International Tables for Crystallography (2006). Vol. C, Table 9.8.3.1, pp. 915–916 .

structure, whether the assumed displacive or occupation modulations obey the site symmetry of the Wyckoff position considered. An atom at a special position transforms into itself by the site symmetry of the position. For such a symmetry transformation, $j' = j$, $\mathbf{v} = 0$, and thus $\Delta(\varepsilon = 1) = \tau$, $\Delta(\varepsilon = -1) = 0$ (*cf.* Subsection 9.8.3.3). In the modulated structure, the site symmetry is preserved only if, for each of its symmetry operations, the appropriate relation is obeyed by the modulations [*cf.* (9.8.1.24)].

For displacive modulations, the conditions are

$$\begin{aligned} \mathbf{u}_j(\mathbf{q}\cdot\mathbf{r}) &= R\mathbf{u}_j(\mathbf{q}\cdot\mathbf{r} - \tau) \quad \text{for } \varepsilon = 1, \\ \mathbf{u}_j(\mathbf{q}\cdot\mathbf{r}) &= R\mathbf{u}_j(\mathbf{q}\cdot\mathbf{r}) \quad \text{for } \varepsilon = -1 \end{aligned} \qquad (9.8.2.13)$$

and, for occupation modulation,

$$\begin{aligned} p_j(\mathbf{q}\cdot\mathbf{r}) &= p_j(\mathbf{q}\cdot\mathbf{r} - \tau) \quad \text{for } \varepsilon = 1, \\ p_j(\mathbf{q}\cdot\mathbf{r}) &= p_j(\mathbf{q}\cdot\mathbf{r}) \quad \text{for } \varepsilon = -1. \end{aligned} \qquad (9.8.2.14)$$

Example 4. Assume, as for the case discussed above, that the basic structure has the space group *Cmmm*. Can the superspace group be *Cmmm*(10γ)? In this superspace group, $\tau = 0$ for all symmetry operations with $\varepsilon = 1$. Displacive modulations at special positions must thus obey $\mathbf{u}_j(\mathbf{q}\cdot\mathbf{r}) = R\mathbf{u}_j(\mathbf{q}\cdot\mathbf{r})$ for the superspace group to be correct. For an atom at special position *mmm*, this is not possible for all site symmetry operations unless $\mathbf{u}_j = 0$. Suppose that the structure model contains a displacive modulation polarized along **a** for that atom. The allowed site symmetry is then lowered to 2*mm*, and as a consequence the superspace group is *C*2*mm*(10γ) rather than *Cmmm*(10γ).

9.8.3. Introduction to the tables

In what follows, the tables dealing with the $(3+1)$-dimensional case will be presented. The explanations can easily be applied to the $(2+d)$-dimensional case also [Tables 9.8.3.1(*a*), (*b*) and 9.8.3.4(*a*), (*b*)].

9.8.3.1. *Tables of Bravais lattices*

The $(3+1)$-dimensional lattice Σ^* is determined by the three-dimensional vectors $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$ and the modulation vector **q**. The former three vectors give by duality **a**, **b**, and **c**, the external components of lattice basis vectors, and the products $-\mathbf{q}\cdot\mathbf{a} = -\alpha$, $-\mathbf{q}\cdot\mathbf{b} = -\beta$, and $-\mathbf{q}\cdot\mathbf{c} = -\gamma$ the corresponding internal components. Therefore, it is sufficient to give the arithmetic crystal class of the group $\Gamma_E(K)$ and the components σ_j ($\sigma_1 = \alpha$, $\sigma_2 = \beta$, and $\sigma_3 = \gamma$) of the modulation vector **q** with respect to a conventional basis $\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$. The arithmetic crystal class is denoted by a modification of the symbol of the three-dimensional symmorphic space group of this class (see Chapter 1.4) plus an indication for the row matrix σ (having entries σ_j). In this way, one obtains the so-called one-line symbols used in Tables 9.8.3.1(*a*), (*b*) and 9.8.3.2(*a*), (*b*).

