites (centring in superspace). These centring conditions for reflections have been discussed in Subsection 9.8.2.1.

In addition to these general reflection conditions, there may be special reflection conditions related to the existence of non-

(*continued on page* 934)