International Tables for Crystallography (2006). Vol. C, Section 9.8.3, pp. 915–937.

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

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

and, for occupation modulation,

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

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)]

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

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), (0β)	
3	$mmp(\frac{1}{2}\beta)$	mm	$1\bar{1}$	$(\frac{1}{2}\beta)$	$(\frac{1}{2}0)$, (01), (0β)	$\frac{1}{2}0\frac{1}{2}$
4	$mmc(0\beta)$	mm	$1\bar{1}$	(0β)	(10), (01), (0β)	$\frac{1}{2}\frac{1}{2}0$

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:

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

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

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

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), (0β), (0μ)	
3	$mmp(\frac{1}{2}\beta, 0\mu)$	mm	12	$(\frac{1}{2}\beta)$	(0μ)	$(\frac{1}{2}0)$, (01), (0β), (0μ)	$\frac{1}{2}0\frac{1}{2}0$
4	$mmp(\alpha 0, 0\mu)$	mm	mm	$(\alpha 0)$	(0μ)	(10), (01), $(\alpha 0)$, (0μ)	
5	$mmp(\alpha\frac{1}{2}, 0\mu)$	mm	mm	$(\alpha\frac{1}{2})$	(0μ)	(10), $(0\frac{1}{2})$, $(\alpha 0)$, (0μ)	$0\frac{1}{2}\frac{1}{2}0$
6	$mmp(\alpha\frac{1}{2}, \frac{1}{2}\mu)$	mm	mm	$(\alpha\frac{1}{2})$	$(\frac{1}{2}\mu)$	$(\frac{1}{2}0)$, $(0\frac{1}{2})$, $(\alpha 0)$, (0μ)	$\frac{1}{2}00\frac{1}{2}$, $0\frac{1}{2}\frac{1}{2}0$
7	$mmp(\alpha\beta)$	mm	mm	$(\alpha\beta)$	$(\alpha\bar{\beta})$	(10), (01), $(\alpha 0)$, (0β)	$00\frac{1}{2}\frac{1}{2}$
8	$mmc(0\beta, 0\mu)$	mm	12	(0β)	(0μ)	(10), (01), (0β), (0μ)	$\frac{1}{2}\frac{1}{2}00$
9	$mmc(\alpha 0, 0\mu)$	mm	mm	$(\alpha 0)$	(0μ)	(10), (01), $(\alpha 0)$, (0μ)	$\frac{1}{2}\frac{1}{2}00$
10	$mmc(\alpha\beta)$	mm	mm	$(\alpha\beta)$	$(\alpha\bar{\beta})$	(10), (01), $(\alpha 0)$, (0β)	$\frac{1}{2}\frac{1}{2}00$, $00\frac{1}{2}\frac{1}{2}$
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), $(\alpha 0)$, (0α)	
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), $(\alpha 0)$, (0α)	
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 $B_{1\ \bar{1}}^{2/mB}$. 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: $B_{1\ \bar{1}}^{2/mB}$.

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_{4m}^{4mp} is actually $P_{4\dot{m}}^{4\dot{m}p}$ and is different from the class $P_{4\ddot{m}}^{4\dot{m}p}$. 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

Table 9.8.3.2(*a*). (3 + 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 $h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* + m\mathbf{q}$, where $\mathbf{q}$ is the modulation wavevector. If the rational part $\mathbf{q}^r$ is not zero, there is a corresponding centring translation in four-dimensional space. A conventional basis $(\mathbf{a}_c^*, \mathbf{b}_c^*, \mathbf{c}_c^*, \mathbf{q}^i)$ for the vector module M^* is then chosen such that $\mathbf{q}^r = 0$. The basis vectors are indicated by their components with respect to the conventional basis $\mathbf{a}^*$, $\mathbf{b}^*$ $\mathbf{c}^*$ of the lattice Λ^* of main reflections. The Bravais classes can also be found in Janssen (1969) and Brown *et al.* (1978). The notation of the Bravais classes there is here given in the columns Ref. *a* and Ref. *b*, respectively.

No.	Symbol	K_E	K_I	$\mathbf{q}$	Conventional basis	Centring translation(s)	Ref. *a*	Ref. *b*
Triclinic								
1	$\bar{1}P(\alpha\beta\gamma)$	$\bar{1}$	$\bar{1}$	$(\alpha\beta\gamma)$	(100), (010), (001), $(\alpha\beta\gamma)$		I *P*	I/I
Monoclinic								
2	$2/mP(\alpha\beta 0)$	$2/m$	$\bar{1}1$	$(\alpha\beta 0)$	(100), (010), (001), $(\alpha\beta 0)$		II *P*	II/I
3	$2/mP(\alpha\beta\frac{1}{2})$	$2/m$	$\bar{1}1$	$(\alpha\beta\frac{1}{2})$	(100), (010), $(00\frac{1}{2})$, $(\alpha\beta 0)$	$00\frac{1}{2}\frac{1}{2}$	II *I*	II/II
4	$2/mB(\alpha\beta 0)$	$2/m$	$\bar{1}1$	$(\alpha\beta 0)$	(100), (010), (001), $(\alpha\beta 0)$	$\frac{1}{2}0\frac{1}{2}0$	II *I*	II/II
5	$2/mP(00\gamma)$	$2/m$	$1\bar{1}$	(00γ)	(100), (010), (001), (00γ)		III *P*	III/I
6	$2/mP(\frac{1}{2}0\gamma)$	$2/m$	$1\bar{1}$	$(\frac{1}{2}0\gamma)$	$(\frac{1}{2}00)$, (010), (001), (00γ)	$\frac{1}{2}00\frac{1}{2}$	III *I*	III/II
7	$2/mB(00\gamma)$	$2/m$	$1\bar{1}$	(00γ)	(100), (010), (001), (00γ)	$\frac{1}{2}0\frac{1}{2}0$	III *I*	III/II
8	$2/mB(0\frac{1}{2}\gamma)$	$2/m$	$1\bar{1}$	$(0\frac{1}{2}\gamma)$	(100), $(0\frac{1}{2}0)$, (001), (00γ)	$\frac{1}{2}0\frac{1}{2}0$, $0\frac{1}{2}0\frac{1}{2}$	III *G*	III/III
Orthorhombic								
9	$mmmP(00\gamma)$	mmm	$11\bar{1}$	(00γ)	(100), (010), (001), (00γ)		IV *P*	IV/I
10	$mmmP(0\frac{1}{2}\gamma)$	mmm	$11\bar{1}$	$(0\frac{1}{2}\gamma)$	(100), $(0\frac{1}{2}0)$, (001), (00γ)	$0\frac{1}{2}0\frac{1}{2}$	IV *B*	IV/III
11	$mmmP(\frac{1}{2}\frac{1}{2}\gamma)$	mmm	$11\bar{1}$	$(\frac{1}{2}\frac{1}{2}\gamma)$	$(\frac{1}{2}00)$, $(0\frac{1}{2}0)$, (001), (00γ)	$\frac{1}{2}00\frac{1}{2}$, $0\frac{1}{2}0\frac{1}{2}$	IV *F*	IV/VI
12	$mmmI(00\gamma)$	mmm	$11\bar{1}$	(00γ)	(100), (010), (001), (00γ)	$\frac{1}{2}\frac{1}{2}\frac{1}{2}0$	IV *I*	IV/IV
13	$mmmC(00\gamma)$	mmm	$11\bar{1}$	(00γ)	(100), (010), (001), (00γ)	$\frac{1}{2}\frac{1}{2}00$	IV *C*	IV/II
14	$mmmC(10\gamma)$	mmm	$11\bar{1}$	(10γ)	(100), (010), (001), (00γ)	$\frac{1}{2}\frac{1}{2}0\frac{1}{2}$	IV *I*	IV/IV
15	$mmmA(00\gamma)$	mmm	$11\bar{1}$	(00γ)	(100), (010), (001), (00γ)	$0\frac{1}{2}\frac{1}{2}0$	IV *B*	IV/III
16	$mmmA(\frac{1}{2}0\gamma)$	mmm	$11\bar{1}$	$(\frac{1}{2}0\gamma)$	$(\frac{1}{2}00)$, (010), (001), (00γ)	$0\frac{1}{2}\frac{1}{2}0$, $\frac{1}{2}00\frac{1}{2}$	IV *G*	IV/V
17	$mmmF(00\gamma)$	mmm	$11\bar{1}$	(00γ)	(100), (010), (001), (00γ)	$\frac{1}{2}\frac{1}{2}00$, $\frac{1}{2}0\frac{1}{2}0$	IV *F*	IV/VI
18	$mmmF(10\gamma)$	mmm	$11\bar{1}$	(10γ)	(100), (010), (001), (00γ)	$\frac{1}{2}\frac{1}{2}0\frac{1}{2}$, $\frac{1}{2}0\frac{1}{2}\frac{1}{2}$	IV *G*	IV/V
Tetragonal								
19	$4/mmmP(00\gamma)$	$4/mmm$	$1\bar{1}11$	(00γ)	(100), (010), (001), (00γ)		VII *P*	VI/I
20	$4/mmmP(\frac{1}{2}\frac{1}{2}\gamma)$	$4/mmm$	$1\bar{1}11$	$(\frac{1}{2}\frac{1}{2}\gamma)$	$(\frac{1}{2}\frac{1}{2}0)$, $(\bar{\frac{1}{2}}\frac{1}{2}0)$, (001), (00γ)	$\frac{1}{2}\frac{1}{2}0\frac{1}{2}$	VII *I*	VI/II
21	$4/mmmI(00\gamma)$	$4/mmm$	$1\bar{1}11$	(00γ)	(100), (010), (001), (00γ)	$\frac{1}{2}\frac{1}{2}\frac{1}{2}0$	VII *I*	VI/II
Trigonal								
22	$\bar{3}mR(00\gamma)$	$\bar{3}m$	$\bar{1}1$	(00γ)	(100), (010), (001), (00γ)	$\frac{1}{3}\frac{2}{3}\frac{2}{3}0$	VI *P*	VII/I
23	$\bar{3}1mP(\frac{1}{3}\frac{1}{3}\gamma)$	$\bar{3}1m$	$\bar{1}11$	$(\frac{1}{3}\frac{1}{3}\gamma)$	$(\frac{1}{3}\frac{1}{3}0)$, $(\bar{\frac{1}{3}}\frac{2}{3}0)$, (001), (00γ)	$\frac{1}{3}\frac{2}{3}0\frac{2}{3}$	VI *P*	VII/I
Hexagonal								
24	$6/mmmP(00\gamma)$	$6/mmm$	$1\bar{1}11$	(00γ)	(100), (010), (001), (00γ)		V *P*	VII/II

class has been discussed in Subsection 9.8.3.2. Given a point-group transformation R_s, the associated translation is determined up to a lattice translation. As in three dimensions, the translational part generally depends on the choice of origin. To avoid this arbitrariness, one decomposes that translation into a component (called intrinsic) independent of the origin, and a remainder. The (3 + 1)-dimensional translation υ_s associated with the point-group transformation R_s is given by

$$\upsilon_s = \sum_{i=1}^{3+1} \upsilon_i a_{is}. \qquad (9.8.3.4)$$

Its origin-invariant part υ_s^o is given by

$$\upsilon_s^o = \sum_{j=1}^{4} \upsilon_j^o a_{sj} \quad \text{with} \quad \upsilon_j^o = \frac{1}{n} \sum_{m=1}^{n} \sum_{k=1}^{4} \Gamma(R^m)_{jk} \upsilon_k, \qquad (9.8.3.5)$$

where n is now the order of the point-group transformation R so that R^n is the identity. As customary also in three-dimensional crystallography, one indicates in the space-group symbol the invariant components υ_j^o. Notice that this means that there is an origin for R_s in (3 + 1)-dimensional superspace such that the translation associated with R_s has these components. This origin, however, may not be the same for different transformations R_s, as is known in three-dimensional crystallography.

(*continued on page* 920)

Table 9.8.3.2(*b*). (3 + 1)-*Dimensional Bravais classes for commensurate 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 $h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* + m\mathbf{q}$, where $\mathbf{q}$ is the modulation wavevector. Here $\mathbf{q}$ is a commensurate vector having rational components with respect to $\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$. The rank of the vector module M^* is three. Therefore, there are three basis vectors for M^*. They are given by their components with respect to the conventional basis $\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$ of the lattice of main reflections. If they do not coincide with the primitive basis vectors of the lattice Λ^* of main reflections, there is a centring in four-dimensional space. The notation of the Bravais classes in Janssen (1969) is here given in the column Ref. *a*. Notice that for a commensurate one-dimensional modulation cubic symmetry is also possible.

No.	Symbol	K_E	K_I	$\mathbf{q}$	Conventional basis	Centring translation(s)	Ref. *a*
Triclinic							
1	$\bar{1}P(000)$	$\bar{1}1$	$1\bar{1}$	(000)	(100), (010), (001)		II *P*
2	$\bar{1}P(\frac{1}{2}\frac{1}{2}\frac{1}{2})$	$\bar{1}1$	$1\bar{1}$	$(\frac{1}{2}\frac{1}{2}\frac{1}{2})$	$(\bar{\frac{1}{2}}\frac{1}{2}\frac{1}{2}), (\frac{1}{2}\bar{\frac{1}{2}}\frac{1}{2}), (\frac{1}{2}\frac{1}{2}\bar{\frac{1}{2}})$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}$	II *I*
Monoclinic							
3	$2/mP(000)$	$2/m1$	$11\bar{1}$	(000)	(100), (010), (001)		IV *P*
4	$2/mP(\frac{1}{2}\frac{1}{2}0)$	$2/m1$	$11\bar{1}$	$(\frac{1}{2}\frac{1}{2}0)$	$(\frac{1}{2}\frac{1}{2}0), (\bar{\frac{1}{2}}\frac{1}{2}0), (001)$	$\frac{1}{2}\frac{1}{2}0\frac{1}{2}$	IV *B*
5	$2/mP(00\frac{1}{2})$	$2/m1$	$11\bar{1}$	$(00\frac{1}{2})$	$(100), (010), (00\frac{1}{2})$	$00\frac{1}{2}\frac{1}{2}$	IV *C*
6	$2/mP(\frac{1}{2}\frac{1}{2}\frac{1}{2})$	$2/m1$	$11\bar{1}$	$(\frac{1}{2}\frac{1}{2}\frac{1}{2})$	$(\frac{1}{2}\frac{1}{2}0), (\bar{\frac{1}{2}}\frac{1}{2}0), (00\frac{1}{2})$	$\frac{1}{2}\frac{1}{2}0\frac{1}{2}, 00\frac{1}{2}\frac{1}{2}$	IV *F*
7	$2/mB(000)$	$2/m1$	$11\bar{1}$	(000)	(100), (010), (001)	$\frac{1}{2}0\frac{1}{2}0$	IV *B*
8	$2/mB(100)$	$2/m1$	$11\bar{1}$	(100)	(100), (010), (001)	$\frac{1}{2}0\bar{\frac{1}{2}}\frac{1}{2}$	IV *I*
9	$2/mB(0\frac{1}{2}0)$	$2/m1$	$11\bar{1}$	$(0\frac{1}{2}0)$	$(100), (0\frac{1}{2}0), (001)$	$\frac{1}{2}0\frac{1}{2}0, 0\frac{1}{2}0\frac{1}{2}$	IV *G*
Orthorhombic							
10	$mmmP(000)$	$mmm1$	$111\bar{1}$	(000)	(100), (010), (001)		VIII *P*
11	$mmmP(00\frac{1}{2})$	$mmm1$	$111\bar{1}$	$(00\frac{1}{2})$	$(100), (010), (00\frac{1}{2})$	$00\frac{1}{2}\frac{1}{2}$	VIII *A*
12	$mmmP(0\frac{1}{2}\frac{1}{2})$	$mmm1$	$111\bar{1}$	$(0\frac{1}{2}\frac{1}{2})$	$(100), (0\frac{1}{2}0), (00\frac{1}{2})$	$0\frac{1}{2}0\frac{1}{2}, 00\frac{1}{2}\frac{1}{2}$	VIII *F*
13	$mmmP(\frac{1}{2}\frac{1}{2}\frac{1}{2})$	$mmm1$	$111\bar{1}$	$(\frac{1}{2}\frac{1}{2}\frac{1}{2})$	$(\frac{1}{2}00), (0\frac{1}{2}0), (00\frac{1}{2})$	$\frac{1}{2}00\frac{1}{2}, 0\frac{1}{2}0\frac{1}{2}, 00\frac{1}{2}\frac{1}{2}$	VIII *S*
14	$mmmI(000)$	$mmm1$	$111\bar{1}$	(000)	(100), (010), (001)	$\frac{1}{2}\frac{1}{2}\frac{1}{2}0$	VIII *E*
15	$mmmI(111)$	$mmm1$	$111\bar{1}$	(111)	(100), (010), (001)	$\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}$	VIII *I*
16	$mmmI(\frac{1}{2}\frac{1}{2}\frac{1}{2})$	mmm	$\bar{1}\bar{1}\bar{1}$	$(\frac{1}{2}\frac{1}{2}\frac{1}{2})$	$(\frac{1}{2}00), (0\frac{1}{2}0), (00\frac{1}{2})$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\frac{1}{4}, \bar{\frac{1}{4}}\frac{1}{4}\frac{1}{4}\bar{\frac{1}{4}}, \frac{1}{4}\frac{1}{4}\bar{\frac{1}{4}}\bar{\frac{1}{4}}$	VIII *K*
17	$mmmF(000)$	$mmm1$	$111\bar{1}$	(000)	(100), (010), (001)	$\frac{1}{2}\frac{1}{2}00, \frac{1}{2}0\frac{1}{2}0$	VIII *F*
18	$mmmF(001)$	$mmm1$	$111\bar{1}$	(001)	(100), (010), (001)	$\frac{1}{2}\frac{1}{2}00, \frac{1}{2}0\frac{1}{2}\frac{1}{2}$	VIII *H*
19	$mmmC(000)$	$mmm1$	$111\bar{1}$	(000)	(100), (010), (001)	$\frac{1}{2}\frac{1}{2}00$	VIII *A*
20	$mmmC(100)$	$mmm1$	$111\bar{1}$	(100)	(100), (010), (001)	$\frac{1}{2}\frac{1}{2}0\frac{1}{2}$	VIII *E*
21	$mmmC(00\frac{1}{2})$	$mmm1$	$111\bar{1}$	$(00\frac{1}{2})$	$(100), (010), (00\frac{1}{2})$	$\frac{1}{2}\frac{1}{2}00, 00\frac{1}{2}\frac{1}{2}$	VIII *G*
22	$mmmC(10\frac{1}{2})$	$mmm1$	$111\bar{1}$	$(10\frac{1}{2})$	$(100), (010), (00\frac{1}{2})$	$\frac{1}{2}\frac{1}{2}0\frac{1}{2}, \frac{1}{2}\frac{1}{2}\frac{1}{2}0$	VIII *H*
Tetragonal							
23	$4/mmmP(000)$	$4/mmm1$	$1111\bar{1}$	(000)	(100), (010), (001)		XII *P*
24	$4/mmmP(00\frac{1}{2})$	$4/mmm1$	$1111\bar{1}$	$(00\frac{1}{2})$	$(100), (010), (00\frac{1}{2})$	$00\frac{1}{2}\frac{1}{2}$	XII *A*
25	$4/mmmP(\frac{1}{2}\frac{1}{2}0)$	$4/mmm1$	$1111\bar{1}$	$(\frac{1}{2}\frac{1}{2}0)$	$(\frac{1}{2}\frac{1}{2}0), (\bar{\frac{1}{2}}\frac{1}{2}0), (001)$	$\frac{1}{2}\frac{1}{2}0\frac{1}{2}$	XII *E*
26	$4/mmmP(\frac{1}{2}\frac{1}{2}\frac{1}{2})$	$4/mmm1$	$1111\bar{1}$	$(\frac{1}{2}\frac{1}{2}\frac{1}{2})$	$(\frac{1}{2}\frac{1}{2}0), (\bar{\frac{1}{2}}\frac{1}{2}0), (00\frac{1}{2})$	$\frac{1}{2}\frac{1}{2}0\frac{1}{2}, 00\frac{1}{2}\frac{1}{2}$	XII *H*
27	$4/mmmI(000)$	$4/mmm1$	$1111\bar{1}$	(000)	(100), (010), (001)	$\frac{1}{2}\frac{1}{2}\frac{1}{2}0$	XII *E*
28	$4/mmmI(111)$	$4/mmm1$	$1111\bar{1}$	(111)	(100), (010), (001)	$\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}$	XII *I*
29	$4/mmmI(\frac{1}{2}\frac{1}{2}\frac{1}{2})$	$4/mmm$	$\bar{1}\bar{1}\bar{1}1$	$(\frac{1}{2}\frac{1}{2}\frac{1}{2})$	(100), (010), (001)		XII *N*
Trigonal							
30	$\bar{3}m1R(000)$	$\bar{3}m1$	$11\bar{1}$	(000)	(100), (010), (001)	$\frac{2}{3}\frac{1}{3}\frac{1}{3}0$	X *R*
31	$\bar{3}m1R(00\frac{1}{2})$	$\bar{3}m1$	$11\bar{1}$	$(00\frac{1}{2})$	$(100), (010), (00\frac{1}{2})$	$00\frac{1}{2}\frac{1}{2}, \frac{2}{3}\frac{1}{3}\frac{1}{6}\frac{1}{6}$	X *RI*
Hexagonal							
32	$6/mmmP(000)$	$6/mmm1$	$1111\bar{1}$	(000)	(100), (010), (001)		X *P*
33	$6/mmmP(00\frac{1}{2})$	$6/mmm1$	$1111\bar{1}$	$(00\frac{1}{2})$	$(100), (010), (00\frac{1}{2})$	$00\frac{1}{2}\frac{1}{2}$	X *A*
34	$6/mmmP(\frac{1}{3}\frac{1}{3}0)$	$6/mmm$	$\bar{1}11\bar{1}$	$(\frac{1}{3}\frac{1}{3}0)$	$(\frac{1}{3}\frac{1}{3}0), (\bar{\frac{1}{3}}\frac{2}{3}0), (001)$	$\frac{1}{3}\frac{2}{3}0\frac{2}{3}$	X *R*
35	$6/mmmP(\frac{1}{3}\frac{1}{3}\frac{1}{2})$	$6/mmm$	$\bar{1}11\bar{1}$	$(\frac{1}{3}\frac{1}{3}\frac{1}{2})$	$(\frac{1}{3}\frac{1}{3}0), (\bar{\frac{1}{3}}\frac{2}{3}0), (00\frac{1}{2})$	$\frac{1}{3}\frac{2}{3}0\frac{2}{3}, 00\frac{1}{2}\frac{1}{2}$	X *RI*
Cubic							
36	$m3mP(000)$	$m\bar{3}m1$	$111\bar{1}$	(000)	(100), (010), (001)		XIV *P*
37	$m3mP(\frac{1}{2}\frac{1}{2}\frac{1}{2})$	$m\bar{3}m1$	$111\bar{1}$	$(\frac{1}{2}\frac{1}{2}\frac{1}{2})$	$(\frac{1}{2}00), (0\frac{1}{2}0), (00\frac{1}{2})$	$\frac{1}{2}00\frac{1}{2}, 0\frac{1}{2}0\frac{1}{2}, 00\frac{1}{2}\frac{1}{2}$	XIV *S*
38	$m3mI(000)$	$m\bar{3}m1$	$111\bar{1}$	(000)	(100), (010), (001)	$\frac{1}{2}\frac{1}{2}\frac{1}{2}0$	XIV *V*
39	$m3mI(111)$	$m\bar{3}m1$	$111\bar{1}$	(111)	(100), (010), (001)	$\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}$	XIV *I*
40	$m3mI(\frac{1}{2}\frac{1}{2}\frac{1}{2})$	$m\bar{3}m$	$\bar{1}\bar{1}1$	$(\frac{1}{2}\frac{1}{2}\frac{1}{2})$	$(\frac{1}{2}00), (0\frac{1}{2}0), (00\frac{1}{2})$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\frac{1}{4}, \bar{\frac{1}{4}}\frac{1}{4}\frac{1}{4}\bar{\frac{1}{4}}, \frac{1}{4}\frac{1}{4}\bar{\frac{1}{4}}\bar{\frac{1}{4}}$	XIV *K*
41	$m3mF(000)$	$m\bar{3}m1$	$111\bar{1}$	(000)	(100), (010), (001)	$\frac{1}{2}\frac{1}{2}00, \frac{1}{2}0\frac{1}{2}0$	XIV *F*