As an example, the symbol $2/mB(0\frac{1}{2}\gamma)$ denotes a Bravais class for which the main reflections belong to a *B*-centred monoclinic lattice (unique axis **c**) and the satellite positions are generated by the point-group transforms of $\frac{1}{2}\mathbf{b}^* + \gamma\mathbf{c}^*$. Then the matrix σ becomes $\sigma = (0\frac{1}{2}\gamma)$. It has as irrational part $\sigma^i = (00\gamma)$ and as rational part $\sigma^r = (0\frac{1}{2}0)$. The external part of the $(3+1)$-dimensional point group of the Bravais lattice is $2/m$. By use of the relation [*cf.* (9.8.2.4)]

$$R\mathbf{q}^i = \varepsilon\mathbf{q}^i, \quad R\mathbf{q}^r \equiv \varepsilon\mathbf{q}^r \text{ (modulo } \mathbf{b}^*), \qquad (9.8.3.1)$$

Table 9.8.3.1(*a*). $(2+1)$-*Dimensional Bravais classes for incommensurate structures*

The holohedral point group K_s is given in terms of its external and internal parts, K_E and K_I, respectively. The reflections are given by $h\mathbf{a}^* + k\mathbf{b}^* + m\mathbf{q}$ where **q** is the modulation wavevector. If the rational part $\mathbf{q}^r$ is not zero, there is a corresponding centring translation in three-dimensional space. The conventional basis $(\mathbf{a}_c^*, \mathbf{b}_c^*, \mathbf{q}^i)$ given for the vector module M^* is shown such that $\mathbf{q}^r = 0$. The basis vectors are given by components with respect to the conventional basis $\mathbf{a}^*$, $\mathbf{b}^*$ of the lattice Λ^* of main reflections.

No.	Symbol	K_E	K_I	q	Conventional basis	Centring
Oblique						
1	$2p(\alpha\beta)$	2	$\bar{1}$	$(\alpha\beta)$	$(10), (01), (\alpha\beta)$	
Rectangular						
2	$mmp(0\beta)$	mm	$1\bar{1}$	(0β)	$(10), (01), (0\beta)$	
3	$mmp(\frac{1}{2}\beta)$	mm	$1\bar{1}$	$(\frac{1}{2}\beta)$	$(\frac{1}{2}0), (01), (0\beta)$	$\frac{1}{2}0\frac{1}{2}$
4	$mmc(0\beta)$	mm	$1\bar{1}$	(0β)	$(10), (01), (0\beta)$	$\frac{1}{2}\frac{1}{2}0$

we see that the operations 2 and *m* are associated with the internal space transformations $\varepsilon = 1$ and $\varepsilon = -1$, respectively. This is denoted by the one-line symbol $(2/m, 1\bar{1})$ for the $(3+1)$-dimensional point group of the Bravais lattice. In direct space, the symmetry operation $\{R, \varepsilon(R)\}$ is represented by the matrix $\Gamma(R)$ which transforms the components $v_j, j = 1, \ldots, 4$, of a vector v_s to:

$$v'_j = \sum_{k=1}^{4} \Gamma(R)_{jk} v_k.$$

The operations (2, 1) and $(m, \bar{1})$ are represented by the matrices:

$$\Gamma(2) = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \end{pmatrix}; \quad \Gamma(m) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{pmatrix}. \qquad (9.8.3.2)$$

The 3×3 part $\Gamma_E(R)$ of each matrix is obtained by considering the action of *R* on the external part **v** of v_s. The 1×1 part $\Gamma_I(R)$ is the value of the ε associated with *R* and the remaining part $\Gamma_M(R)$ follows from the relation

$$\Gamma_M(R) = -\Gamma_I(R)\sigma^r + \sigma^r\Gamma_E(R). \qquad (9.8.3.3)$$

Bravais classes can be denoted in an alternative way by two-line symbols. In the two-line symbol, the Bravais class is given by specifying the arithmetic crystal class of the external symmetry by the symbol of its symmorphic space group, the associated elements $\Gamma_I(R) = \varepsilon$ by putting their symbol under the corresponding symbols of $\Gamma_E(R)$, and by the rational part σ^r indicated by a prefix. In the following table, this prefix is given for the components of $\mathbf{q}^r$ that play a role in the classification.

P	(000)	*R*	$(\frac{1}{3}, \frac{1}{3}, 0)$		
A	$(\frac{1}{2}, 0, 0)$	*B*	$(0, \frac{1}{2}, 0)$	*C*	$(0, 0, \frac{1}{2})$
L	(1, 0, 0)	*M*	(0, 1, 0)	*N*	(0, 0, 1)
U	$(0, \frac{1}{2}, \frac{1}{2})$	*V*	$(\frac{1}{2}, 0, \frac{1}{2})$	*W*	$(\frac{1}{2}, \frac{1}{2}, 0)$.