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

The four-dimensional point group K_s has external part K_E, which belongs to a three-dimensional system. Depending on the Bravais class of the four-dimensional lattice left invariant by K_s, this point group gives rise to an integral 4×4 matrix group $\Gamma(K)$ which belongs to one of the arithmetic crystal classes given in the last column.

System	Point group		External Bravais class	Arithmetic crystal class(es)
	K_E	K_s		
Triclinic	1	$(1, 1)$	$\bar{1}P$	$1P(\alpha\beta\gamma)$
	$\bar{1}$	$(\bar{1}, \bar{1})$	$\bar{1}P$	$\bar{1}P(\alpha\beta\gamma)$
Monoclinic	2	$(2, \bar{1})$	$2/mP$	$2P(\alpha\beta 0), 2P(\alpha\beta\frac{1}{2})$
			$2/mB$	$2B(\alpha\beta 0)$
		$(2, 1)$	$2/mP$	$2P(00\gamma), 2P(\frac{1}{2}0\gamma)$
			$2/mB$	$2B(00\gamma), 2B(0\frac{1}{2}\gamma)$
	m	$(m, 1)$	$2/mP$	$mP(\alpha\beta 0), mP(\alpha\beta\frac{1}{2})$
			$2/mB$	$mB(\alpha\beta 0)$
		$(m, \bar{1})$	$2/mP$	$mP(00\gamma), mP(\frac{1}{2}0\gamma)$
			$2/mB$	$mB(00\gamma), mB(0\frac{1}{2}\gamma)$
	$2/m$	$(2/m, \bar{1}1)$	$2/mP$	$2/mP(\alpha\beta 0), 2/mP(\alpha\beta\frac{1}{2})$
			$2/mB$	$2/mB(\alpha\beta 0)$
		$(2/m, 1\bar{1})$	$2/mP$	$2/mP(00\gamma), 2/mP(\frac{1}{2}0\gamma)$
			$2/mB$	$2/mB(00\gamma), 2/mB(0\frac{1}{2}\gamma)$
Orthorhombic	222	$(222, \bar{1}\bar{1}1)$	$mmmP$	$222P(00\gamma), 222P(0\frac{1}{2}\gamma), 222P(\frac{1}{2}\frac{1}{2}\gamma)$
			$mmmI$	$222I(00\gamma)$
			$mmmF$	$222F(00\gamma), 222F(10\gamma)$
			$mmmC$	$222C(00\gamma), 222C(10\gamma)$
		$(222, 1\bar{1}\bar{1})$	$mmmC$	$222C(\alpha 00), 222C(\alpha 0\frac{1}{2})$
	$mm2$	$(mm2, 111)$	$mmmP$	$mm2P(00\gamma), mm2P(0\frac{1}{2}\gamma), mm2P(\frac{1}{2}\frac{1}{2}\gamma)$
			$mmmI$	$mm2I(00\gamma)$
			$mmmF$	$mm2F(00\gamma), mm2F(10\gamma)$
			$mmmC$	$mm2C(00\gamma), mm2C(10\gamma)$
		$(2mm, 111)$	$mmmC$	$2mmC(\alpha 00), 2mmC(\alpha 0\frac{1}{2})$
		$(2mm, \bar{1}1\bar{1})$	$mmmP$	$2mmP(00\gamma), 2mmP(0\frac{1}{2}\gamma), 2mmP(\frac{1}{2}\frac{1}{2}\gamma)$
			$mmmI$	$2mmI(00\gamma)$
			$mmmF$	$2mmF(00\gamma), 2mmF(10\gamma)$
			$mmmC$	$2mmC(00\gamma), 2mmC(10\gamma)$
		$(mm2, \bar{1}1\bar{1})$	$mmmC$	$mm2C(\alpha 00), mm2C(\alpha 0\frac{1}{2})$
		$(m2m, 1\bar{1}\bar{1})$	$mmmP$	$m2mP(0\frac{1}{2}\gamma)$
		$(m2m, \bar{1}\bar{1}1)$	$mmmC$	$m2mC(\alpha 00), m2mC(\alpha 0\frac{1}{2})$
	mmm	$(mmm, 11\bar{1})$	$mmmP$	$mmmP(00\gamma), mmmP(0\frac{1}{2}\gamma), mmmP(\frac{1}{2}\frac{1}{2}\gamma)$
			$mmmI$	$mmmI(00\gamma)$
			$mmmF$	$mmmF(00\gamma), mmmF(10\gamma)$
			$mmmC$	$mmmC(00\gamma), mmmC(10\gamma)$
		$(mmm, \bar{1}11)$	$mmmC$	$mmmC(\alpha 00), mmmC(\alpha 0\frac{1}{2})$
Tetragonal	4	$(4, 1)$	$4/mmmP$	$4P(00\gamma), 4P(\frac{1}{2}\frac{1}{2}\gamma)$
			$4/mmmI$	$4I(00\gamma)$
	$\bar{4}$	$(\bar{4}, \bar{1})$	$4/mmmP$	$\bar{4}P(00\gamma), \bar{4}P(\frac{1}{2}\frac{1}{2}\gamma)$
			$4/mmmI$	$\bar{4}I(00\gamma)$
	$4/m$	$(4/m, 1\bar{1})$	$4/mmmP$	$4/mP(00\gamma), 4/mP(\frac{1}{2}\frac{1}{2}\gamma)$
			$4/mmmI$	$4/mI(00\gamma)$
	422	$(422, 1\bar{1}\bar{1})$	$4/mmmP$	$422P(00\gamma), 422P(\frac{1}{2}\frac{1}{2}\gamma)$
			$4/mmmI$	$422I(00\gamma)$
	$4mm$	$(4mm, 111)$	$4/mmmP$	$4mmP(00\gamma), 4mmP(\frac{1}{2}\frac{1}{2}\gamma)$
			$4/mmmI$	$4mmI(00\gamma)$
	$\bar{4}2m$	$(\bar{4}2m, \bar{1}\bar{1}1)$	$4/mmmP$	$\bar{4}2mP(00\gamma), \bar{4}2mP(\frac{1}{2}\frac{1}{2}\gamma)$
			$4/mmmI$	$\bar{4}2mI(00\gamma)$
	$\bar{4}m2$	$(\bar{4}m2, \bar{1}1\bar{1})$	$4/mmmP$	$\bar{4}m2P(00\gamma), \bar{4}m2P(\frac{1}{2}\frac{1}{2}\gamma)$
			$4/mmmI$	$\bar{4}m2I(00\gamma)$
	$4/mmm$	$(4/mmm, 1\bar{1}11)$	$4/mmmP$	$4/mmmP(00\gamma), 4/mmmP(\frac{1}{2}\frac{1}{2}\gamma)$
			$4/mmmI$	$4/mmmI(00\gamma)$
Trigonal	3	$(3, 1)$	$\bar{3}mR$	$3R(00\gamma)$
			$6/mmmP$	$3P(00\gamma), 3P(\frac{1}{3}\frac{1}{3}\gamma)$
	$\bar{3}$	$(\bar{3}, \bar{1})$	$\bar{3}mR$	$\bar{3}R(00\gamma)$
			$6/mmmP$	$\bar{3}P(00\gamma), \bar{3}P(\frac{1}{3}\frac{1}{3}\gamma)$
	32	$(32, 1\bar{1})$	$\bar{3}mR$	$32R(00\gamma)$
			$6/mmmP$	$312P(00\gamma), 312P(\frac{1}{3}\frac{1}{3}\gamma), 321P(00\gamma)$

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 υ_s associated with the point-group element (R, R_I) is $(\mathbf{v}, \upsilon_I)$, where υ_I can be written as $\delta - \mathbf{q}\cdot\mathbf{v}$. In accordance with (9.8.1.12), δ is defined as υ_4. The origin-invariant part υ_s^o of υ_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 τ 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 τ. 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 τ, one for each generator appearing in the three-dimensional space-group symbol. A letter symbolizes the value of τ according to

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

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 $(2/m, \bar{1}1)$. 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	$cmm(\alpha 0, 0\mu)$

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

No.	Basic space group	Point group K_s	Bravais class No.	Group symbol
Rectangular (*cont.*)				
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 τ 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 $P^{P112_1/m}_{\bar{1}\bar{1}\bar{1}\ \ s}$, 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)

Table 9.8.3.5. (3 + 1)-*Dimensional superspace groups*

The number labelling the superspace group is denoted by *n.m*, where *n* is the number attached to the three-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 K_s, the number of the four-dimensional Bravais class to which the superspace group belongs (Table 9.8.3.2*a*), and the superspace-group symbol are also given. The superspace-group symbol is indicated in the short notation, *i.e.* for the basic group one uses the short symbol from *International Tables for Crystallography*, Volume A, and then the values of τ are given for each of the generators in this symbol, unless all these values are zero. Then, instead of writing a number of zeros, one omits them all. Finally, the special reflection conditions due to non-primitive translations are given, for *hklm* if $\mathbf{q}^r = 0$ and for *HKLm* otherwise. Recall the *HKLm* are the indices with respect to a conventional basis $\mathbf{a}_c^*, \mathbf{b}_c^*, \mathbf{c}_c^*, \mathbf{q}^i$ as in Table 9.8.3.2(*a*). The reflection conditions due to centring translations are given in Table 9.8.3.6.

No.	Basic space group	Point group K_s	Bravais class No.	Group symbol	Special reflection conditions
1.1	$P1$	$(1, 1)$	1	$P1(\alpha\beta\gamma)$	
2.1	$P\bar{1}$	$(\bar{1}, \bar{1})$	1	$P\bar{1}(\alpha\beta\gamma)$	
3.1	$P2$	$(2, \bar{1})$	2	$P2(\alpha\beta 0)$	
3.2		$(2, \bar{1})$	3	$P2(\alpha\beta\frac{1}{2})$	
3.3		$(2, 1)$	5	$P2(00\gamma)$	
3.4		$(2, 1)$	5	$P2(00\gamma)s$	$00lm$: $m=2n$
3.5		$(2, 1)$	6	$P2(\frac{1}{2}0\gamma)$	
4.1	$P2_1$	$(2, \bar{1})$	2	$P2_1(\alpha\beta 0)$	$00l0$: $l=2n$
4.2		$(2, 1)$	5	$P2_1(00\gamma)$	$00lm$: $l=2n$
4.3		$(2, 1)$	6	$P2_1(\frac{1}{2}0\gamma)$	$00Lm$: $L=2n$
5.1	$B2$	$(2, \bar{1})$	4	$B2(\alpha\beta 0)$	
5.2		$(2, 1)$	7	$B2(00\gamma)$	
5.3		$(2, 1)$	7	$B2(00\gamma)s$	$00lm$: $m=2n$
5.4		$(2, 1)$	8	$B2(0\frac{1}{2}\gamma)$	
6.1	Pm	$(m, 1)$	2	$Pm(\alpha\beta 0)$	
6.2		$(m, 1)$	2	$Pm(\alpha\beta 0)s$	$hk0m$: $m=2n$
6.3		$(m, 1)$	3	$Pm(\alpha\beta\frac{1}{2})$	
6.4		$(m, \bar{1})$	5	$Pm(00\gamma)$	
6.5		$(m, \bar{1})$	6	$Pm(\frac{1}{2}0\gamma)$	
7.1	Pb	$(m, 1)$	2	$Pb(\alpha\beta 0)$	$hk0m$: $k=2n$
7.2		$(m, 1)$	3	$Pb(\alpha\beta\frac{1}{2})$	$HK0m$: $K=2n$
7.3		$(m, \bar{1})$	5	$Pb(00\gamma)$	$hk00$: $k=2n$
7.4		$(m, \bar{1})$	6	$Pb(\frac{1}{2}0\gamma)$	$HK00$: $K=2n$
8.1	Bm	$(m, 1)$	4	$Bm(\alpha\beta 0)$	
8.2		$(m, 1)$	4	$Bm(\alpha\beta 0)s$	$hk0m$: $m=2n$
8.3		$(m, \bar{1})$	7	$Bm(00\gamma)$	
8.4		$(m, \bar{1})$	8	$Bm(0\frac{1}{2}\gamma)$	
9.1	Bb	$(m, 1)$	4	$Bb(\alpha\beta 0)$	$hk0m$: $k=2n$
9.2		$(m, \bar{1})$	7	$Bb(00\gamma)$	$hk00$: $k=2n$
10.1	$P2/m$	$(2/m, \bar{1}1)$	2	$P2/m(\alpha\beta 0)$	
10.2		$(2/m, \bar{1}1)$	2	$P2/m(\alpha\beta 0)0s$	$hk0m$: $m=2n$
10.3		$(2/m, \bar{1}1)$	3	$P2/m(\alpha\beta\frac{1}{2})$	
10.4		$(2/m, 1\bar{1})$	5	$P2/m(00\gamma)$	
10.5		$(2/m, 1\bar{1})$	5	$P2/m(00\gamma)s0$	$00lm$: $m=2n$
10.6		$(2/m, 1\bar{1})$	6	$P2/m(\frac{1}{2}0\gamma)$	
11.1	$P2_1/m$	$(2/m, \bar{1}1)$	2	$P2_1/m(\alpha\beta 0)$	$00l0$: $l=2n$
11.2		$(2/m, \bar{1}1)$	2	$P2_1/m(\alpha\beta 0)0s$	$00l0$: $l=2n$; $hk0m$: $m=2n$
11.3		$(2/m, 1\bar{1})$	5	$P2_1/m(00\gamma)$	$00lm$: $l=2n$
11.4		$(2/m, 1\bar{1})$	6	$P2_1/m(\frac{1}{2}0\gamma)$	$00Lm$: $L=2n$
12.1	$B2/m$	$(2/m, \bar{1}1)$	4	$B2/m(\alpha\beta 0)$	
12.2		$(2/m, \bar{1}1)$	4	$B2/m(\alpha\beta 0)0s$	$hk0m$: $m=2n$
12.3		$(2/m, 1\bar{1})$	7	$B2/m(00\gamma)$	
12.4		$(2/m, 1\bar{1})$	7	$B2/m(00\gamma)s0$	$00lm$: $m=2n$
12.5		$(2/m, 1\bar{1})$	8	$B2/m(\frac{1}{2}0\gamma)$	
13.1	$P2/b$	$(2/m, \bar{1}1)$	2	$P2/b(\alpha\beta 0)$	$hk0m$: $k=2n$
13.2		$(2/m, \bar{1}1)$	3	$P2/b(\alpha\beta\frac{1}{2})$	$HK0m$: $m=2n$
13.3		$(2/m, 1\bar{1})$	5	$P2/b(00\gamma)$	$hk00$: $k=2n$
13.4		$(2/m, 1\bar{1})$	5	$P2/b(00\gamma)s0$	$00lm$: $m=2n$; $hk00$: $k=2n$
13.5		$(2/m, 1\bar{1})$	6	$P2/b(\frac{1}{2}0\gamma)$	$HK00$: $K=2n$
14.1	$P2_1/b$	$(2/m, \bar{1}1)$	2	$P2_1/b(\alpha\beta 0)$	$00l0$: $l=2n$; $hk0m$: $k=2n$
14.2		$(2/m, 1\bar{1})$	5	$P2_1/b(00\gamma)$	$00lm$: $l=2n$; $hk00$: $k=2n$
14.3		$(2/m, 1\bar{1})$	6	$P2_1/b(\frac{1}{2}0\gamma)$	$00Lm$: $L=2n$; $HK00$: $K=2n$
15.1	$B2/b$	$(2/m, \bar{1}1)$	4	$B2/b(\alpha\beta 0)$	$hk0m$: $k=2n$
15.2		$(2/m, 1\bar{1})$	7	$B2/b(00\gamma)$	$hk00$: $k=2n$
15.3		$(2/m, 1\bar{1})$	7	$B2/b(00\gamma)s0$	$00lm$: $m=2n$; $hk00$: $k=2n$

Table 9.8.3.5. (3 + 1)-*Dimensional superspace groups (cont.)*

No.	Basic space group	Point group K_s	Bravais class No.	Group symbol	Special reflection conditions
16.1	$P222$	$(222, \bar{1}\bar{1}1)$	9	$P222(00\gamma)$	
16.2			9	$P222(00\gamma)00s$	$00lm$: $m=2n$
16.3			10	$P222(0\frac{1}{2}\gamma)$	
16.4			11	$P222(\frac{11}{22}\gamma)$	
17.1	$P222_1$	$(222, \bar{1}\bar{1}1)$	9	$P222_1(00\gamma)$	$00lm$: $l=2n$
17.2			10	$P222_1(0\frac{1}{2}\gamma)$	$00Lm$: $L=2n$
17.3			11	$P222_1(\frac{11}{22}\gamma)$	$00Lm$: $L=2n$
17.4			9	$P2_122(00\gamma)$	$h000$: $h=2n$
17.5			9	$P2_122(00\gamma)00s$	$h000$: $h=2n$; $00lm$: $m=2n$
17.6			10	$P2_122(0\frac{1}{2}\gamma)$	$H000$: $H=2n$
18.1	$P2_12_12$	$(222, \bar{1}\bar{1}1)$	9	$P2_12_12(00\gamma)$	$h000$: $h=2n$; $0k00$: $k=2n$
18.2			9	$P2_12_12(00\gamma)00s$	$h000$: $h=2n$; $0k00$: $k=2n$; $00lm$: $m=2n$
18.3			9	$P2_122_1(00\gamma)$	$h000$: $h=2n$; $00lm$: $l=2n$
18.4			10	$P2_122_1(0\frac{1}{2}\gamma)$	$H000$: $H=2n$; $00Lm$: $L=2n$
19.1	$P2_12_12_1$	$(222, \bar{1}\bar{1}1)$	9	$P2_12_12_1(00\gamma)$	$h000$: $h=2n$; $0k00$: $k=2n$; $00lm$: $l=2n$
20.1	$C222_1$	$(222, \bar{1}\bar{1}1)$	13	$C222_1(00\gamma)$	$00lm$: $l=2n$
20.2			14	$C222_1(10\gamma)$	$00Lm$: $L=2n$
20.3			15	$A2_122(00\gamma)$	$h000$: $h=2n$
20.4			15	$A2_122(00\gamma)00s$	$h000$: $h=2n$; $00lm$: $m=2n$
21.1	$C222$	$(222, \bar{1}\bar{1}1)$	13	$C222(00\gamma)$	
21.2			13	$C222(00\gamma)00s$	$00lm$: $m=2n$
21.3			14	$C222(10\gamma)$	
21.4			14	$C222(10\gamma)00s$	$00Lm$: $m=2n$
21.5			15	$A222(00\gamma)$	
21.6			15	$A222(00\gamma)00s$	$00lm$: $m=2n$
21.7			16	$A222(\frac{1}{2}0\gamma)$	
22.1	$F222$	$(222, \bar{1}\bar{1}1)$	17	$F222(00\gamma)$	
22.2			17	$F222(00\gamma)00s$	$00lm$: $m=2n$
22.3			18	$F222(10\gamma)$	
23.1	$I222$	$(222, \bar{1}\bar{1}1)$	12	$I222(00\gamma)$	
23.2			12	$I222(00\gamma)00s$	$00lm$: $m=2n$
24.1	$I2_12_12_1$	$(222, \bar{1}\bar{1}1)$	12	$I2_12_12_1(00\gamma)$	$h000$: $h=2n$; $0k00$: $k=2n$; $00lm$: $l=2n$
24.2			12	$I2_12_12_1(00\gamma)00s$	$h000$: $h=2n$; $0k00$: $k=2n$; $00lm$: $l+m=2n$
25.1	$Pmm2$	$(mm2, 111)$	9	$Pmm2(00\gamma)$	
25.2			9	$Pmm2(00\gamma)s0s$	$0klm$: $m=2n$
25.3			9	$Pmm2(00\gamma)ss0$	$0klm$: $m=2n$; $h0lm$: $m=2n$
25.4			10	$Pmm2(0\frac{1}{2}\gamma)$	
25.5			10	$Pmm2(0\frac{1}{2}\gamma)s0s$	$0KLm$: $m=2n$
25.6			11	$Pmm2(\frac{1}{2}\frac{1}{2}\gamma)$	
25.7		$(m2m, 1\bar{1}\bar{1})$	10	$Pm2m(0\frac{1}{2}\gamma)$	
25.8			10	$Pm2m(0\frac{1}{2}\gamma)s00$	$0KLm$: $m=2n$
25.9		$(2mm, \bar{1}1\bar{1})$	9	$P2mm(00\gamma)$	
25.10			9	$P2mm(00\gamma)0s0$	$h0lm$: $m=2n$
25.11			10	$P2mm(0\frac{1}{2}\gamma)$	
25.12			11	$P2mm(\frac{1}{2}\frac{1}{2}\gamma)$	
26.1	$Pmc2_1$	$(mm2, 111)$	9	$Pmc2_1(00\gamma)$	$h0lm$: $l=2n$
26.2			9	$Pmc2_1(00\gamma)s0s$	$0klm$: $m=2n$; $h0lm$: $l=2n$
26.3			10	$Pmc2_1(0\frac{1}{2}\gamma)$	$H0Lm$: $L=2n$
26.4			10	$Pmc2_1(0\frac{1}{2}\gamma)s0s$	$0KLm$: $m=2n$; $H0Lm$: $L=2n$
26.5			10	$Pcm2_1(0\frac{1}{2}\gamma)$	$0KLm$: $L=2n$
26.6			11	$Pmc2_1(\frac{1}{2}\frac{1}{2}\gamma)$	$H0Lm$: $L=2n$
26.7		$(2mm, \bar{1}1\bar{1})$	9	$P2_1am(00\gamma)$	$h0lm$: $h=2n$
26.8			9	$P2_1am(00\gamma)0s0$	$h0lm$: $h+m=2n$
26.9			9	$P2_1ma(00\gamma)$	$hk00$: $h=2n$
26.10			9	$P2_1ma(00\gamma)0s0$	$h0lm$: $m=2n$; $hk00$: $h=2n$
26.11			10	$P2_1am(0\frac{1}{2}\gamma)$	$H0Lm$: $H=2n$
26.12			10	$P2_1ma(0\frac{1}{2}\gamma)$	$HK00$: $H=2n$
27.1	$Pcc2$	$(mm2, 111)$	9	$Pcc2(00\gamma)$	$0klm$: $l=2n$; $h0lm$: $l=2n$
27.2			9	$Pcc2(00\gamma)s0s$	$0klm$: $l+m=2n$; $h0lm$: $l=2n$
27.3			10	$Pcc2(0\frac{1}{2}\gamma)$	$0KLm$: $L=2n$; $H0Lm$: $L=2n$
27.4			11	$Pcc2(\frac{1}{2}\frac{1}{2}\gamma)$	$0KLm$: $L=2n$; $H0Lm$: $L=2n$
27.5		$(2mm, \bar{1}1\bar{1})$	9	$P2aa(00\gamma)$	$h0lm$: $h=2n$; $hk00$: $h=2n$
27.6			9	$P2aa(00\gamma)0s0$	$h0lm$: $h+m=2n$; $hk00$: $h=2n$
27.7			10	$P2aa(0\frac{1}{2}\gamma)$	$H0Lm$: $H=2n$; $HK00$: $H=2n$
28.1	$Pma2$	$(mm2, 111)$	9	$Pma2(00\gamma)$	$h0lm$: $h=2n$
28.2			9	$Pma2(00\gamma)s0s$	$0klm$: $m=2n$; $h0lm$: $h=2n$

Table 9.8.3.5. (3 + 1)-*Dimensional superspace groups (cont.)*

No.	Basic space group	Point group K_s	Bravais class No.	Group symbol	Special reflection conditions
28.3			9	$Pma2(00\gamma)ss0$	$0klm$: $m=2n$; $h0lm$: $h+m=2n$
28.4			9	$Pma2(00\gamma)0ss$	$h0lm$: $h+m=2n$
28.5			10	$Pma2(0\frac{1}{2}\gamma)$	$H0Lm$: $H=2n$
28.6			10	$Pma2(0\frac{1}{2}\gamma)s0s$	$0KLm$: $m=2n$; $H0Lm$: $H=2n$
28.7		$(m2m, 1\bar{1}\bar{1})$	10	$Pm2a(0\frac{1}{2}\gamma)$	$HK00$: $H=2n$
28.8			10	$Pm2a(0\frac{1}{2}\gamma)s00$	$0KLm$: $m=2n$; $HK00$: $H=2n$
28.9			10	$Pc2m(0\frac{1}{2}\gamma)$	$0KLm$: $L=2n$
28.10		$(2mm, \bar{1}1\bar{1})$	9	$P2cm(00\gamma)$	$h0lm$: $l=2n$
28.11			9	$P2mb(00\gamma)$	$hk00$: $k=2n$
28.12			9	$P2mb(00\gamma)0s0$	$h0lm$: $m=2n$; $hk00$: $k=2n$
28.13			10	$P2cm(0\frac{1}{2}\gamma)$	$H0Lm$: $L=2n$
28.14			11	$P2cm(\frac{1}{2}\frac{1}{2}\gamma)$	$H0Lm$: $L=2n$
29.1	$Pca2_1$	$(mm2, 111)$	9	$Pca2_1(00\gamma)$	$0klm$: $l=2n$; $h0lm$: $h=2n$
29.2			9	$Pca2_1(00\gamma)0ss$	$0klm$: $l=2n$; $h0lm$: $h+m=2n$
29.3			10	$Pca2_1(0\frac{1}{2}\gamma)$	$0KLm$: $L=2n$; $H0Lm$: $H=2n$
29.4		$(2mm, \bar{1}1\bar{1})$	9	$P2_1ca(00\gamma)$	$hk00$: $h=2n$; $h0lm$: $l=2n$
29.5			9	$P2_1ab(00\gamma)$	$h0lm$: $h=2n$; $hk00$: $k=2n$
29.6			9	$P2_1ab(00\gamma)0s0$	$h0lm$: $h+m=2n$; $hk00$: $k=2n$
29.7			10	$P2_1ca(0\frac{1}{2}\gamma)$	$H0Lm$: $L=2n$; $HK00$: $H=2n$
30.1	$Pcn2$	$(mm2, 111)$	9	$Pcn2(00\gamma)$	$0klm$: $l=2n$; $h0lm$: $h+l=2n$
30.2			9	$Pcn2(00\gamma)s0s$	$0klm$: $l+m=2n$; $h0lm$: $h+l=2n$
30.3			10	$Pcn2(0\frac{1}{2}\gamma)$	$0KLm$: $L=2n$; $H0Lm$: $H+L=2n$
30.4		$(2mm, \bar{1}1\bar{1})$	9	$P2na(00\gamma)$	$h0lm$: $h+l=2n$; $hk00$: $h=2n$
30.5			9	$P2an(00\gamma)$	$h0lm$: $h=2n$; $hk00$: $h+k=2n$
30.6			9	$P2an(00\gamma)0s0$	$h0lm$: $h+m=2n$; $hk00$: $h+k=2n$
30.7			10	$P2na(0\frac{1}{2}\gamma)$	$H0Lm$: $H+L=2n$; $HK00$: $H=2n$
30.8			11	$P2an(\frac{1}{2}\frac{1}{2}\gamma)0q0$	$H0Lm$: $2H+m=4n$; $HK00$: $H+K=2n$
31.1	$Pmn2_1$	$(mm2, 111)$	9	$Pmn2_1(00\gamma)$	$h0lm$: $h+l=2n$
31.2			9	$Pmn2_1(00\gamma)s0s$	$0klm$: $m=2n$; $h0lm$: $h+l=2n$
31.3			10	$Pmn2_1(0\frac{1}{2}\gamma)$	$H0Lm$: $H+L=2n$
31.4			10	$Pmn2_1(0\frac{1}{2}\gamma)s0s$	$0KLm$: $m=2n$; $H0Lm$: $H+L=2n$
31.5		$(2mm, \bar{1}1\bar{1})$	9	$P2_1nm(00\gamma)$	$h0lm$: $h+l=2n$
31.6			9	$P2_1mn(00\gamma)$	$hk00$: $h+k=2n$
31.7			9	$P2_1mn(00\gamma)0s0$	$hk00$: $h+k=2n$; $h0lm$: $m=2n$
31.8			10	$P2_1nm(0\frac{1}{2}\gamma)$	$H0Lm$: $H+L=2n$
32.1	$Pba2$	$(mm2, 111)$	9	$Pba2(00\gamma)$	$0klm$: $k=2n$; $h0lm$: $h=2n$
32.2			9	$Pba2(00\gamma)s0s$	$0klm$: $k+m=2n$; $h0lm$: $h=2n$
32.3			9	$Pba2(00\gamma)ss0$	$0klm$: $k+m=2n$; $h0lm$: $h+m=2n$
32.4			11	$Pba2(\frac{1}{2}\frac{1}{2}\gamma)qq0$	$0KLm$: $2K+m=4n$; $H0Lm$: $2H+m=4n$
32.5		$(m2m, 1\bar{1}\bar{1})$	10	$Pc2a(0\frac{1}{2}\gamma)$	$0KLm$: $L=2n$; $HK00$: $H=2n$
32.6		$(2mm, \bar{1}1\bar{1})$	9	$P2cb(00\gamma)$	$h0lm$: $l=2n$; $hk00$: $k=2n$
33.1	$Pbn2_1$	$(mm2, 111)$	9	$Pbn2_1(00\gamma)$	$0klm$: $k=2n$; $h0lm$: $h+l=2n$
33.2			9	$Pbn2_1(00\gamma)s0s$	$0klm$: $k+m=2n$; $h0lm$: $h+l=2n$
33.3			11	$Pbn2_1(\frac{1}{2}\frac{1}{2}\gamma)qq0$	$0KLm$: $2K+m=4n$; $H0Lm$: $2H+2L+m=4n$
33.4		$(2mm, \bar{1}1\bar{1})$	9	$P2_1nb(00\gamma)$	$h0lm$: $h+l=2n$; $hk00$: $k=2n$
33.5			9	$P2_1cn(00\gamma)$	$h0lm$: $l=2n$; $hk00$: $h+k=2n$
34.1	$Pnn2$	$(mm2, 111)$	9	$Pnn2(00\gamma)$	$0klm$: $k+l=2n$; $h0lm$: $h+l=2n$
34.2			9	$Pnn2(00\gamma)s0s$	$0klm$: $k+l+m=2n$; $h0lm$: $h+l=2n$
34.3			11	$Pnn2(\frac{1}{2}\frac{1}{2}\gamma)qq0$	$0KLm$: $2K+2L+m=4n$; $H0Lm$: $2H+2L+m=4n$
34.4		$(2mm, \bar{1}1\bar{1})$	9	$P2nn(00\gamma)$	$h0lm$: $h+l=2n$; $hk00$: $h+k=2n$
34.5			11	$P2nn(\frac{1}{2}\frac{1}{2}\gamma)0q0$	$H0Lm$: $2H+2L+m=4n$; $HK00$: $H+K=2n$
35.1	$Cmm2$	$(mm2, 111)$	13	$Cmm2(00\gamma)$	
35.2			13	$Cmm2(00\gamma)s0s$	$0klm$: $m=2n$
35.3			13	$Cmm2(00\gamma)ss0$	$0klm$: $m=2n$; $h0lm$: $m=2n$
35.4			14	$Cmm2(10\gamma)$	
35.5			14	$Cmm2(10\gamma)s0s$	$0KLm$: $m=2n$
35.6			14	$Cmm2(10\gamma)ss0$	$0KLm$: $m=2n$; $H0Lm$: $m=2n$
35.7		$(2mm, \bar{1}1\bar{1})$	15	$A2mm(00\gamma)$	
35.8			15	$A2mm(00\gamma)0s0$	$h0lm$: $m=2n$
35.9			16	$A2mm(\frac{1}{2}0\gamma)$	
35.10			16	$A2mm(\frac{1}{2}0\gamma)0s0$	$H0Lm$: $m=2n$
36.1	$Cmc2_1$	$(mm2, 111)$	13	$Cmc2_1(00\gamma)$	
36.2			13	$Cmc2_1(00\gamma)s0s$	$0klm$: $m=2n$; $h0lm$: $l=2n$
36.3			14	$Cmc2_1(10\gamma)$	$H0Lm$: $L=2n$
36.4			14	$Cmc2_1(10\gamma)s0s$	$0KLm$: $m=2n$; $H0Lm$: $L=2n$
36.5		$(2mm, \bar{1}1\bar{1})$	15	$A2_1am(00\gamma)$	$h0lm$: $h=2n$

Table 9.8.3.5. (3 + 1)-*Dimensional superspace groups (cont.)*

No.	Basic space group	Point group K_s	Bravais class No.	Group symbol	Special reflection conditions
36.6			15	$A2_1am(00\gamma)0s0$	$h0lm$: $h+m=2n$
36.7			15	$A2_1ma(00\gamma)$	$hk00$: $h=2n$
36.8			15	$A2_1ma(00\gamma)0s0$	$h0lm$: $m=2n$; $hk00$: $h=2n$
37.1	$Ccc2$	$(mm2, 111)$	13	$Ccc2(00\gamma)$	$0klm$: $l=2n$; $h0lm$: $l=2n$
37.2			13	$Ccc2(00\gamma)s0s$	$0klm$: $l+m=2n$; $h0lm$: $l=2n$
37.3			14	$Ccc2(10\gamma)$	$0KLm$: $L=2n$; $H0Lm$: $L=2n$
37.4			14	$Ccc2(10\gamma)s0s$	$0KLm$: $L+m=2n$; $H0Lm$: $L=2n$
37.5		$(2mm, \bar{1}1\bar{1})$	15	$A2aa(00\gamma)$	$h0lm$: $h=2n$; $hk00$: $h=2n$
37.6			15	$A2aa(00\gamma)0s0$	$h0lm$: $h+m=2n$; $hk00$: $h=2n$
38.1	$C2mm$	$(2mm, \bar{1}1\bar{1})$	13	$C2mm(00\gamma)$	
38.2			13	$C2mm(00\gamma)0s0$	$h0lm$: $m=2n$
38.3			14	$C2mm(10\gamma)$	
38.4			14	$C2mm(10\gamma)0s0$	$H0Lm$: $m=2n$
38.5		$(mm2, 111)$	15	$Amm2(00\gamma)$	
38.6			15	$Amm2(00\gamma)s0s$	$0klm$: $m=2n$
38.7			15	$Amm2(00\gamma)ss0$	$0klm$: $m=2n$; $h0lm$: $m=2n$
38.8			15	$Amm2(00\gamma)0ss$	$h0lm$: $m=2n$
38.9			16	$Amm2(\frac{1}{2}0\gamma)$	
38.10			16	$Amm2(\frac{1}{2}0\gamma)0ss$	$H0Lm$: $m=2n$
38.11		$(m2m, 1\bar{1}\bar{1})$	15	$Am2m(00\gamma)$	
38.12			15	$Am2m(00\gamma)s00$	$0klm$: $m=2n$
38.13			16	$Am2m(\frac{1}{2}0\gamma)$	
39.1	$C2mb$	$(2mm, \bar{1}1\bar{1})$	13	$C2mb(00\gamma)$	$hk00$: $k=2n$
39.2			13	$C2mb(00\gamma)0s0$	$h0lm$: $m=2n$; $hk00$: $k=2n$
39.3			14	$C2mb(10\gamma)$	$HK00$: $K=2n$
39.4			14	$C2mb(10\gamma)0s0$	$H0Lm$: $m=2n$; $HK00$: $K=2n$
39.5		$(mm2, 111)$	15	$Abm2(00\gamma)$	$0klm$: $k=2n$
39.6			15	$Abm2(00\gamma)s0s$	$0klm$: $k+m=2n$
39.7			15	$Abm2(00\gamma)ss0$	$0klm$: $k+m=2n$; $h0lm$: $m=2n$
39.8			15	$Abm2(00\gamma)0ss$	$0klm$: $k=2n$; $h0lm$: $m=2n$
39.9			16	$Abm2(\frac{1}{2}0\gamma)$	$0KLm$: $K=2n$
39.10			16	$Abm2(\frac{1}{2}0\gamma)0ss$	$0KLm$: $K+m=2n$
39.11		$(m2m, 1\bar{1}\bar{1})$	15	$Ac2m(00\gamma)$	$0klm$: $l=2n$
39.12			15	$Ac2m(00\gamma)s00$	$0klm$: $l+m=2n$
39.13			16	$Ac2m(\frac{1}{2}0\gamma)$	$0KLm$: $L=2n$
40.1	$C2cm$	$(2mm, \bar{1}1\bar{1})$	13	$C2cm(00\gamma)$	$h0lm$: $l=2n$
40.2			14	$C2cm(10\gamma)$	$H0Lm$: $L=2n$
40.3		$(mm2, 111)$	15	$Ama2(00\gamma)$	$h0lm$: $h=2n$
40.4			15	$Ama2(00\gamma)s0s$	$0klm$: $m=2n$; $h0lm$: $h=2n$
40.5			15	$Ama2(00\gamma)ss0$	$0klm$: $m=2n$; $h0lm$: $h+m=2n$
40.6			15	$Ama2(00\gamma)0ss$	$h0lm$: $h+m=2n$
40.7		$(m2m, 1\bar{1}\bar{1})$	15	$Am2a(00\gamma)$	$hk00$: $h=2n$
40.8			15	$Am2a(00\gamma)s00$	$0klm$: $m=2n$; $hk00$: $h=2n$
41.1	$C2cb$	$(2mm, \bar{1}1\bar{1})$	13	$C2cb(00\gamma)$	$h0lm$: $l=2n$; $hk00$: $k=2n$
41.2			14	$C2cb(10\gamma)$	$H0Lm$: $L=2n$; $HK00$: $K=2n$
41.3		$(mm2, 111)$	15	$Aba2(00\gamma)$	$0klm$: $k=2n$; $h0lm$: $h=2n$
41.4			15	$Aba2(00\gamma)s0s$	$0klm$: $k+m=2n$; $h0lm$: $h=2n$
41.5			15	$Aba2(00\gamma)ss0$	$0klm$: $k+m=2n$; $h0lm$: $h+m=2n$
41.6			15	$Aba2(00\gamma)0ss$	$0klm$: $k=2n$; $h0lm$: $h+m=2n$
41.7		$(m2m, 1\bar{1}\bar{1})$	15	$Ac2a(00\gamma)$	$0klm$: $l=2n$; $hk00$: $h=2n$
41.8			15	$Ac2a(00\gamma)s00$	$0klm$: $l+m=2n$; $hk00$: $h=2n$
42.1	$Fmm2$	$(mm2, 111)$	17	$Fmm2(00\gamma)$	
42.2			17	$Fmm2(00\gamma)s0s$	$0klm$: $m=2n$
42.3			17	$Fmm2(00\gamma)ss0$	$0klm$: $m=2n$; $h0lm$: $m=2n$
42.4			18	$Fmm2(10\gamma)$	
42.5			18	$Fmm2(10\gamma)s0s$	$0KLm$: $m=2n$
42.6			18	$Fmm2(10\gamma)ss0$	$0KLm$: $m=2n$; $H0Lm$: $m=2n$
42.7		$(2mm, \bar{1}1\bar{1})$	17	$F2mm(00\gamma)$	
42.8			17	$F2mm(00\gamma)0s0$	$h0lm$: $m=2n$
42.9			18	$F2mm(10\gamma)$	
42.10			18	$F2mm(10\gamma)0s0$	$H0Lm$: $m=2n$
43.1	$Fdd2$	$(mm2, 111)$	17	$Fdd2(00\gamma)$	$0klm$: $k+l=4n$
43.2			17	$Fdd2(00\gamma)s0s$	$0klm$: $k+l+2m=4n$; $h0lm$: $h+l=4n$
43.3		$(2mm, \bar{1}1\bar{1})$	17	$F2dd(00\gamma)$	$h0lm$: $h+l=4n$
44.1	$Imm2$	$(mm2, 111)$	12	$Imm2(00\gamma)$	
44.2			12	$Imm2(00\gamma)s0s$	$0klm$: $m=2n$