Note that the integers appearing here are not equivalent to zero because they express components with respect to a conventional lattice basis (and not a primitive one). For the Bravais class

Table 9.8.3.1(*b*). (2 + 2)-*Dimensional Bravais classes for incommensurate structures*

The holohedral point group K_s is given in terms of its external and internal parts, K_E and K_I, respectively. The basis of the vector module M^* contains two modulation wavevectors and the reflections are given by $h\mathbf{a}^* + k\mathbf{b}^* + m_1\mathbf{q}_1 + m_2\mathbf{q}_2$. If $\mathbf{q}_1^r$ or $\mathbf{q}_2^r$ are not zero, there are corresponding centring translations in four-dimensional space. The conventional basis ($\mathbf{a}_c^*$, $\mathbf{b}_c^*$, $\mathbf{q}_1^i$, $\mathbf{q}_2^i$) for the vector module M^* is chosen such that $\mathbf{q}_1^r = \mathbf{q}_2^r = 0$. The basis vectors are indicated by their components with respect to the conventional basis $\mathbf{a}^*$, $\mathbf{b}^*$ of the lattice Λ^* of main reflections.

No.	Symbol	K_E	K_I	$\mathbf{q}_1$	$\mathbf{q}_2$	Conventional basis	Centring
Oblique							
1	$2p(\alpha\beta, \lambda\mu)$	2	2	$(\alpha\beta)$	$(\lambda\mu)$	$(10), (01), (\alpha\beta), (\lambda\mu)$	
Rectangular							
2	$mmp(0\beta, 0\mu)$	mm	12	(0β)	(0μ)	$(10), (01), (0\beta), (0\mu)$	
3	$mmp(\frac{1}{2}\beta, 0\mu)$	mm	12	$(\frac{1}{2}\beta)$	(0μ)	$(\frac{1}{2}0), (01), (0\beta), (0\mu)$	$\frac{1}{2}0\frac{1}{2}0$
4	$mmp(\alpha 0, 0\mu)$	mm	mm	$(\alpha 0)$	(0μ)	$(10), (01), (\alpha 0), (0\mu)$	
5	$mmp(\alpha\frac{1}{2}, 0\mu)$	mm	mm	$(\alpha\frac{1}{2})$	(0μ)	$(10), (0\frac{1}{2}), (\alpha 0), (0\mu)$	$0\frac{1}{2}\frac{1}{2}0$
6	$mmp(\alpha\frac{1}{2}, \frac{1}{2}\mu)$	mm	mm	$(\alpha\frac{1}{2})$	$(\frac{1}{2}\mu)$	$(\frac{1}{2}0), (0\frac{1}{2}), (\alpha 0), (0\mu)$	$\frac{1}{2}00\frac{1}{2}$, $0\frac{1}{2}\frac{1}{2}0$
7	$mmp(\alpha\beta)$	mm	mm	$(\alpha\beta)$	$(\alpha\bar{\beta})$	$(10), (01), (\alpha 0), (0\beta)$	$00\frac{1}{2}\frac{1}{2}$
8	$mmc(0\beta, 0\mu)$	mm	12	(0β)	(0μ)	$(10), (01), (0\beta), (0\mu)$	$\frac{1}{2}\frac{1}{2}00$
9	$mmc(\alpha 0, 0\mu)$	mm	mm	$(\alpha 0)$	(0μ)	$(10), (01), (\alpha 0), (0\mu)$	$\frac{1}{2}\frac{1}{2}00$
10	$mmc(\alpha\beta)$	mm	mm	$(\alpha\beta)$	$(\alpha\bar{\beta})$	$(10), (01), (\alpha 0), (0\beta)$	$\frac{1}{2}\frac{1}{2}00$, $00\frac{1}{2}\frac{1}{2}$
Square							
11	$4p(\alpha\beta)$	4	4	$(\alpha\beta)$	$(\bar{\beta}\alpha)$	$(10), (01), (\alpha\beta), (\bar{\beta}\alpha)$	
12	$4mp(\alpha 0)$	$4m$	$4m$	$(\alpha 0)$	(0α)	$(10), (01), (\alpha 0), (0\alpha)$	
13	$4mp(\alpha\frac{1}{2})$	$4m$	$4m$	$(\alpha\frac{1}{2})$	$(\frac{1}{2}\alpha)$	$(\frac{1}{2}\frac{1}{2}), (\bar{\frac{1}{2}}\frac{1}{2}), (\gamma\gamma), (\delta\bar{\delta})$ $\gamma = (2\alpha + 1)/4$, $\delta = (2\alpha - 1)/4$	$\frac{1}{2}\frac{1}{2}00$, $00\frac{1}{2}\frac{1}{2}$
14	$4mp(\alpha\alpha)$	$4\dot{m}$	$4\ddot{m}$	$(\alpha\alpha)$	$(\bar{\alpha}\alpha)$	$(10), (01), (\alpha\alpha), (\bar{\alpha}\alpha)$	
Hexagonal							
15	$6p(\alpha\beta)$	6	6	$(\alpha\beta)$	$(\bar{\beta}\alpha + \beta)$	$(10), (01), (\alpha\beta), (\bar{\beta}\alpha + \beta)$	
16	$6mp(\alpha 0)$	$6m$	$6m$	$(\alpha 0)$	(0α)	$(10), (01), (\alpha 0), (0\alpha)$	
17	$6mp(\alpha\alpha)$	$6\dot{m}$	$6\ddot{m}$	$(\alpha\alpha)$	$(\bar{\alpha}2\alpha)$	$(10), (01), (\alpha\alpha), (\bar{\alpha}2\alpha)$	