Table 9.8.3.5. (3 + 1)-*Dimensional superspace groups (cont.)*

No.	Basic space group	Point group K_s	Bravais class No.	Group symbol	Special reflection conditions
44.3			12	$Imm2(00\gamma)ss0$	$0klm$: $m=2n$; $h0lm$: $m=2n$
44.4		$(2mm, \bar{1}1\bar{1})$	12	$I2mm(00\gamma)$	
44.5			12	$I2mm(00\gamma)0s0$	$h0lm$: $m=2n$
45.1	$Iba2$	$(mm2, 111)$	12	$Iba2(00\gamma)$	$0klm$: $k=2n$; $h0lm$: $h=2n$
45.2			12	$Iba2(00\gamma)s0s$	$0klm$: $k+m=2n$; $h0lm$: $h=2n$
45.3			12	$Iba2(00\gamma)ss0$	$0klm$: $k+m=2n$; $h0lm$: $h+m=2n$
45.4		$(2mm, \bar{1}1\bar{1})$	12	$I2cb(00\gamma)$	$h0lm$: $l=2n$; $hk00$: $k=2n$
45.5			12	$I2cb(00\gamma)0s0$	$h0lm$: $l+m=2n$; $hk00$: $k=2n$
46.1	$Ima2$	$(mm2, 111)$	12	$Ima2(00\gamma)$	$h0lm$: $h=2n$
46.2			12	$Ima2(00\gamma)s0s$	$0klm$: $m=2n$; $h0lm$: $h=2n$
46.3			12	$Ima2(00\gamma)ss0$	$0klm$: $m=2n$; $h0lm$: $h+m=2n$
46.4			12	$Ima2(00\gamma)0ss$	$h0lm$: $h+m=2n$
46.5		$(2mm, \bar{1}1\bar{1})$	12	$I2mb(00\gamma)$	$hk00$: $k=2n$
46.6			12	$I2mb(00\gamma)0s0$	$h0lm$: $m=2n$; $hk00$: $k=2n$
46.7			12	$I2cm(00\gamma)$	$h0lm$: $l=2n$
46.8			12	$I2cm(00\gamma)0s0$	$h0lm$: $l+m=2n$
47.1	$Pmmm$	$(mmm, 11\bar{1})$	9	$Pmmm(00\gamma)$	
47.2			9	$Pmmm(00\gamma)s00$	$0klm$: $m=2n$
47.3			9	$Pmmm(00\gamma)ss0$	$0klm$: $m=2n$; $h0lm$: $m=2n$
47.4			10	$Pmmm(0\frac{1}{2}\gamma)$	
47.5			10	$Pmmm(0\frac{1}{2}\gamma)s00$	$0KLm$: $m=2n$
47.6			11	$Pmmm(\frac{1}{2}\frac{1}{2}\gamma)$	
48.1	$Pnnn$	$(mmm, 11\bar{1})$	9	$Pnnn(00\gamma)$	$0klm$: $k+l=2n$; $h0lm$: $h+l=2n$; $hk00$: $h+k=2n$
48.2			9	$Pnnn(00\gamma)s00$	$0klm$: $k+l+m=2n$; $h0lm$: $h+l=2n$; $hk00$: $h+k=2n$
48.3			11	$Pnnn(\frac{1}{2}\frac{1}{2}\gamma)qq0$	$0KLm$: $2K+2L+m=4n$; $H0Lm$: $2H+2L+m=2n$; $HK00$: $H+K=2n$
49.1	$Pccm$	$(mmm, 11\bar{1})$	9	$Pccm(00\gamma)$	$0klm$: $l=2n$; $h0lm$: $l=2n$
49.2			9	$Pccm(00\gamma)s00$	$0klm$: $l+m=2n$; $h0lm$: $l=2n$
49.3			9	$Pmaa(00\gamma)$	$h0lm$: $h=2n$; $hk00$: $h=2n$
49.4			9	$Pmaa(00\gamma)s00$	$0klm$: $m=2n$; $h0lm$: $h=2n$; $hk00$: $h=2n$
49.5			9	$Pmaa(00\gamma)ss0$	$0klm$: $m=2n$; $h0lm$: $h+m=2n$; $hk00$: $h=2n$
49.6			9	$Pmaa(00\gamma)0s0$	$h0lm$: $h+m=2n$; $hk00$: $h=2n$
49.7			10	$Pccm(0\frac{1}{2}\gamma)$	$0KLm$: $L=2n$; $H0Lm$: $L=2n$
49.8			10	$Pmaa(0\frac{1}{2}\gamma)$	$H0Lm$: $H=2n$; $HK00$: $H=2n$
49.9			10	$Pmaa(0\frac{1}{2}\gamma)s00$	$0KLm$: $m=2n$; $H0Lm$: $H=2n$; $HK00$: $H=2n$
49.10			11	$Pccm(\frac{1}{2}\frac{1}{2}\gamma)$	$0KLm$: $L=2n$; $H0Lm$: $L=2n$
50.1	$Pban$	$(mmm, 11\bar{1})$	9	$Pban(00\gamma)$	$0klm$: $k=2n$; $h0lm$: $h=2n$
50.2			9	$Pban(00\gamma)s00$	$0klm$: $k+m=2n$; $h0lm$: $h=2n$
50.3			9	$Pban(00\gamma)ss0$	$0klm$: $k+m=2n$; $h0lm$: $h+m=2n$
50.4			9	$Pcna(00\gamma)$	$0klm$: $l=2n$; $h0lm$: $h+l=2n$; $hk00$: $h=2n$
50.5			9	$Pcna(00\gamma)s00$	$0klm$: $l+m=2n$; $h0lm$: $h+l=2n$; $hk00$: $h=2n$
50.6			10	$Pcna(0\frac{1}{2}\gamma)$	$0KLm$: $L=2n$; $H0Lm$: $H+L=2n$; $HK00$: $H=2n$
50.7			11	$Pban(\frac{1}{2}\frac{1}{2}\gamma)qq0$	$0KLm$: $2K+m=4n$; $H0Lm$: $2H+m=4n$; $HK00$: $H+K=2n$
51.1	$Pmma$	$(mmm, 11\bar{1})$	9	$Pmma(00\gamma)$	$hk00$: $h=2n$
51.2			9	$Pmma(00\gamma)s00$	$0klm$: $m=2n$; $hk00$: $h=2n$
51.3			9	$Pmma(00\gamma)ss0$	$0klm$: $m=2n$; $h0lm$: $m=2n$; $hk00$: $h=2n$
51.4			9	$Pmma(00\gamma)0s0$	$h0lm$: $m=2n$; $hk00$: $h=2n$
51.5			9	$Pmam(00\gamma)$	$h0lm$: $h=2n$
51.6			9	$Pmam(00\gamma)s00$	$0klm$: $m=2n$; $h0lm$: $h=2n$
51.7			9	$Pmam(00\gamma)ss0$	$0klm$: $m=2n$; $h0lm$: $h+m=2n$
51.8			9	$Pmam(00\gamma)0s0$	$h0lm$: $h+m=2n$
51.9			9	$Pmcm(00\gamma)$	$h0lm$: $l=2n$
51.10			9	$Pmcm(00\gamma)s00$	$0klm$: $m=2n$; $h0lm$: $l=2n$
51.11			10	$Pmma(0\frac{1}{2}\gamma)$	$HK00$: $H=2n$
51.12			10	$Pmma(0\frac{1}{2}\gamma)s00$	$0KLm$: $m=2n$; $HK00$: $H=2n$
51.13			10	$Pmam(0\frac{1}{2}\gamma)$	$H0Lm$: $H=2n$
51.14			10	$Pmam(0\frac{1}{2}\gamma)s00$	$0KLm$: $m=2n$; $H0Lm$: $H=2n$
51.15			10	$Pmcm(0\frac{1}{2}\gamma)$	$H0Lm$: $L=2n$
51.16			10	$Pmcm(0\frac{1}{2}\gamma)s00$	$0KLm$: $m=2n$; $H0Lm$: $L=2n$
51.17			10	$Pcmm(0\frac{1}{2}\gamma)$	$0KLm$: $L=2n$
51.18			11	$Pcmm(\frac{1}{2}\frac{1}{2}\gamma)$	$0KLm$: $L=2n$
52.1	$Pnna$	$(mmm, 11\bar{1})$	9	$Pnna(00\gamma)$	$0klm$: $k+l=2n$; $h0lm$: $h+l=2n$; $hk00$: $h=2n$
52.2			9	$Pnna(00\gamma)s00$	$0klm$: $k+l+m=2n$; $h0lm$: $h+l=2n$; $hk00$: $h=2n$
52.3			9	$Pbnn(00\gamma)$	$0klm$: $k=2n$; $h0lm$: $h+l=2n$; $hk00$: $h+k=2n$

Table 9.8.3.5. (3 + 1)-*Dimensional superspace groups (cont.)*

No.	Basic space group	Point group K_s	Bravais class No.	Group symbol	Special reflection conditions
52.4			9	$Pbnn(00\gamma)s00$	$0klm$: $k+m=2n$; $h0lm$: $h+l=2n$; $hk00$: $h+k=2n$
52.5			9	$Pcnn(00\gamma)$	$0klm$: $l=2n$; $h0lm$: $h+l=2n$; $hk00$: $h+k=2n$
52.6			9	$Pcnn(00\gamma)s00$	$0klm$: $l+m=2n$; $h0lm$: $h+l=2n$; $hk00$: $h+k=2n$
52.7			11	$Pbnn(\frac{1}{2}\frac{1}{2}\gamma)qq0$	$0KLm$: $2K+m=4n$; $H0Lm$: $2H+2L+m=4n$; $HK00$: $H+K=2n$
53.1	*Pmna*	$(mmm, 11\bar{1})$	9	$Pmna(00\gamma)$	$h0lm$: $h+l=2n$; $hk00$: $h=2n$
53.2			9	$Pmna(00\gamma)s00$	$0klm$: $m=2n$; $h0lm$: $h+l=2n$; $hk00$: $h=2n$
53.3			9	$Pcnm(00\gamma)$	$0klm$: $l=2n$; $h0lm$: $h+l=2n$
53.4			9	$Pcnm(00\gamma)s00$	$0klm$: $l+m=2n$; $h0lm$: $h+l=2n$
53.5			9	$Pbmn(00\gamma)$	$0klm$: $k=2n$; $hk00$: $h+k=2n$
53.6			9	$Pbmn(00\gamma)s00$	$0klm$: $k+m=2n$; $hk00$: $h+k=2n$
53.7			9	$Pbmn(00\gamma)ss0$	$0klm$: $k+m=2n$; $h0lm$: $m=2n$; $hk00$: $h+k=2n$
53.8			9	$Pbmn(00\gamma)0s0$	$0klm$: $k=2m$; $h0lm$: $m=2n$; $hk00$: $h+k=2n$
53.9			10	$Pmna(0\frac{1}{2}\gamma)$	$H0Lm$: $H+L=2n$; $HK00$: $H=2n$
53.10			10	$Pmna(0\frac{1}{2}\gamma)s00$	$0KLm$: $m=2n$; $H0Lm$: $H+L=2n$; $HK00$: $H=2n$
53.11			10	$Pcnm(0\frac{1}{2}\gamma)$	$0KLm$: $L=2n$; $H0Lm$: $H+L=2n$
54.1	*Pcca*	$(mmm, 11\bar{1})$	9	$Pcca(00\gamma)$	$0klm$: $l=2n$; $h0lm$: $l=2n$; $hk00$: $h=2n$
54.2			9	$Pcca(00\gamma)s00$	$0klm$: $l+m=2n$; $h0lm$: $l=2n$; $hk00$: $h=2n$
54.3			9	$Pcaa(00\gamma)$	$0klm$: $l=2n$; $h0lm$: $h=2n$; $hk00$: $h=2n$
54.4			9	$Pcaa(00\gamma)0s0$	$0klm$: $l=2n$; $h0lm$: $h+m=2n$; $hk00$: $h=2n$
54.5			9	$Pbab(00\gamma)$	$0klm$: $k=2n$; $h0lm$: $h=2n$; $hk00$: $k=2n$
54.6			9	$Pbab(00\gamma)s00$	$0klm$: $k+m=2n$; $h0lm$: $h=2n$; $hk00$: $k=2n$
54.7			9	$Pbab(00\gamma)ss0$	$0klm$: $k+m=2n$; $h0lm$: $h+m=2n$; $hk00$: $k=2n$
54.8			9	$Pbab(00\gamma)0s0$	$0klm$: $k=2n$; $h0lm$: $h+m=2n$; $hk00$: $k=2n$
54.9			10	$Pcca(0\frac{1}{2}\gamma)$	$0KLm$: $L=2n$; $H0Lm$: $L=2n$; $HK00$: $H=2n$
54.10			10	$Pcaa(0\frac{1}{2}\gamma)$	$0KLm$: $L=2n$; $H0Lm$: $H=2n$; $HK00$: $H=2n$
55.1	*Pbam*	$(mmm, 11\bar{1})$	9	$Pbam(00\gamma)$	$0klm$: $k=2n$; $h0lm$: $h=2n$
55.2			9	$Pbam(00\gamma)s00$	$0klm$: $k+m=2n$; $h0lm$: $h=2n$
55.3			9	$Pbam(00\gamma)ss0$	$0klm$: $k+m=2n$; $h0lm$: $h+m=2n$
55.4			9	$Pcma(00\gamma)$	$0klm$: $l=2n$; $hk00$: $h=2n$
55.5			9	$Pcma(00\gamma)0s0$	$0klm$: $l=2n$; $h0lm$: $m=2n$; $hk00$: $h=2n$
55.6			10	$Pcma(0\frac{1}{2}\gamma)$	$0KLm$: $L=2n$; $HK00$: $H=2n$
56.1	*Pccn*	$(mmm, 11\bar{1})$	9	$Pccn(00\gamma)$	$0klm$: $l=2n$; $h0lm$: $l=2n$; $hk00$: $h+k=2n$
56.2			9	$Pccn(00\gamma)s00$	$0klm$: $l+m=2n$; $h0lm$: $l=2n$; $hk00$: $h+k=2n$
56.3			9	$Pbnb(00\gamma)$	$0klm$: $k=2n$; $h0lm$: $h+l=2n$; $hk00$: $k=2n$
56.4			9	$Pbnb(00\gamma)s00$	$0klm$: $k+m=2n$; $h0lm$: $h+l=2n$; $hk00$: $k=2n$
57.1	*Pcam*	$(mmm, 11\bar{1})$	9	$Pcam(00\gamma)$	$0klm$: $l=2n$; $h0lm$: $h=2n$
57.2			9	$Pcam(00\gamma)0s0$	$0klm$: $l=2n$; $h0lm$: $h+m=2n$
57.3			9	$Pmca(00\gamma)$	$h0lm$: $l=2n$; $hk00$: $h=2n$
57.4			9	$Pmca(00\gamma)s00$	$0klm$: $m=2n$; $h0lm$: $l=2n$; $hk00$: $h=2n$
57.5			9	$Pbma(00\gamma)$	$0klm$: $k=2n$; $hk00$: $h=2n$
57.6			9	$Pbma(00\gamma)s00$	$0klm$: $k+m=2n$; $hk00$: $h=2n$
57.7			9	$Pbma(00\gamma)ss0$	$0klm$: $k+m=2n$; $h0lm$: $m=2n$; $hk00$: $h=2n$
57.8			9	$Pbma(00\gamma)0s0$	$0klm$: $k=2n$; $h0lm$: $m=2n$; $hk00$: $h=2n$
57.9			10	$Pcam(0\frac{1}{2}\gamma)$	$0KLm$: $L=2n$; $H0Lm$: $H=2n$
57.10			10	$Pmca(0\frac{1}{2}\gamma)$	$H0Lm$: $L=2n$; $HK00$: $H=2n$
57.11			10	$Pmca(0\frac{1}{2}\gamma)s00$	$0KLm$: $m=2n$; $H0Lm$: $L=2n$; $HK00$: $H=2n$
58.1	*Pnnm*	$(mmm, 11\bar{1})$	9	$Pnnm(00\gamma)$	$0klm$: $k+l=2n$; $h0lm$: $h+l=2n$
58.2			9	$Pnnm(00\gamma)s00$	$0klm$: $k+l+m=2n$; $h0lm$: $h+l=2n$
58.3			9	$Pmnn(00\gamma)$	$h0lm$: $h+l=2n$; $hk00$: $h+k=2n$
58.4			9	$Pmnn(00\gamma)s00$	$0klm$: $m=2n$; $h0lm$: $h+l=2n$; $hk00$: $h+k=2n$
59.1	*Pmmn*	$(mmm, 11\bar{1})$	9	$Pmmn(00\gamma)$	$hk00$: $h+k=2n$
59.2			9	$Pmmn(00\gamma)s00$	$0klm$: $m=2n$; $hk00$: $h+k=2n$
59.3			9	$Pmmn(00\gamma)ss0$	$0klm$: $m=2n$; $h0lm$: $m=2n$; $hk00$: $h+k=2n$
59.4			9	$Pmnm(00\gamma)$	$h0lm$: $h+l=2n$
59.5			9	$Pmnm(00\gamma)s00$	$0klm$: $m=2n$; $h0lm$: $h+l=2n$
59.6			10	$Pmnm(0\frac{1}{2}\gamma)$	$H0Lm$: $H+L=2n$
59.7			10	$Pmnm(0\frac{1}{2}\gamma)s00$	$0KLm$: $m=2n$; $H0Lm$: $H+L=2n$
60.1	*Pbcn*	$(mmm, 11\bar{1})$	9	$Pbcn(00\gamma)$	$0klm$: $k=2n$; $h0lm$: $l=2n$; $hk00$: $h+k=2n$
60.2			9	$Pbcn(00\gamma)s00$	$0klm$: $k+m=2n$; $h0lm$: $l=2n$; $hk00$: $h+k=2n$
60.3			9	$Pnca(00\gamma)$	$0klm$: $k+l=2n$; $h0lm$: $l=2n$; $hk00$: $h=2n$
60.4			9	$Pnca(00\gamma)s00$	$0klm$: $k+l+m=2n$; $h0lm$: $l=2n$; $hk00$: $h=2n$
60.5			9	$Pbna(00\gamma)$	$0klm$: $k=2n$; $h0lm$: $h+l=2n$; $hk00$: $h=2n$
60.6			9	$Pbna(00\gamma)s00$	$0klm$: $k+m=2n$; $h0lm$: $h+l=2n$; $hk00$: $h=2n$
61.1	*Pbca*	$(mmm, 11\bar{1})$	9	$Pbca(00\gamma)$	$0klm$: $k=2n$; $h0lm$: $l=2n$; $hk00$: $h=2n$
61.2			9	$Pbca(00\gamma)s00$	$0klm$: $k+m=2n$; $h0lm$: $l=2n$; $hk00$: $h=2n$

Table 9.8.3.5. (3 + 1)-*Dimensional superspace groups (cont.)*

No.	Basic space group	Point group K_s	Bravais class No.	Group symbol	Special reflection conditions
62.1	*Pnma*	$(mmm, 11\bar{1})$	9	$Pnma(00\gamma)$	$0klm$: $k+l=2n$; $hk00$: $h=2n$
62.2			9	$Pnma(00\gamma)0s0$	$0klm$: $k+l=2n$; $h0lm$: $m=2n$; $hk00$: $h=2n$
62.3			9	$Pbnm(00\gamma)$	$0klm$: $k=2n$; $h0lm$: $h+l=2n$
62.4			9	$Pbnm(00\gamma)s00$	$0klm$: $k+m=2n$; $h0lm$: $h+l=2n$
62.5			9	$Pmcn(00\gamma)$	$h0lm$: $l=2n$; $hk00$: $h+k=2n$
62.6			9	$Pmcn(00\gamma)s00$	$0klm$: $m=2n$; $h0lm$: $l=2n$; $hk00$: $h+k=2n$
63.1	*Cmcm*	$(mmm, 11\bar{1})$	13	$Cmcm(00\gamma)$	$h0lm$: $l=2n$
63.2			13	$Cmcm(00\gamma)s00$	$0klm$: $m=2n$; $h0lm$: $l=2n$
63.3			14	$Cmcm(10\gamma)$	$H0Lm$: $L=2n$
63.4			14	$Cmcm(10\gamma)s00$	$0KLm$: $m=2n$; $H0Lm$: $L=2n$
63.5			15	$Amam(00\gamma)$	$h0lm$: $h=2n$
63.6			15	$Amam(00\gamma)s00$	$0klm$: $m=2n$; $h0lm$: $h=2n$
63.7			15	$Amam(00\gamma)ss0$	$0klm$: $m=2n$; $h0lm$: $h+m=2n$
63.8			15	$Amam(00\gamma)0s0$	$h0lm$: $h+m=2n$
63.9			15	$Amma(00\gamma)$	$hk00$: $h=2n$
63.10			15	$Amma(00\gamma)s00$	$0klm$: $m=2n$; $hk00$: $h=2n$
63.11			15	$Amma(00\gamma)ss0$	$0klm$: $m=2n$; $h0lm$: $m=2n$; $hk00$: $h=2n$
63.12			15	$Amma(00\gamma)0s0$	$h0lm$: $m=2n$; $hk00$: $h=2n$
64.1	*Cmca*	$(mmm, 11\bar{1})$	13	$Cmca(00\gamma)$	$h0lm$: $l=2n$; $hk00$: $h=2n$
64.2			13	$Cmca(00\gamma)s00$	$0klm$: $m=2n$; $h0lm$: $l=2n$; $hk00$: $h=2n$
64.3			14	$Cmca(10\gamma)$	$H0Lm$: $L=2n$; $HK00$: $H=2n$
64.4			14	$Cmca(10\gamma)s00$	$0KLm$: $m=2n$; $H0Lm$: $L=2n$; $HK00$: $H=2n$
64.5			15	$Abma(00\gamma)$	$0klm$: $k=2n$; $hk00$: $h=2n$
64.6			15	$Abma(00\gamma)s00$	$0klm$: $k+m=2n$; $hk00$: $h=2n$
64.7			15	$Abma(00\gamma)ss0$	$0klm$: $k+m=2n$; $h0lm$: $m=2n$; $hk00$: $h=2n$
64.8			15	$Abma(00\gamma)0s0$	$0klm$: $k=2n$; $h0lm$: $m=2n$; $hk00$: $h=2n$
64.9			15	$Acam(00\gamma)$	$0klm$: $l=2n$; $h0lm$: $h=2n$
64.10			15	$Acam(00\gamma)s00$	$0klm$: $l+m=2n$; $h0lm$: $h=2n$
64.11			15	$Acam(00\gamma)ss0$	$0klm$: $l+m=2n$; $h0lm$: $h+m=2n$
64.12			15	$Acam(00\gamma)0s0$	$0klm$: $l=2n$; $h0lm$: $h+m=2n$
65.1	*Cmmm*	$(mmm, 11\bar{1})$	13	$Cmmm(00\gamma)$	
65.2			13	$Cmmm(00\gamma)s00$	$0klm$: $m=2n$
65.3			13	$Cmmm(00\gamma)ss0$	$0klm$: $m=2n$; $h0lm$: $m=2n$
65.4			14	$Cmmm(10\gamma)$	
65.5			14	$Cmmm(10\gamma)s00$	$0KLm$: $m=2n$
65.6			14	$Cmmm(10\gamma)ss0$	$0KLm$: $m=2n$; $H0Lm$: $m=2n$
65.7			15	$Ammm(00\gamma)$	
65.8			15	$Ammm(00\gamma)s00$	$0klm$: $m=2n$
65.9			15	$Ammm(00\gamma)ss0$	$0klm$: $m=2n$; $h0lm$: $m=2n$
65.10			15	$Ammm(00\gamma)0s0$	$h0lm$: $m=2n$
65.11			16	$Ammm(\frac{1}{2}0\gamma)$	
65.12			16	$Ammm(\frac{1}{2}0\gamma)0s0$	$H0Lm$: $m=2n$
66.1	*Cccm*	$(mmm, 11\bar{1})$	13	$Cccm(00\gamma)$	$0klm$: $l=2n$; $h0lm$: $l=2n$
66.2			13	$Cccm(00\gamma)s00$	$0klm$: $l+m=2n$; $h0lm$: $l=2n$
66.3			14	$Cccm(10\gamma)$	$0KLm$: $L=2n$; $H0Lm$: $L=2n$
66.4			14	$Cccm(10\gamma)s00$	$0KLm$: $L+m=2n$; $H0Lm$: $L=2n$
66.5			15	$Amaa(00\gamma)$	$h0lm$: $h=2n$; $hk00$: $h=2n$
66.6			15	$Amaa(00\gamma)s00$	$0klm$: $m=2n$; $h0lm$: $h=2n$; $hk00$: $h=2n$
66.7			15	$Amaa(00\gamma)ss0$	$0klm$: $m=2n$; $h0lm$: $h+m=2n$; $hk00$: $h=2n$
66.8			15	$Amaa(00\gamma)0s0$	$h0lm$: $h+m=2n$; $hk00$: $h=2n$
67.1	*Cmma*	$(mmm, 11\bar{1})$	13	$Cmma(00\gamma)$	$hk00$: $h=2n$
67.2			13	$Cmma(00\gamma)s00$	$0klm$: $m=2n$; $hk00$: $h=2n$
67.3			13	$Cmma(00\gamma)ss0$	$0klm$: $m=2n$; $h0lm$: $m=2n$; $hk00$: $h=2n$
67.4			14	$Cmma(10\gamma)$	$HK00$: $H=2n$
67.5			14	$Cmma(10\gamma)s00$	$0KLm$: $m=2n$; $HK00$: $H=2n$
67.6			14	$Cmma(10\gamma)ss0$	$0KLm$: $m=2n$; $H0Lm$: $m=2n$; $HK00$: $H=2n$
67.7			15	$Acmm(00\gamma)$	$0klm$: $l=2n$
67.8			15	$Acmm(00\gamma)s00$	$0klm$: $l+m=2n$
67.9			15	$Acmm(00\gamma)ss0$	$0klm$: $l+m=2n$; $h0lm$: $m=2n$
67.10			15	$Acmm(00\gamma)0s0$	$0klm$: $l=2n$; $h0lm$: $m=2n$
67.11			16	$Acmm(\frac{1}{2}0\gamma)$	$0KLm$: $L=2n$
67.12			16	$Acmm(\frac{1}{2}0\gamma)0s0$	$0KLm$: $L=2n$; $H0Lm$: $m=2n$
68.1	*Ccca*	$(mmm, 11\bar{1})$	13	$Ccca(00\gamma)$	$0klm$: $l=2n$; $h0lm$: $l=2n$; $hk00$: $h=2n$
68.2			13	$Ccca(00\gamma)s00$	$0klm$: $l+m=2n$; $h0lm$: $l=2n$; $hk00$: $h=2n$
68.3			14	$Ccca(10\gamma)$	$0KLm$: $L=2n$; $H0Lm$: $L=2n$; $HK00$: $H=2n$
68.4			14	$Ccca(10\gamma)s00$	$0KLm$: $L+m=2n$; $H0Lm$: $L=2n$; $HK00$: $H=2n$

Table 9.8.3.5. (3 + 1)-*Dimensional superspace groups (cont.)*

No.	Basic space group	Point group K_s	Bravais class No.	Group symbol	Special reflection conditions
68.5			15	$Acaa(00\gamma)$	$0klm$: $l=2n$; $h0lm$: $h=2n$; $hk00$: $h=2n$
68.6			15	$Acaa(00\gamma)s00$	$0klm$: $l+m=2n$; $h0lm$: $h=2n$; $hk00$: $h=2n$
68.7			15	$Acaa(00\gamma)ss0$	$0klm$: $l+m=2n$; $h0lm$: $h+m=2n$; $hk00$: $h=2n$
68.8			15	$Acaa(00\gamma)0s0$	$0klm$: $l=2n$; $h0lm$: $h+m=2n$; $hk00$: $h=2n$
69.1	$Fmmm$	$(mmm, 11\bar{1})$	17	$Fmmm(00\gamma)$	
69.2			17	$Fmmm(00\gamma)s00$	$0klm$: $m=2n$
69.3			17	$Fmmm(00\gamma)ss0$	$0klm$: $m=2n$; $h0lm$: $m=2n$
69.4			18	$Fmmm(10\gamma)$	
69.5			18	$Fmmm(10\gamma)s00$	$0KLm$: $m=2n$
69.6			18	$Fmmm(10\gamma)ss0$	$0KLm$: $m=2n$; $H0Lm$: $m=2n$
70.1	$Fddd$	$(mmm, 11\bar{1})$	17	$Fddd(00\gamma)$	$0klm$: $k+l=4n$; $h0lm$: $h+l=4n$; $hk00$: $h+k=4n$
70.2			17	$Fddd(00\gamma)s00$	$0klm$: $k+l+2m=4n$; $h0lm$: $h+l=4n$; $hk00$: $h+k=4n$
71.1	$Immm$	$(mmm, 11\bar{1})$	12	$Immm(00\gamma)$	
71.2			12	$Immm(00\gamma)s00$	$0klm$: $m=2n$
71.3			12	$Immm(00\gamma)ss0$	$0klm$: $m=2n$; $h0lm$: $m=2n$
72.1	$Ibam$	$(mmm, 11\bar{1})$	12	$Ibam(00\gamma)$	$0klm$: $k=2n$; $h0lm$: $h=2n$
72.2			12	$Ibam(00\gamma)s00$	$0klm$: $k+m=2n$; $h0lm$: $h=2n$
72.3			12	$Ibam(00\gamma)ss0$	$0klm$: $k+m=2n$; $h0lm$: $h+m=2n$
72.4			12	$Imcb(00\gamma)$	$h0lm$: $l=2n$; $hk00$: $k=2n$
72.5			12	$Imcb(00\gamma)s00$	$0klm$: $m=2n$; $h0lm$: $l=2n$; $hk00$: $k=2n$
72.6			12	$Imcb(00\gamma)ss0$	$0klm$: $m=2n$; $h0lm$: $l+m=2n$; $hk00$: $k=2n$
72.7			12	$Imcb(00\gamma)0s0$	$h0lm$: $l+m=2n$; $hk00$: $k=2n$
73.1	$Ibca$	$(mmm, 11\bar{1})$	12	$Ibca(00\gamma)$	$0klm$: $k=2n$; $h0lm$: $l=2n$; $hk00$: $h=2n$
73.2			12	$Ibca(00\gamma)s00$	$0klm$: $k+m=2n$; $h0lm$: $l=2n$; $hk00$: $h=2n$
73.3			12	$Ibca(00\gamma)ss0$	$0klm$: $k+m=2n$; $h0lm$: $l+m=2n$; $hk00$: $h=2n$
74.1	$Imma$	$(mmm, 11\bar{1})$	12	$Imma(00\gamma)$	$hk00$: $h=2n$
74.2			12	$Imma(00\gamma)s00$	$0klm$: $m=2n$; $hk00$: $h=2n$
74.3			12	$Imma(00\gamma)ss0$	$0klm$: $m=2n$; $h0lm$: $m=2n$; $hk00$: $h=2n$
74.4			12	$Icmm(00\gamma)$	$0klm$: $l=2n$
74.5			12	$Icmm(00\gamma)s00$	$0klm$: $l+m=2n$
74.6			12	$Icmm(00\gamma)ss0$	$0klm$: $l+m=2n$; $h0lm$: $m=2n$
74.7			12	$Icmm(00\gamma)0s0$	$0klm$: $l=2n$; $h0lm$: $m=2n$
75.1	$P4$	$(4, 1)$	19	$P4(00\gamma)$	
75.2			19	$P4(00\gamma)q$	$00lm$: $m=4n$
75.3			19	$P4(00\gamma)s$	$00lm$: $m=2n$
75.4			20	$P4(\frac{1}{2}\frac{1}{2}\gamma)$	
75.5			20	$P4(\frac{1}{2}\frac{1}{2}\gamma)q$	$00Lm$: $m=4n$
76.1	$P4_1$	$(4, 1)$	19	$P4_1(00\gamma)$	$00lm$: $l=4n$
76.2			20	$P4_1(\frac{1}{2}\frac{1}{2}\gamma)$	$00Lm$: $L=4n$
77.1	$P4_2$	$(4, 1)$	19	$P4_2(00\gamma)$	$00lm$: $l=2n$
77.2			19	$P4_2(00\gamma)q$	$00lm$: $2l+m=4n$
77.3			20	$P4_2(\frac{1}{2}\frac{1}{2}\gamma)$	$00Lm$: $L=2n$
77.4			20	$P4_2(\frac{1}{2}\frac{1}{2}\gamma)q$	$00Lm$: $2L+m=4n$
78.1	$P4_3$	$(4, 1)$	19	$P4_3(00\gamma)$	$00lm$: $l=4n$
78.2			20	$P4_3(\frac{1}{2}\frac{1}{2}\gamma)$	$00Lm$: $L=4n$
79.1	$I4$	$(4, 1)$	21	$I4(00\gamma)$	
79.2			21	$I4(00\gamma)q$	$00lm$: $m=4n$
79.3			21	$I4(00\gamma)s$	$00lm$: $m=2n$
80.1	$I4_1$	$(4, 1)$	21	$I4_1(00\gamma)$	$00lm$: $l=4n$
80.2			21	$I4_1(00\gamma)q$	$00lm$: $l+m=4n$
81.1	$P\bar{4}$	$(\bar{4}, \bar{1})$	19	$P\bar{4}(00\gamma)$	
81.2			20	$P\bar{4}(\frac{1}{2}\frac{1}{2}\gamma)$	
82.1	$I\bar{4}$	$(\bar{4}, \bar{1})$	21	$I\bar{4}(00\gamma)$	
83.1	$P4/m$	$(4/m, 1\bar{1})$	19	$P4/m(00\gamma)$	
83.2			19	$P4/m(00\gamma)s0$	$00lm$: $m=2n$
83.3			20	$P4/m(\frac{1}{2}\frac{1}{2}\gamma)$	
84.1	$P4_2/m$	$(4/m, 1\bar{1})$	19	$P4_2/m(00\gamma)$	$00lm$: $l=2n$
84.2			20	$P4_2/m(\frac{1}{2}\frac{1}{2}\gamma)$	$00Lm$: $L=2n$
85.1	$P4/n$	$(4/m, 1\bar{1})$	19	$P4/n(00\gamma)$	$hk00$: $h+k=2n$
85.2			19	$P4/n(00\gamma)s0$	$00lm$: $m=2n$; $hk00$: $h+k=2n$
85.3			20	$P4/n(\frac{1}{2}\frac{1}{2}\gamma)q0$	$00Lm$: $m=4n$; $HK00$: $H=2n$, $K=2n$
86.1	$P4_2/n$	$(4/m, 1\bar{1})$	19	$P4_2/n(00\gamma)$	$00lm$: $l=2n$; $hk00$: $h+k=2n$
86.2			20	$P4_2/n(\frac{1}{2}\frac{1}{2}\gamma)q0$	$00Lm$: $2L+m=4n$; $HK00$: $H=2n$, $K=2n$
87.1	$I4/m$	$(4/m, 1\bar{1})$	21	$I4/m(00\gamma)$	