mentioned above, the two-line symbol is $B^{2/mB}_{1\,\bar{1}}$. This symbol has the advantage that the internal transformation (the value of ε) is explicitly given for the corresponding generators. It has, however, certain typographical drawbacks. It is rare for the printer to put the symbol together in the correct manner: $B^{2/mB}_{1\,\bar{1}}$.

In Tables 9.8.3.1(*a*), (*b*) and 9.8.3.2(*a*), (*b*) the symbols for the $(2 + d)$- and (3 + 1)-dimensional Bravais classes are given in the one-line form. It is, however, easy to derive from each one-line symbol the corresponding two-line symbol because the bottom line for the two-line symbol appears in the tables as the internal part of the point-group symbol.

The number of symbols in the bottom line of the two-line symbol should be equal to that of the generators given in the top line. A symbol '1' is used in the bottom line if the corresponding R_I is the unit transformation. If necessary, a mirror perpendicular to a crystal axis is indicated by $\dot{m}$ and one that is not by $\ddot{m}$. This situation only occurs for $d \geq 2$. So the (2 + 2)-dimensional class P^{4mp}_{4m} is actually $P^{4\dot{m}p}_{4\dot{m}}$ and is different from the class $P^{4\ddot{m}p}_{4\ddot{m}}$. In a one-line symbol, their difference is apparent, the first being $4mp(\alpha 0)$, whereas the second is $4mp(\alpha\alpha)$.

9.8.3.2. *Table for geometric and arithmetic crystal classes*

In Table 9.8.3.3, the geometric and the arithmetic crystal classes of (3 + 1)-dimensional superspace are given.

The symbols for *geometric crystal classes* indicate the pairs $[R, \varepsilon(R)]$ of the generators of the point group. This is done by giving the crystal class for the point group K_E and the symbols for the corresponding elements of K_I. So, for example, the geometric crystal class belonging to the holohedral point group of the Bravais class $2/mB(0\frac{1}{2}\gamma)$, mentioned above, is $(2/m, 1\bar{1})$.

The notation for the *arithmetic crystal classes* is similar to that for the Bravais classes. In the tables, their one-line symbols are given. They consist of the (modified) symbol of the three-dimensional symmorphic space group and, in parentheses, the appropriate components of the modulation wavevector. The three arithmetic crystal classes implying a lattice belonging to the Bravais class $2/mB(0\frac{1}{2}\gamma)$ are $2B(0\frac{1}{2}\gamma)$, $mB(0\frac{1}{2}\gamma)$, and $2/mB(0\frac{1}{2}\gamma)$. The corresponding geometric crystal classes are $(2, \bar{1})$, $(m, \bar{1})$, and $(2/m, 1\bar{1})$.

9.8.3.3. *Tables of superspace groups*

9.8.3.3.1. *Symmetry elements*

The transformations g_s belonging to a (3 + 1)-dimensional superspace group consist of a point-group transformation R_s given by the integral matrix $\Gamma(R)$ and of the associated translation. So the superspace group is determined by the arithmetic crystal class of its point group and the corresponding translational components. The symbol for the arithmetic crystal

references