Table 9.8.3.5. (3 + 1)-*Dimensional superspace groups (cont.)*

No.	Basic space group	Point group K_s	Bravais class No.	Group symbol	Special reflection conditions
87.2			21	$I4/m(00\gamma)s0$	$00lm$: $m=2n$
88.1	$I4_1/a$	$(4/m, 1\bar{1})$	21	$I4_1/a(00\gamma)$	$00lm$: $l=4n$; $hk00$: $h=2n$
89.1	$P422$	$(422, 1\bar{1}\bar{1})$	19	$P422(00\gamma)$	
89.2			19	$P422(00\gamma)q00$	$00lm$: $m=4n$
89.3			19	$P422(00\gamma)s00$	$00lm$: $m=2n$
89.4			20	$P422(\frac{1}{2}\frac{1}{2}\gamma)$	
89.5			20	$P422(\frac{1}{2}\frac{1}{2}\gamma)q00$	$00Lm$: $m=4n$
90.1	$P42_12$	$(422, 1\bar{1}\bar{1})$	19	$P42_12(00\gamma)$	$h000$: $h=2n$
90.2			19	$P42_12(00\gamma)q00$	$00lm$: $m=4n$; $h000$: $h=2n$
90.3			19	$P42_12(00\gamma)s00$	$00lm$: $m=2n$; $h000$: $h=2n$
91.1	$P4_122$	$(422, 1\bar{1}\bar{1})$	19	$P4_122(00\gamma)$	$00lm$: $l=4n$
91.2			20	$P4_122(\frac{1}{2}\frac{1}{2}\gamma)$	$00Lm$: $L=4n$
92.1	$P4_12_12$	$(422, 1\bar{1}\bar{1})$	19	$P4_12_12(00\gamma)$	$00lm$: $l=4n$; $h000$: $h=2n$
93.1	$P4_222$	$(422, 1\bar{1}\bar{1})$	19	$P4_222(00\gamma)$	$00lm$: $l=2n$
93.2			19	$P4_222(00\gamma)q00$	$00lm$: $2l+m=4n$
93.3			20	$P4_222(\frac{1}{2}\frac{1}{2}\gamma)$	$00Lm$: $L=2n$
93.4			20	$P4_222(\frac{1}{2}\frac{1}{2}\gamma)q00$	$00Lm$: $2L+m=4n$
94.1	$P4_22_12$	$(422, 1\bar{1}\bar{1})$	19	$P4_22_12(00\gamma)$	$00lm$: $l=2n$; $h000$: $h=2n$
94.2			19	$P4_22_12(00\gamma)q00$	$00lm$: $2l+m=4n$; $h000$: $h=2n$
95.1	$P4_322$	$(422, 1\bar{1}\bar{1})$	19	$P4_322(00\gamma)$	$00lm$: $l=4n$
95.2			20	$P4_322(\frac{1}{2}\frac{1}{2}\gamma)$	$00Lm$: $L=4n$
96.1	$P4_32_12$	$(422, 1\bar{1}\bar{1})$	19	$P4_32_12(00\gamma)$	$00lm$: $l=4n$; $h000$: $h=2n$
97.1	$I422$	$(422, 1\bar{1}\bar{1})$	21	$I422(00\gamma)$	
97.2			21	$I422(00\gamma)q00$	$00lm$: $m=4n$
97.3			21	$I422(00\gamma)s00$	$00lm$: $m=2n$
98.1	$I4_122$	$(422, 1\bar{1}\bar{1})$	21	$I4_122(00\gamma)$	$00lm$: $l=4n$
98.2			21	$I4_122(00\gamma)q00$	$00lm$: $l+m=4n$
99.1	$P4mm$	$(4mm, 111)$	19	$P4mm(00\gamma)$	
99.2			19	$P4mm(00\gamma)ss0$	$00lm$: $m=2n$; $0klm$: $m=2n$
99.3			19	$P4mm(00\gamma)0ss$	$0klm$: $m=2n$; $hhlm$: $m=2n$
99.4			19	$P4mm(00\gamma)s0s$	$00lm$: $m=2n$; $hhlm$: $m=2n$
99.5			20	$P4mm(\frac{1}{2}\frac{1}{2}\gamma)$	
99.6			20	$P4mm(\frac{1}{2}\frac{1}{2}\gamma)0ss$	$0KLm$: $m=2n$; $HHLm$: $m=2n$
100.1	$P4bm$	$(4mm, 111)$	19	$P4bm(00\gamma)$	$0klm$: $k=2n$
100.2			19	$P4bm(00\gamma)ss0$	$00lm$: $m=2n$; $0klm$: $m=2n$
100.3			19	$P4bm(00\gamma)0ss$	$0klm$: $k+m=2n$; $hhlm$: $m=2n$
100.4			19	$P4bm(00\gamma)s0s$	$00lm$: $m=2n$; $0klm$: $k=2n$; $hhlm$: $m=2n$
100.5			20	$P4bm(\frac{1}{2}\frac{1}{2}\gamma)qq0$	$00Lm$: $m=4n$; $KKLm$: $2K+m=4n$
100.6			20	$P4bm(\frac{1}{2}\frac{1}{2}\gamma)qqs$	$00Lm$: $m=4n$; $KKLm$: $2K+m=4n$; $H0Lm$: $m=2n$
101.1	$P4_2cm$	$(4mm, 111)$	19	$P4_2cm(00\gamma)$	$00lm$: $l=2n$; $0klm$: $l=2n$
101.2			19	$P4_2cm(00\gamma)0ss$	$00lm$: $l=2n$; $0klm$: $l+m=2n$; $hhlm$: $m=2n$
101.3			20	$P4_2cm(\frac{1}{2}\frac{1}{2}\gamma)$	$00Lm$: $L=2n$; $HHLm$: $L=2n$
101.4			20	$P4_2cm(\frac{1}{2}\frac{1}{2}\gamma)0ss$	$00Lm$: $L=2n$; $HHLm$: $L+m=2n$; $H0Lm$: $m=2n$
102.1	$P4_2nm$	$(4mm, 111)$	19	$P4_2nm(00\gamma)$	$00lm$: $l=2n$; $0klm$: $k+l=2n$
102.2			19	$P4_2nm(00\gamma)0ss$	$00lm$: $l=2n$; $0klm$: $k+l+m=2n$; $hhlm$: $m=2n$
102.3			20	$P4_2nm(\frac{1}{2}\frac{1}{2}\gamma)qq0$	$00Lm$: $2L+m=4n$; $HHLm$: $2H+2L+m=4n$
102.4			20	$P4_2nm(\frac{1}{2}\frac{1}{2}\gamma)qqs$	$00Lm$: $2L+m=4n$; $HHLm$: $2H+2L+m=4n$; $H0Lm$: $m=2n$
103.1	$P4cc$	$(4mm, 111)$	19	$P4cc(00\gamma)$	$0klm$: $l=2n$; $hhlm$: $l=2n$
103.2			19	$P4cc(00\gamma)ss0$	$00lm$: $m=2n$; $0klm$: $l+m=2n$; $hhlm$: $l=2n$
103.3			20	$P4cc(\frac{1}{2}\frac{1}{2}\gamma)$	$HHLm$: $L=2n$; $H0Lm$: $L=2n$
104.1	$P4nc$	$(4mm, 111)$	19	$P4nc(00\gamma)$	$0klm$: $k+l=2n$; $hhlm$: $l=2n$
104.2			19	$P4nc(00\gamma)ss0$	$00lm$: $m=2n$; $0klm$: $k+l+m=2n$; $hhlm$: $l=2n$
104.3			20	$P4nc(\frac{1}{2}\frac{1}{2}\gamma)qq0$	$00Lm$: $m=4n$; $HHLm$: $2H+2L+m=4n$; $H0Lm$: $L=2n$
105.1	$P4_2mc$	$(4mm, 111)$	19	$P4_2mc(00\gamma)$	$00lm$: $l=2n$; $hhlm$: $l=2n$
105.2			19	$P4_2mc(00\gamma)ss0$	$00lm$: $l+m=2n$; $0klm$: $m=2n$; $hhlm$: $l=2n$
105.3			20	$P4_2mc(\frac{1}{2}\frac{1}{2}\gamma)$	$00Lm$: $L=2n$; $H0Lm$: $L=2n$
106.1	$P4_2bc$	$(4mm, 111)$	19	$P4_2bc(00\gamma)$	$00lm$: $l=2n$; $0klm$: $k=2n$; $hhlm$: $l=2n$
106.2			19	$P4_2bc(00\gamma)ss0$	$00lm$: $l+m=2n$; $0klm$: $k+m=2n$; $hhlm$: $l=2n$
106.3			20	$P4_2bc(\frac{1}{2}\frac{1}{2}\gamma)qq0$	$00Lm$: $2L+m=4n$; $HHLm$: $2H+m=4n$; $H0Lm$: $L=2n$
107.1	$I4mm$	$(4mm, 111)$	21	$I4mm(00\gamma)$	
107.2			21	$I4mm(00\gamma)ss0$	$00lm$: $m=2n$; $0klm$: $m=2n$
107.3			21	$I4mm(00\gamma)0ss$	$0klm$: $m=2n$; $hhlm$: $m=2n$

Table 9.8.3.5. (3 + 1)-*Dimensional superspace groups (cont.)*

No.	Basic space group	Point group K_s	Bravais class No.	Group symbol	Special reflection conditions
107.4			21	$I4mm(00\gamma)s0s$	$00lm$: $m=2n$; $hhlm$: $m=2n$
108.1	$I4cm$	$(4mm, 111)$	21	$I4cm(00\gamma)$	$0klm$: $l=2n$
108.2			21	$I4cm(00\gamma)ss0$	$00lm$: $m=2n$; $0klm$: $l+m=2n$
108.3			21	$I4cm(00\gamma)0ss$	$0klm$: $l+m=2n$; $hhlm$: $m=2n$
108.4			21	$I4cm(00\gamma)s0s$	$00lm$: $m=2n$; $0klm$: $l=2n$; $hhlm$: $m=2n$
109.1	$I4_1md$	$(4mm, 111)$	21	$I4_1md(00\gamma)$	$00lm$: $l=4n$; $hhlm$: $2h+l=4n$
109.2			21	$I4_1md(00\gamma)ss0$	$00lm$: $l+2m=4n$; $0klm$: $m=2n$; $hhlm$: $2h+l=4n$
110.1	$I4_1cd$	$(4mm, 111)$	21	$I4_1cd(00\gamma)$	$00lm$: $l=4n$; $0klm$: $l=2n$; $hhlm$: $2h+l=4n$
110.2			21	$I4_1cd(00\gamma)ss0$	$00lm$: $l+2m=4n$; $0klm$: $l+m=2n$; $hhlm$: $2h+l=4n$
111.1	$P\bar{4}2m$	$(\bar{4}2m, \bar{1}\bar{1}1)$	19	$P\bar{4}2m(00\gamma)$	
111.2			19	$P\bar{4}2m(00\gamma)00s$	$hhlm$: $m=2n$
111.3			20	$P\bar{4}2m(\frac{1}{2}\frac{1}{2}\gamma)$	
111.4			20	$P\bar{4}2m(\frac{1}{2}\frac{1}{2}\gamma)00s$	$H0Lm$: $m=2n$
112.1	$P\bar{4}2c$	$(\bar{4}2m, \bar{1}\bar{1}1)$	19	$P\bar{4}2c(00\gamma)$	$hhlm$: $l=2n$
112.2			20	$P\bar{4}2c(\frac{1}{2}\frac{1}{2}\gamma)$	$H0Lm$: $L=2n$
113.1	$P\bar{4}2_1m$	$(\bar{4}2m, \bar{1}\bar{1}1)$	19	$P\bar{4}2_1m(00\gamma)$	$h000$: $h=2n$
113.2			19	$P\bar{4}2_1m(00\gamma)00s$	$h000$: $h=2n$; $hhlm$: $m=2n$
114.1	$P\bar{4}2_1c$	$(\bar{4}2m, \bar{1}\bar{1}1)$	19	$P\bar{4}2_1c(00\gamma)$	$h000$: $h=2n$; $hhlm$: $l=2n$
115.1	$P\bar{4}m2$	$(\bar{4}m2, \bar{1}1\bar{1})$	19	$P\bar{4}m2(00\gamma)$	
115.2			19	$P\bar{4}m2(00\gamma)0s0$	$0klm$: $m=2n$
115.3			20	$P\bar{4}m2(\frac{1}{2}\frac{1}{2}\gamma)$	
116.1	$P\bar{4}c2$	$(\bar{4}m2, \bar{1}1\bar{1})$	19	$P\bar{4}c2(00\gamma)$	$0klm$: $l=2n$
116.2			20	$P\bar{4}c2(\frac{1}{2}\frac{1}{2}\gamma)$	$HHLm$: $L=2n$
117.1	$P\bar{4}b2$	$(\bar{4}m2, \bar{1}1\bar{1})$	19	$P\bar{4}b2(00\gamma)$	$0klm$: $k=2n$
117.2			19	$P\bar{4}b2(00\gamma)0s0$	$0klm$: $k+m=2n$
117.3			20	$P\bar{4}b2(\frac{1}{2}\frac{1}{2}\gamma)0q0$	$HHLm$: $2H+m=4n$
118.1	$P\bar{4}n2$	$(\bar{4}m2, \bar{1}1\bar{1})$	19	$P\bar{4}n2(00\gamma)$	$0klm$: $k+l=2n$
118.2			20	$P\bar{4}n2(\frac{1}{2}\frac{1}{2}\gamma)0q0$	$HHLm$: $2H+2L+m=4n$
119.1	$I\bar{4}m2$	$(\bar{4}m2, \bar{1}1\bar{1})$	21	$I\bar{4}m2(00\gamma)$	
119.2			21	$I\bar{4}m2(00\gamma)0s0$	$0klm$: $m=2n$
120.1	$I\bar{4}c2$	$(\bar{4}m2, \bar{1}1\bar{1})$	21	$I\bar{4}c2(00\gamma)$	$0klm$: $l=2n$
120.2			21	$I\bar{4}c2(00\gamma)0s0$	$0klm$: $l+m=2n$
121.1	$I\bar{4}2m$	$(\bar{4}2m, \bar{1}\bar{1}1)$	21	$I\bar{4}2m(00\gamma)$	
121.2			21	$I\bar{4}2m(00\gamma)00s$	$hhlm$: $m=2n$
122.1	$I\bar{4}2d$	$(\bar{4}2m, \bar{1}\bar{1}1)$	21	$I\bar{4}2d(00\gamma)$	$hhlm$: $2h+l=4n$
123.1	$P4/mmm$	$(4/mmm, 1\bar{1}11)$	19	$P4/mmm(00\gamma)$	
123.2			19	$P4/mmm(00\gamma)s0s0$	$00lm$: $m=2n$; $0klm$: $m=2n$
123.3			19	$P4/mmm(00\gamma)00ss$	$0klm$: $m=2n$; $hhlm$: $m=2n$
123.4			19	$P4/mmm(00\gamma)s00s$	$00lm$: $m=2n$; $hhlm$: $m=2n$
123.5			20	$P4/mmm(\frac{1}{2}\frac{1}{2}\gamma)$	
123.6			20	$P4/mmm(\frac{1}{2}\frac{1}{2}\gamma)00ss$	$HHLm$: $m=2n$; $H0Lm$: $m=2n$
124.1	$P4/mcc$	$(4/mmm, 1\bar{1}11)$	19	$P4/mcc(00\gamma)$	$0klm$: $l=2n$; $hhlm$: $l=2n$
124.2			19	$P4/mcc(00\gamma)s0s0$	$00lm$: $m=2n$; $0klm$: $l+m=2n$; $hhlm$: $l=2n$
124.3			20	$P4/mcc(\frac{1}{2}\frac{1}{2}\gamma)$	$HHLm$: $L=2n$; $H0Lm$: $L=2n$
125.1	$P4/nbm$	$(4/mmm, 1\bar{1}11)$	19	$P4/nbm(00\gamma)$	$hk00$: $h+k=2n$; $0klm$: $k=2n$
125.2			19	$P4/nbm(00\gamma)s0s0$	$00lm$: $m=2n$; $hk00$: $h+k=2n$; $0klm$: $k+m=2n$
125.3			19	$P4/nbm(00\gamma)00ss$	$hk00$: $h+k=2n$; $0klm$: $k+m=2n$; $hhlm$: $m=2n$
125.4			19	$P4/nbm(00\gamma)s00s$	$00lm$: $m=2n$; $hk00$: $h+k=2n$; $0klm$: $k=2n$; $hhlm$: $m=2n$
125.5			20	$P4/nbm(\frac{1}{2}\frac{1}{2}\gamma)q0q0$	$00Lm$: $m=4n$; $HK00$: $H=2n$, $K=2n$; $HHLm$: $2H+m=4n$
125.6			20	$P4/nbm(\frac{1}{2}\frac{1}{2}\gamma)q0qs$	$00Lm$: $m=4n$; $HK00$: $H=2n$, $K=2n$; $HHLm$: $2H+m=4n$; $H0Lm$: $m=2n$
126.1	$P4/nnc$	$(4/mmm, 1\bar{1}11)$	19	$P4/nnc(00\gamma)$	$hk00$: $h+k=2n$; $h0lm$: $h+l=2n$; $hhlm$: $l=2n$
126.2			19	$P4/nnc(00\gamma)s0s0$	$00lm$: $m=2n$; $hk00$: $h+k=2n$; $h0lm$: $h+l+m=2n$; $hhlm$: $l=2n$
126.3			20	$P4/nnc(\frac{1}{2}\frac{1}{2}\gamma)q0q0$	$00Lm$: $m=4n$; $HK00$: $H=2n$, $K=2n$; $HHLm$: $2H+2L+m=4n$; $H0Lm$: $L=2n$
127.1	$P4/mbm$	$(4/mmm, 1\bar{1}11)$	19	$P4/mbm(00\gamma)$	$0klm$: $k=2n$
127.2			19	$P4/mbm(00\gamma)s0s0$	$00lm$: $m=2n$; $0klm$: $k+m=2n$
127.3			19	$P4/mbm(00\gamma)00ss$	$0klm$: $k+m=2n$; $hhlm$: $m=2n$
127.4			19	$P4/mbm(00\gamma)s00s$	$00lm$: $m=2n$; $0klm$: $k=2n$; $hhlm$: $m=2n$
128.1	$P4/mnc$	$(4/mmm, 1\bar{1}11)$	19	$P4/mnc(00\gamma)$	$0klm$: $k+l=2n$; $hhlm$: $l=2n$
128.2			19	$P4/mnc(00\gamma)s0s0$	$00lm$: $m=2n$; $0klm$: $k+l+m=2n$; $hhlm$: $l=2n$
129.1	$P4/nmm$	$(4/mmm, 1\bar{1}11)$	19	$P4/nmm(00\gamma)$	$hk00$: $h+k=2n$

Table 9.8.3.5. (3 + 1)-*Dimensional superspace groups (cont.)*

No.	Basic space group	Point group K_s	Bravais class No.	Group symbol	Special reflection conditions
129.2			19	$P4/nmm(00\gamma)s0s0$	$00lm$: $m=2n$; $hk00$: $h+k=2n$; $0klm$: $m=2n$
129.3			19	$P4/nmm(00\gamma)00ss$	$hk00$: $h+k=2n$; $0klm$: $m=2n$; $hhlm$: $m=2n$
129.4			19	$P4/nmm(00\gamma)s00s$	$00lm$: $m=2n$; $hk00$: $h+k=2n$; $hhlm$: $m=2n$
130.1	$P4/ncc$	$(4/mmm, 1\bar{1}11)$	19	$P4/ncc(00\gamma)$	$hk00$: $h+k=2n$; $0klm$: $l=2n$; $hhlm$: $l=2n$
130.2			19	$P4/ncc(00\gamma)s0s0$	$00lm$: $m=2n$; $hk00$: $h+k=2n$; $0klm$: $l+m=2n$; $hhlm$: $l=2n$
131.1	$P4_2/mmc$	$(4/mmm, 1\bar{1}11)$	19	$P4_2/mmc(00\gamma)$	$00lm$: $l=2n$; $hhlm$: $l=2n$
131.2			19	$P4_2/mmc(00\gamma)s0s0$	$00lm$: $l+m=2n$; $0klm$: $m=2n$; $hhlm$: $l=2n$
131.3			20	$P4_2/mmc(\frac{1}{2}\frac{1}{2}\gamma)$	$00Lm$: $L=2n$; $H0Lm$: $L=2n$
132.1	$P4_2/mcm$	$(4/mmm, 1\bar{1}11)$	19	$P4_2/mcm(00\gamma)$	$00lm$: $l=2n$; $0klm$: $l=2n$
132.2			19	$P4_2/mcm(00\gamma)00ss$	$00lm$: $l=2n$; $0klm$: $l+m=2n$; $hhlm$: $m=2n$
132.3			20	$P4_2/mcm(\frac{1}{2}\frac{1}{2}\gamma)$	$00Lm$: $L=2n$; $HHLm$: $L=2n$
132.4			20	$P4_2/mcm(\frac{1}{2}\frac{1}{2}\gamma)00ss$	$00Lm$: $L=2n$; $HHLm$: $L+m=2n$; $H0Lm$: $m=2n$
133.1	$P4_2/nbc$	$(4/mmm, 1\bar{1}11)$	19	$P4_2/nbc(00\gamma)$	$00lm$: $l=2n$; $hk00$: $h+k=2n$; $0klm$: $k=2n$; $hhlm$: $l=2n$
133.2			19	$P4_2/nbc(00\gamma)s0s0$	$00lm$: $l+m=2n$; $hk00$: $h+k=2n$; $0klm$: $k+m=2n$; $hhlm$: $l=2n$
133.3			20	$P4_2/nbc(\frac{1}{2}\frac{1}{2}\gamma)q0q0$	$00Lm$: $2L+m=4n$; $HK00$: $H=2n$, $K=2n$; $HHLm$: $2H+m=4n$; $H0Lm$: $L=2n$
134.1	$P4_2/nnm$	$(4/mmm, 1\bar{1}11)$	19	$P4_2/nnm(00\gamma)$	$00lm$: $l=2n$; $hk00$: $h+k=2n$; $0klm$: $k+l=2n$
134.2			19	$P4_2/nnm(00\gamma)00ss$	$00lm$: $l=2n$; $hk00$: $h+k=2n$; $0klm$: $k+l+m=2n$; $hhlm$: $m=2n$
134.3			20	$P4_2/nnm(\frac{1}{2}\frac{1}{2}\gamma)q0q0$	$00Lm$: $2L+m=4n$; $HK00$: $H=2n$, $K=2n$; $HHLm$: $2H+2L+m=4n$
134.4			20	$P4_2/nnm(\frac{1}{2}\frac{1}{2}\gamma)q0qs$	$00Lm$: $2L+m=4n$; $HK00$: $H+K=2n$; $HHLm$: $2H+2L+m=4n$; $H0Lm$: $m=2n$
135.1	$P4_2/mbc$	$(4/mmm, 1\bar{1}11)$	19	$P4_2/mbc(00\gamma)$	$00lm$: $l=2n$; $0klm$: $k=2n$; $hhlm$: $l=2n$
135.2			19	$P4_2/mbc(00\gamma)s0s0$	$00lm$: $l+m=2n$; $0klm$: $k+m=2n$; $hhlm$: $l=2n$
136.1	$P4_2/mnm$	$(4/mmm, 1\bar{1}11)$	19	$P4_2/mnm(00\gamma)$	$00lm$: $l=2n$; $0klm$: $k+l=2n$
136.2			19	$P4_2/mnm(00\gamma)00ss$	$00lm$: $l=2n$; $0klm$: $k+l+m=2n$; $hhlm$: $m=2n$
137.1	$P4_2/nmc$	$(4/mmm, 1\bar{1}11)$	19	$P4_2/nmc(00\gamma)$	$00lm$: $l=2n$; $hk00$: $h+k=2n$; $hhlm$: $l=2n$
137.2			19	$P4_2/nmc(00\gamma)s0s0$	$00lm$: $l+m=2n$; $hk00$: $h+k=2n$; $0klm$: $m=2n$; $hhlm$: $l=2n$
138.1	$P4_2/ncm$	$(4/mmm, 1\bar{1}11)$	19	$P4_2/ncm(00\gamma)$	$00lm$: $l=2n$; $hk00$: $h+k=2n$; $0klm$: $l=2n$
138.2			19	$P4_2/ncm(00\gamma)00ss$	$00lm$: $l=2n$; $hk00$: $h+k=2n$; $0klm$: $l+m=2n$; $hhlm$: $m=2n$
139.1	$I4/mmm$	$(4/mmm, 1\bar{1}11)$	21	$I4/mmm(00\gamma)$	
139.2			21	$I4/mmm(00\gamma)s0s0$	$00lm$: $m=2n$; $0klm$: $m=2n$
139.3			21	$I4/mmm(00\gamma)00ss$	$0klm$: $m=2n$; $hhlm$: $m=2n$
139.4			21	$I4/mmm(00\gamma)s00s$	$00lm$: $m=2n$; $hhlm$: $m=2n$
140.1	$I4/mcm$	$(4/mmm, 1\bar{1}11)$	21	$I4/mcm(00\gamma)$	$0klm$: $l=2n$
140.2			21	$I4/mcm(00\gamma)s0s0$	$00lm$: $m=2n$; $0klm$: $l+m=2n$
140.3			21	$I4/mcm(00\gamma)00ss$	$0klm$: $l+m=2n$; $hhlm$: $m=2n$
140.4			21	$I4/mcm(00\gamma)s00s$	$00lm$: $m=2n$; $0klm$: $l=2n$; $hhlm$: $m=2n$
141.1	$I4_1/amd$	$(4/mmm, 1\bar{1}11)$	21	$I4_1/amd(00\gamma)$	$00lm$: $l=4n$; $hk00$: $h=2n$; $hhlm$: $2h+l=4n$
141.2			21	$I4_1/amd(00\gamma)s0s0$	$00lm$: $l+2m=4n$; $hk00$: $h=2n$; $0klm$: $m=2n$; $hhlm$: $2h+l=4n$
142.1	$I4_1/acd$	$(4/mmm, 1\bar{1}11)$	21	$I4_1/acd(00\gamma)$	$00lm$: $l=4n$; $hk00$: $h=2n$; $0klm$: $l=2n$; $hhlm$: $2h+l=4n$
142.2			21	$I4_1/acd(00\gamma)s0s0$	$00lm$: $l+2m=4n$; $hk00$: $h=2n$; $0klm$: $l+m=2n$; $hhlm$: $2h+l=4n$
143.1	$P3$	$(3, 1)$	23	$P3(\frac{1}{3}\frac{1}{3}\gamma)$	
143.2			24	$P3(00\gamma)$	
143.3			24	$P3(00\gamma)t$	$00lm$: $m=3n$
144.1	$P3_1$	$(3, 1)$	23	$P3_1(\frac{1}{3}\frac{1}{3}\gamma)$	$00Lm$: $L=3n$
144.2			24	$P3_1(00\gamma)$	$00lm$: $l=3n$
145.1	$P3_2$	$(3, 1)$	23	$P3_2(\frac{1}{3}\frac{1}{3}\gamma)$	$00Lm$: $L=3n$
145.2			24	$P3_2(00\gamma)$	$00lm$: $l=3n$
146.1	$R3$	$(3, 1)$	22	$R3(00\gamma)$	
146.2			22	$R3(00\gamma)t$	$00lm$: $m=3n$
147.1	$P\bar{3}$	$(\bar{3}, \bar{1})$	23	$P\bar{3}(\frac{1}{3}\frac{1}{3}\gamma)$	
147.2			24	$P\bar{3}(00\gamma)$	
148.1	$R\bar{3}$	$(\bar{3}, \bar{1})$	22	$R\bar{3}(00\gamma)$	
149.1	$P312$	$(312, 11\bar{1})$	23	$P312(\frac{1}{3}\frac{1}{3}\gamma)$	
149.2			24	$P312(00\gamma)$	

Table 9.8.3.5. (3 + 1)-*Dimensional superspace groups (cont.)*

No.	Basic space group	Point group K_s	Bravais class No.	Group symbol	Special reflection conditions
149.3			24	$P312(00\gamma)t00$	$00lm$: $m=3n$
150.1	$P321$	$(321, 1\bar{1}1)$	24	$P321(00\gamma)$	
150.2			24	$P321(00\gamma)t00$	$00lm$: $m=3n$
151.1	$P3_112$	$(312, 11\bar{1})$	23	$P3_112(\frac{1}{3}\frac{1}{3}\gamma)$	$00Lm$: $L=3n$
151.2			24	$P3_112(00\gamma)$	$00lm$: $l=3n$
152.1	$P3_121$	$(321, 1\bar{1}1)$	24	$P3_121(00\gamma)$	$00lm$: $l=3n$
153.1	$P3_212$	$(312, 11\bar{1})$	23	$P3_212(\frac{1}{3}\frac{1}{3}\gamma)$	
153.2			24	$P3_212(00\gamma)$	$00lm$: $l=3n$
154.1	$P3_221$	$(321, 1\bar{1}1)$	24	$P3_221(00\gamma)$	$00lm$: $l=3n$
155.1	$R32$	$(32, 1\bar{1})$	22	$R32(00\gamma)$	
155.2			22	$R32(00\gamma)t0$	$00lm$: $m=3n$
156.1	$P3m1$	$(3m1, 111)$	24	$P3m1(00\gamma)$	
156.2			24	$P3m1(00\gamma)0s0$	$0klm$: $m=2n$
157.1	$P31m$	$(31m, 111)$	23	$P31m(\frac{1}{3}\frac{1}{3}\gamma)$	
157.2			23	$P31m(\frac{1}{3}\frac{1}{3}\gamma)00s$	$H\bar{H}Lm$: $m=2n$
157.3			24	$P31m(00\gamma)$	
157.4			24	$P31m(00\gamma)00s$	$hhlm$: $m=2n$
158.1	$P3c1$	$(3m1, 111)$	24	$P3c1(00\gamma)$	$0klm$: $l=2n$
159.1	$P31c$	$(31m, 111)$	23	$P31c(\frac{1}{3}\frac{1}{3}\gamma)$	$H\bar{H}Lm$: $L=2n$
159.2			24	$P31c(00\gamma)$	$hhlm$: $l=2n$
160.1	$R3m$	$(3m, 11)$	22	$R3m(00\gamma)$	
160.2			22	$R3m(00\gamma)0s$	$hhlm$: $m=2n$
161.1	$R3c$	$(3m, 11)$	22	$R3c(00\gamma)$	$hhlm$: $l=2n$
162.1	$P\bar{3}1m$	$(\bar{3}1m, \bar{1}11)$	23	$P\bar{3}1m(\frac{1}{3}\frac{1}{3}\gamma)$	
162.2			23	$P\bar{3}1m(\frac{1}{3}\frac{1}{3}\gamma)00s$	$H\bar{H}Lm$: $m=2n$
162.3			24	$P\bar{3}1m(00\gamma)$	
162.4			24	$P\bar{3}1m(00\gamma)00s$	$hhlm$: $m=2n$
163.1	$P\bar{3}1c$	$(\bar{3}1m, \bar{1}11)$	23	$P\bar{3}1c(\frac{1}{3}\frac{1}{3}\gamma)$	$H\bar{H}Lm$: $L=2n$
163.2			24	$P\bar{3}1c(00\gamma)$	$hhlm$: $l=2n$
164.1	$P\bar{3}m1$	$(\bar{3}m1, \bar{1}11)$	24	$P\bar{3}m1(00\gamma)$	
164.2			24	$P\bar{3}m1(00\gamma)0s0$	$0klm$: $m=2n$
165.1	$P\bar{3}c1$	$(\bar{3}m1, \bar{1}11)$	24	$P\bar{3}c1(00\gamma)$	$0klm$: $l=2n$
166.1	$R\bar{3}m$	$(\bar{3}m, \bar{1}1)$	22	$R\bar{3}m(00\gamma)$	
166.2			22	$R\bar{3}m(00\gamma)0s$	$hhlm$: $m=2n$
167.1	$R\bar{3}c$	$(\bar{3}m, \bar{1}1)$	22	$R\bar{3}c(00\gamma)$	$hhlm$: $l=2n$
168.1	$P6$	$(6, 1)$	24	$P6(00\gamma)$	
168.2			24	$P6(00\gamma)h$	$00lm$: $m=6n$
168.3			24	$P6(00\gamma)t$	$00lm$: $m=3n$
168.4			24	$P6(00\gamma)s$	$00lm$: $m=2n$
169.1	$P6_1$	$(6, 1)$	24	$P6_1(00\gamma)$	$00lm$: $l=6n$
170.1	$P6_5$	$(6, 1)$	24	$P6_5(00\gamma)$	$00lm$: $l=6n$
171.1	$P6_2$	$(6, 1)$	24	$P6_2(00\gamma)$	$00lm$: $l=3n$
171.2			24	$P6_2(00\gamma)h$	$00lm$: $2l+m=6n$
172.1	$P6_4$	$(6, 1)$	24	$P6_4(00\gamma)$	$00lm$: $l=3n$
172.2			24	$P6_4(00\gamma)h$	$00lm$: $2l+m=6n$
173.1	$P6_3$	$(6, 1)$	24	$P6_3(00\gamma)$	$00lm$: $l=2n$
173.2			24	$P6_3(00\gamma)h$	$00lm$: $3l+m=6n$
174.1	$P\bar{6}$	$(\bar{6}, \bar{1})$	24	$P\bar{6}(00\gamma)$	
175.1	$P6/m$	$(6/m, 1\bar{1})$	24	$P6/m(00\gamma)$	
175.2			24	$P6/m(00\gamma)s0$	$00lm$: $m=2n$
176.1	$P6_3/m$	$(6/m, 1\bar{1})$	24	$P6_3/m(00\gamma)$	$00lm$: $l=2n$
177.1	$P622$	$(622, 1\bar{1}\bar{1})$	24	$P622(00\gamma)$	
177.2			24	$P622(00\gamma)h00$	$00lm$: $m=6n$
177.3			24	$P622(00\gamma)t00$	$00lm$: $m=3n$
177.4			24	$P622(00\gamma)s00$	$00lm$: $m=2n$
178.1	$P6_122$	$(622, 1\bar{1}\bar{1})$	24	$P6_122(00\gamma)$	$00lm$: $l=6n$
179.1	$P6_522$	$(622, 1\bar{1}\bar{1})$	24	$P6_522(00\gamma)$	$00lm$: $l=6n$
180.1	$P6_222$	$(622, 1\bar{1}\bar{1})$	24	$P6_222(00\gamma)$	$00lm$: $l=3n$
180.2			24	$P6_222(00\gamma)h00$	$00lm$: $2l+m=6n$
181.1	$P6_422$	$(622, 1\bar{1}\bar{1})$	24	$P6_422(00\gamma)$	$00lm$: $l=3n$
181.2			24	$P6_422(00\gamma)h00$	$00lm$: $2l+m=6n$
182.1	$P6_322$	$(622, 1\bar{1}\bar{1})$	24	$P6_322(00\gamma)$	
182.2			24	$P6_322(00\gamma)h00$	$00lm$: $3l+m=6n$
183.1	$P6mm$	$(6mm, 111)$	24	$P6mm(00\gamma)$	
183.2			24	$P6mm(00\gamma)ss0$	$00lm$: $m=2n$; $0klm$: $m=2n$

Table 9.8.3.5. (3 + 1)-*Dimensional superspace groups (cont.)*

No.	Basic space group	Point group K_s	Bravais class No.	Group symbol	Special reflection conditions
183.3			24	$P6mm(00\gamma)0ss$	$0klm$: $m=2n$; $hhlm$: $m=2n$
183.4			24	$P6mm(00\gamma)s0s$	$00lm$: $m=2n$; $hhlm$: $m=2n$
184.1	$P6cc$	$(6mm, 111)$	24	$P6cc(00\gamma)$	$0klm$: $l=2n$; $hhlm$: $l=2n$
184.2			24	$P6cc(00\gamma)s0s$	$00lm$: $m=2n$; $0klm$: $l=2n$; $hhlm$: $l+m=2n$
185.1	$P6_3cm$	$(6mm, 111)$	24	$P6_3cm(00\gamma)$	$00lm$: $l=2n$; $0klm$: $l=2n$
185.2			24	$P6_3cm(00\gamma)0ss$	$00lm$: $l=2n$; $0klm$: $l+m=2n$; $hhlm$: $m=2n$
186.1	$P6_3mc$	$(6mm, 111)$	24	$P6_3mc(00\gamma)$	$00lm$: $l=2n$; $hhlm$: $l=2n$
186.2			24	$P6_3mc(00\gamma)0ss$	$00lm$: $l=2n$; $0klm$: $m=2n$; $hhlm$: $l+m=2n$
187.1	$P\bar{6}m2$	$(\bar{6}m2, \bar{1}1\bar{1})$	24	$P\bar{6}m2(00\gamma)$	
187.2			24	$P\bar{6}m2(00\gamma)0s0$	$0klm$: $m=2n$
188.1	$P\bar{6}c2$	$(\bar{6}m2, \bar{1}1\bar{1})$	24	$P\bar{6}c2(00\gamma)$	$0klm$: $l=2n$
189.1	$P\bar{6}2m$	$(\bar{6}2m, \bar{1}\bar{1}1)$	24	$P\bar{6}2m(00\gamma)$	
189.2			24	$P\bar{6}2m(00\gamma)00s$	$hhlm$: $m=2n$
190.1	$P\bar{6}2c$	$(\bar{6}2m, \bar{1}\bar{1}1)$	24	$P\bar{6}2c(00\gamma)$	$hhlm$: $l=2n$
191.1	$P6/mmm$	$(6/mmm, 1\bar{1}11)$	24	$P6/mmm(00\gamma)$	
191.2			24	$P6/mmm(00\gamma)s0s0$	$00lm$: $m=2n$; $0klm$: $m=2n$
191.3			24	$P6/mmm(00\gamma)00ss$	$0klm$: $m=2n$; $hhlm$: $m=2n$
191.4			24	$P6/mmm(00\gamma)s00s$	$00lm$: $m=2n$; $hhlm$: $m=2n$
192.1	$P6/mcc$	$(6/mmm, 1\bar{1}11)$	24	$P6/mcc(00\gamma)$	$0klm$: $l=2n$; $hhlm$: $l=2n$
192.2			24	$P6/mcc(00\gamma)s00s$	$00lm$: $m=2n$; $0klm$: $l=2n$; $hhlm$: $l+m=2n$
193.1	$P6_3/mcm$	$(6/mmm, 1\bar{1}11)$	24	$P6_3/mcm(00\gamma)$	$00lm$: $l=2n$; $0klm$: $l=2n$
193.2			24	$P6_3/mcm(00\gamma)00ss$	$00lm$: $l=2n$; $0klm$: $l+m=2n$; $hhlm$: $m=2n$
194.1	$P6_3/mmc$	$(6/mmm, 1\bar{1}11)$	24	$P6_3/mmc(00\gamma)$	$00lm$: $l=2n$; $hhlm$: $l=2n$
194.2			24	$P6_3/mmc(00\gamma)00ss$	$00lm$: $l=2n$; $0klm$: $m=2n$; $hhlm$: $l+m=2n$

primitive translations in the (3 + 1)-dimensional space group, just as is the case for glide planes and screw axes in three dimensions.

Special reflection conditions can be derived from transformation properties of the structure factor under symmetry operations. Transforming the geometric structure factor by an element $g_s = (\{R|\mathbf{v}\}, \{R_I|\upsilon_I\})$, one obtains

$$S_{\mathbf{H}} = S_{R^{-1}\mathbf{H}} \exp[-2\pi i(\mathbf{H}\cdot\mathbf{v} + H_I\cdot\upsilon_I)]. \qquad (9.8.3.10)$$

Therefore, if $R\mathbf{H} = \mathbf{H}$, the corresponding structure factor vanishes unless $\mathbf{H}\cdot\mathbf{v} + H_I\cdot\upsilon_I$ is an integer.

The form of such a reflection condition in terms of allowed or forbidden sets of indices depends on the basis chosen. When a lattice basis is chosen, one has

$$H_s = (\mathbf{H}, H_I) = \sum_{i=1}^{4} h_i \mathbf{a}_{si}^*, \qquad (9.8.3.11)$$

$$\upsilon_s = (\mathbf{v}, \upsilon_I) + \sum_{i=1}^{4} \upsilon_i \mathbf{a}_{si}. \qquad (9.8.3.12)$$

Then the reflection condition becomes

$$H_s\cdot\upsilon_s = \sum_{i=1}^{4} h_i\upsilon_i = \text{integer} \qquad \text{for } R\mathbf{H} = \mathbf{H}. \qquad (9.8.3.13)$$

In terms of external and internal shift components, the reflection condition can be written as

$$H_s\cdot\upsilon_s = \mathbf{H}\cdot\mathbf{v} + H_I\cdot\upsilon_I = \mathbf{H}\cdot\mathbf{v} + m\upsilon_I = \text{integer for } R\mathbf{H} = \mathbf{H}. \qquad (9.8.3.14)$$

With $\mathbf{H} = \mathbf{K} + m\mathbf{q}$ and $\upsilon_I = \delta - \mathbf{q}\cdot\mathbf{v}$, (9.8.3.14) gives

$$\mathbf{K}\cdot\mathbf{v} + m\delta = \text{integer} \qquad \text{for } R\mathbf{H} = \mathbf{H}. \qquad (9.8.3.15)$$

For $\mathbf{v} = \upsilon_1\mathbf{a} + \upsilon_2\mathbf{b} + \upsilon_3\mathbf{c}$ and $\mathbf{K} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$, (9.8.3.15) takes the form (9.8.3.13):

$$h\upsilon_1 + k\upsilon_2 + l\upsilon_3 + m\delta = \text{integer} \qquad \text{for } R\mathbf{H} = \mathbf{H}. \qquad (9.8.3.16)$$

When the modulation wavevector has a rational part, one can choose another basis (Subsection 9.8.2.1) such that $\mathbf{K}' = \mathbf{K} + m\mathbf{q}^r$ has integer coefficients:

$$\mathbf{H} = \mathbf{K}' + m\mathbf{q}^i = H\mathbf{a}_c^* + K\mathbf{b}_c^* + L\mathbf{c}_c^* + m\mathbf{q}^i.$$

Then, (9.8.3.15) with $\tau = \delta - \mathbf{q}^r\cdot\mathbf{v}$ becomes

$$\mathbf{K}'\cdot\mathbf{v} + m\tau = \text{integer} \qquad \text{for } R\mathbf{H} = \mathbf{H} \qquad (9.8.3.17)$$

and (9.8.3.16) transforms into

$$H\upsilon_1' + K\upsilon_2' + L\upsilon_3' + m\tau = \text{integer} \qquad \text{for } R\mathbf{H} = \mathbf{H}, \qquad (9.8.3.18)$$

in which υ_1', υ_2', and υ_3' are the components of $\mathbf{v}$ with respect to the basis $\mathbf{a}_c$, $\mathbf{b}_c$, and $\mathbf{c}_c$.

As an example, consider a (3 + 1)-dimensional space-group transformation with R a mirror perpendicular to the x axis, $\varepsilon = 1$, $\mathbf{v} = \frac{1}{2}\mathbf{b}$, and $\tau = \frac{1}{4}$ with $\mathbf{b}$ orthogonal to $\mathbf{a}$. The modulation wavevector is supposed to be $(\frac{1}{2}\frac{1}{2}\gamma)$. Then $\delta = \frac{1}{4} + \mathbf{q}^r\cdot\mathbf{v} = \frac{1}{2}$. The vectors $\mathbf{H}$ left invariant by R satisfy the relation $2h + m = 0$. For such a vector, the reflection condition becomes

$$\mathbf{K}\cdot\mathbf{v} + m\delta = \tfrac{1}{2}\mathbf{K}\cdot\mathbf{b} + \tfrac{1}{2}m = \frac{k+m}{2} = \text{integer}, \quad \text{or } k + m = 2n.$$

For the basis $\frac{1}{2}(\mathbf{a}^* + \mathbf{b}^*)$, $\frac{1}{2}(\mathbf{a}^* - \mathbf{b}^*)$, $\mathbf{c}^*$, the rational part of the wavevector vanishes. The indices with respect to this basis are $H = h + k + m$, $K = h - k$, $L = l$ and m. The condition now becomes

$$\mathbf{K}'\cdot\mathbf{v} + m\tau = \frac{H - K + m}{4} = \text{integer},$$

$$\text{or} \quad H - K + m = 4n, \quad \text{for } K = -H.$$

Of course, both calculations give the same result: $k + m = 2n$ for $h, k, l, -2h$ and $H - K + m = 4n$ for $H, -H, L, m$.

Table 9.8.3.6 *Centring reflection conditions for* $(3+1)$*-dimensional Bravais classes*

The centring reflection conditions are given for the 24 Bravais classes, belonging to six systems (with number and symbol according to Table 9.8.3.2*a*). If $\mathbf{q}^i = \mathbf{q}$ these are the usual conditions for *hklm*, the indices of the reflections expressed with respect to $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$, $\mathbf{q}$. Otherwise the conditions are for indices *HKLm* with respect to a conventional basis $\mathbf{a}_c^*$, $\mathbf{b}_c^*$, $\mathbf{c}_c^*$, $\mathbf{q}^i$ of the vector module M^*. The relation between indices *HKLm* and *hklm* is given in the fourth column. Planar monoclinic and axial monoclinic mean a monoclinic lattice of main reflections and with the (irrational part of the) modulation wavevector in the mirror plane, or along the unique axis, respectively.

System	$\mathbf{q}^i$ vector	Reflection conditions	Relation of indices	Bravais class	
				No.	Symbol
Triclinic	$(\alpha\beta\gamma)$			1	$\bar{1}P(\alpha\beta\gamma)$
Planar monoclinic	$(\alpha\beta 0)$			2	$2/mP(\alpha\beta 0)$
		$L+m=2n$	$L=2l+m$	3	$2/mP(\alpha\beta\frac{1}{2})$
		$h+l=2n$		4	$2/mB(\alpha\beta 0)$
Axial monoclinic	(00γ)			5	$2/mP(00\gamma)$
		$H+m=2n$	$H=2h+m$	6	$2/mP(\frac{1}{2}0\gamma)$
		$h+l=2n$		7	$2/mB(00\gamma)$
		$H+L=2n,\ K+m=2n'$	$K=2k+m$	8	$2/mB(0\frac{1}{2}\gamma)$
Orthorhombic	(00γ)			9	$mmmP(00\gamma)$
		$K+m=2n$	$K=2k+m$	10	$mmmP(0\frac{1}{2}\gamma)$
		$K+m=2n,\ H+m=2n'$	$K=2k+m,\ H=2h+m$	11	$mmmP(\frac{1}{2}\frac{1}{2}\gamma)$
		$h+k+l=2n$		12	$mmmI(00\gamma)$
		$h+k=2n$		13	$mmmC(00\gamma)$
		$H+K+m=2n$	$H=h+m$	14	$mmmC(10\gamma)$
		$k+l=2n$		15	$mmmA(00\gamma)$
		$H+m=2n,\ K+L=2n'$	$H=2h+m$	16	$mmmA(\frac{1}{2}0\gamma)$
		$h+k=2n,\ h+l=2n'$		17	$mmmF(00\gamma)$
		$H+K+m=2n,$ $K+L=2n'$	$H=h+m$	18	$mmmF(10\gamma)$
Tetragonal	(00γ)			19	$4/mmmP(00\gamma)$
		$H+K+m=2n$	$H=h+k+m,\ K=k-h$	20	$4/mmmP(\frac{1}{2}\frac{1}{2}\gamma)$
		$h+k+l=2n$		21	$4/mmmI(00\gamma)$
Hexagonal/Trigonal	(00γ)	$h-k-l=3n$		22	$\bar{3}mR(00\gamma)$
		$H-K-m=3n$	$H=2h+k+m,\ K=k-h$	23	$\bar{3}1mP(\frac{1}{3}\frac{1}{3}\gamma)$
				24	$6/mmmP(00\gamma)$

The special reflection conditions for the elements occurring in $(3+1)$-dimensional space groups are given in Table 9.8.3.5.

9.8.3.4. *Guide to the use of the tables*

In the tables, Bravais classes, point groups, and space groups are given for three-dimensional incommensurate modulated crystals with a modulation of dimension one and for two-dimensional crystals (*e.g.* surfaces) with one- and two-dimensional modulation (Janssen, Janner & de Wolff, 1980). In the following, we discuss briefly the information given. Examples of their use can be found in Subsection 9.8.3.5.

To determine the symmetry of the modulated phase, one first determines its average structure, which is obtained from the main reflections. Since this structure has three-dimensional space-group symmetry, this analysis is performed in the usual way.

The diffraction pattern of the three-dimensional modulated phase can be indexed by $3+1$ integers. The Bravais class is determined by the symmetry of the vector module spanned by the $3+1$ basis vectors. The crystallographic system of the pattern is equal to or lower than that implied by the main reflections. One chooses a conventional basis ($\mathbf{q}^r = 0$) for the vector module, and finds the Bravais class from the general reflection conditions using Table 9.8.3.6. The relation between indices *hklm* with respect to the basis $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$, and $\mathbf{q}$ and *HKLm* with respect to the conventional basis $\mathbf{a}_c^*$, $\mathbf{b}_c^*$, $\mathbf{c}_c^*$, and $\mathbf{q}^i$ is also given there.

Table 9.8.3.2(*a*) gives the number labelling the $(3+1)$-dimensional Bravais class, its symbol, its external and internal point group, and the modulation wavevector. Moreover, the superspace conventional basis (for which the rational part $\mathbf{q}^r$ vanishes) and the corresponding $(3+1)$-dimensional centring are given. Because the four-dimensional lattices belong to Euclidean Bravais classes, the corresponding class is also given in the notation of Janssen (1969) and Brown *et al.* (1978).

The point group of the modulated structure is a subgroup of the holohedry of its lattice Λ. In Table 9.8.3.3, for each system the $(3+1)$-dimensional point groups are given. Each system contains one or more Bravais classes. Each geometric crystal class contains one or more arithmetic crystal classes. The $(3+1)$-dimensional arithmetic classes belonging to a given geometric crystal class are also listed in Table 9.8.3.3.

Starting from the space group of the average structure, one can determine the $(3+1)$-dimensional superspace group. In Table 9.8.3.5, the full list of these $(3+1)$-dimensional superspace groups is given for the incommensurate case and are ordered according to their basic space group. They have a number *n.m* where *n* is the number of the basic space group one

finds in *International Tables for Crystallography*, Volume A. The various $(3+1)$-dimensional superspace groups for each basic group are distinguished by the number m. Furthermore, the symbol of the basic space group, the point group, and the symbol for the corresponding superspace group are given. In the last column, the special reflection conditions are listed for typical symmetry elements. These may help in the structure analysis. The $(2+d)$-dimensional superspace groups, relevant for modulated surface structures, are given in Tables 9.8.3.4(*a*) and (*b*).

9.8.3.5. *Examples*

(*A*) Na_2CO_3

Na_2CO_3 has a phase transition at about 753 K from the hexagonal to the monoclinic phase. At about 633 K, one vibration mode becomes unstable and below the transition temperature $T_i = 633$ K there is a modulated γ-phase (de Wolff & Tuinstra, 1986). At low temperature (128 K), a transition to a commensurate phase has been reported.

The main reflections in the modulated phase belong to a monoclinic lattice, and the satellites to a modulation with wavevector $\mathbf{q} = \alpha\mathbf{a}^* + \gamma\mathbf{c}^*$, b axis unique. The dimension of the modulation is one. The main reflections satisfy the condition

$$hkl0, h+k = \text{even}.$$

Therefore, the lattice of the average structure is C-centred monoclinic. For the satellites, the same general condition holds ($hklm, h+k = \text{even}$). From Table 9.8.3.6, one sees after a change of axes that the Bravais class of the modulated structure is

$$\text{No. 4: } 2/mC(\alpha 0\gamma).$$

Table 9.8.3.2(*a*) shows that the point group of the vector module is $2/m(\bar{1}1)$. The point group of the modulated structure is equal to or a subgroup of this one.

The space group of the average structure determined from the main reflections is $C2/m$ (No. 12 in *International Tables for Crystallography*, Volume A). The superspace group may then be determined from the special reflection condition

$$h0lm, m = \text{even}$$

using Table 9.8.3.5. There are five superspace groups with basic group No. 12. Among them there are two in Bravais class 4. The reflection condition mentioned leads to the group

$$\text{No. } 12.2 = C2/m(\alpha 0\gamma)0s = P^{C2/m}_{\bar{1}\ s}.$$

In principle, the superspace group could be a subgroup of this, but, since the transition normal–incommensurate is of second order, Landau theory predicts that the basic space group is the symmetry group of the unmodulated monoclinic phase, which is $C2/m$.

(*B*) $ThBr_4$

Thorium tetrabromide has an incommensurately modulated phase below $T_i = 95$ K (Currat, Bernard & Delamoye, 1986). Above that temperature, the structure has space group $I4_1/amd$ (No. 141 in *International Tables for Crystallography*, Volume A). At T_i, a mode becomes unstable and a modulated β-phase sets in with modulation wavevector $\gamma\mathbf{c}^*$. The dimension of the modulation is one, consequently.

The main reflections belong to a tetragonal lattice. The general reflection condition is

$$hklm, h+k+l \text{ even}.$$

Looking at Table 9.8.3.6, one finds the Bravais class to be No. $21 = I4/mmm(00\gamma)$. Table 9.8.3.2(*a*) gives $4/mmm(\bar{1}111)$ for the point group of the vector module.

For the determination of the symmetry group of the modulated structure, one has the special reflection conditions

$$hk00, h \text{ even}; \quad hhl0, 2h+l = 4n; \quad (00l0, l = 4n)$$
$$0klm \text{ (and } h0lm\text{) absent for } m = 1.$$

Higher-order satellites have not been observed. The main reflections lead to the basic group $I4_1/amd$. If one generalizes the reflection condition observed for $0klm$ to $0klm$, $m = \text{even}$, the superspace group is found from Table 9.8.3.5 under the groups $141.x$ as

$$\text{No. } 141.2 = I4_1/amd(00\gamma)s0s0 = P^{I4_1/amd}_{s\ \bar{1}\ s\ 1}.$$

(*C*) PAMC

Bis(n-propylammonium) tetrachloromanganate (PAMC) has several phase transitions. Above about 395 K, it is orthorhombic with space group *Abma*. At T_i, this β-phase goes over into the incommensurately modulated γ-phase (Depmeier, 1986; Kind & Muralt, 1986). The wavevector of the modulation is $\alpha\mathbf{a}^* + \mathbf{c}^*$. Therefore, the dimension of the modulation is one. Interchanging the a and c axes, one sees from Table 9.8.3.2(*a*) that the Bravais class is No. $14 = mmmC(10\gamma)$. In this new setting, the conventional basis of the vector module is $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$, and $\gamma\mathbf{c}^*$ and the general reflection condition becomes

$$HKLm, H+K+m = \text{even}.$$

Therefore, if one considers the vector module as the projection of a four-dimensional lattice, the reflection condition corresponds to a $(\frac{1}{2}\frac{1}{2}0\frac{1}{2})$ centring in four dimensions.

The point group of the vector module is $mmm(11\bar{1})$. The basic space group being *Abma* (or *Ccmb* in the new setting), the superspace group follows from Table 9.8.3.5 as

$$\text{No. } 64.3 = Ccmb(10\gamma) = L^{Ccmb}_{11\bar{1}}$$

or, in the original setting

$$\text{No. } 64.3 = Abma(\alpha 01) = N^{Abma}_{\bar{1}11}.$$

No. 64.4 can be excluded because the reflections do not show the special reflection condition $0KLm$, $m = \text{even}$.

9.8.3.6. *Ambiguities in the notation*

The invariant part v_s^o of the translation part v_s of a $(3+1)$-dimensional superspace-group element is uniquely determined by (9.8.3.5). This does not imply that for each element of the point group there is a translation for which the invariant part is unique up to lattice vectors. The reason is that, for a given element R of the point group and given origin, v_s may be changed when R is combined with a three-dimensional lattice translation $w_s = (\mathbf{w}, 0)$. This situation is well known in ordinary three-dimensional crystallography. For example, the twofold rotation $(x, y, z) \rightarrow (-x, z, y)$ in the space group $P4_132$ has according to Volume A of *International Tables for Crystallography* a translation part $(\frac{1}{4}, \frac{3}{4}, \frac{1}{4})$. Its invariant part is $(0, \frac{1}{2}, \frac{1}{2})$. However, when the translation part is equivalently taken as $(\frac{1}{4}, \frac{3}{4}, -\frac{3}{4})$, the invariant part vanishes. Therefore, in the symbol for that space group, the corresponding generator is given as the rotation '2' and not as the screw axis '2_1'.

The same situation may occur in $3+1$ dimensions. This can be seen very clearly from the definition of τ [equation (9.8.3.8)]. Since $\mathbf{v}$ is only determined modulo a lattice vector, one may add to it a lattice vector that has a non-vanishing product with $\mathbf{q}^r$.

This results in a change for τ. For example, the $(3+1)$-dimensional space group $Pmmm(\frac{1}{2}0\gamma)000 = A^{Pmmm}_{1\,1\,\bar{1}}$ has a mirror perpendicular to the a axis with associated value $\tau = 0$. The parallel mirror at a distance $a/2$ has $\mathbf{v} = \mathbf{a}$ and consequently $\tau = \frac{1}{2}$. Hence, the symbols $Pmmm(\frac{1}{2}0\gamma)000$ and $Pmmm(\frac{1}{2}0\gamma)s00$ indicate the same group. This non-uniqueness in the symbol, however, does not have serious practical consequences.

Another source of ambiguity is the fact that the assignment of a satellite to a main reflection is not unique. For example, the reflection conditions for the group $I2cb(00\gamma)0s0 = P^{I2cb}_{\bar{1}s\bar{1}}$ are $h+k+l =$ even because of the centring and $l+m =$ even and $h+m =$ even for $h0lm$ because of the two glide planes perpendicular to the b axis. When one takes for the modulation vector $\mathbf{q} = \gamma'\mathbf{c}^* = (1-\gamma)\mathbf{c}^*$, the new indices are h, k, l', and m' with $l' = l+m$ and $m' = -m$. Then the reflection conditions become $l' =$ even and $h+m =$ even for $h0l'm'$. The first of these conditions implies the symbol $I2cb(00\gamma)000 = P^{I2cb}_{\bar{1}1\bar{1}}$ for the group considered. This, however, is the symbol for the nonequivalent group with condition $h =$ even for $h0lm$. This difficulty may be avoided by sometimes using a non-standard setting of the three-dimensional space group (see Yamamoto *et al.*, 1985). In this case, the setting $I2ab$ instead of $I2cb$ avoids the problem.

9.8.4. Theoretical foundation

9.8.4.1. *Lattices and metric*

A periodic crystal structure is defined in a three-dimensional Euclidean space V and is invariant with respect to translations $\mathbf{n}$ which are integral linear combinations of three fundamental ones $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$:

$$\mathbf{n} = \sum_{i=1}^{3} n_i \mathbf{a}_i, \quad n_i \text{ integers.} \qquad (9.8.4.1)$$

These translations are linearly independent and span a lattice Λ. The *dimension* of Λ is the dimension of the space spanned by $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ and the *rank* is the (smallest) number of free generators of those integral linear combinations. In the present case, both are equal to three. Accordingly,

$$\{\Lambda\} = V \quad \text{and} \quad \Lambda \approx Z^3. \qquad (9.8.4.2)$$

The elements of Z^3 are triples of integers that correspond to the coordinates of the lattice points. The Bragg reflection peaks of such a crystal structure are at the positions of a reciprocal lattice Λ^*, also of dimension and rank equal to three. Furthermore, the Fourier wavevectors $\mathbf{H}$ belong to Λ^* (after identification of lattice vectors with lattice points):

$$\mathbf{H} = \sum_{i=1}^{3} h_i \mathbf{a}_i^*, \quad h_i \text{ integers} \qquad (9.8.4.3)$$

where $\{\mathbf{a}_i^*\}$ is the reciprocal basis

$$\mathbf{a}_i \cdot \mathbf{a}_k^* = \delta_{ik}.$$

The two corresponding metric tensors g and g^*,

$$g_{ik} = \mathbf{a}_i \cdot \mathbf{a}_k \quad \text{and} \quad g_{ik}^* = \mathbf{a}_i^* \cdot \mathbf{a}_k^*, \qquad (9.8.4.4)$$

are positive definite and dual:

$$\sum_{k=1}^{3} g_{ik} g_{kj}^* = \delta_{ij}.$$

We now consider crystal structures defined in the same three-dimensional Euclidean space V with Fourier wavevectors that are integral linear combinations of $n = (3+d)$ fundamental ones $\mathbf{a}_1^*, \ldots, \mathbf{a}_n^*$:

$$\mathbf{H} = \sum_{i=1}^{n} h_i \mathbf{a}_i^*, \quad h_i \text{ integers.} \qquad (9.8.4.5)$$

The components $(h_1, \ldots, h_n)$ are the indices labelling the corresponding Bragg reflection peaks.

A crystal is *incommensurate* when $d > 0$ and the vectors $\mathbf{a}_i^*$ linearly independent over the rational numbers. In that case, the crystal does not have lattice periodicity and is said to be *aperiodic*. The above description can still be convenient, even in the case that the vectors $\mathbf{a}_i^*$ are not independent over the rationals: one or more of them is then expressed as rational linear combinations of the others. A typical example is that of a superstructure arising from the (commensurate) modulation of a basic structure with lattice periodicity.

Let us denote by M^* the set of all integral linear combinations of the vectors $\mathbf{a}_1^*, \ldots, \mathbf{a}_n^*$. These are said to form a *basis*. It is a set of free Abelian generators, therefore the *rank* of M^* is n. The *dimension* of M^* is the dimension of the Euclidean space spanned by M^*

$$\{M^*\} = V \quad \text{and} \quad M^* \approx Z^n. \qquad (9.8.4.6)$$

The elements of Z^n are precisely the set of indices introduced above. Mathematically speaking, M^* has the structure of a (free Abelian) module. Its elements are vectors. So we call M^* a *vector module*. This nomenclature is intended as a *generic* characterization. When a series of structures is considered with different values of the components of the last d vectors with respect to the first three, the generic values of these components are irrational, but accidentally they may become rational as well. This situation typically arises when considering crystal structures under continuous variation of parameters like temperature, pressure or chemical composition. In the case of an ordinary crystal, rank and dimension are equal, the crystal structure is *periodic*, and the vector module becomes a (reciprocal) lattice.

Lattices and vector modules are, mathematically speaking, free Z modules. For such a module, there exists a dual one that is also free and of the same rank. In the periodic crystal case, that duality can be expressed by a scalar product, but for an aperiodic crystal this is no longer possible. It is possible to keep the metrical duality by enlarging the space and considering the vector module M^* as the projection of an n-dimensional (reciprocal) lattice Σ^* in an n-dimensional Euclidean space V_s.

$$M^* \to \Sigma^*, \quad \{\Sigma^*\} = V_s \quad \text{and} \quad \Sigma^* \approx Z^n, \qquad (9.8.4.7)$$

with the orthogonal projection π_E of V_s onto V defined by

$$M^* = \pi_E \Sigma^*. \qquad (9.8.4.8)$$

This corresponds to attaching to the diffraction peak with indices $(h_1, \ldots, h_n)$ the point of an n-dimensional reciprocal lattice having the same set of coordinates. The orthocomplement of V in V_s is called internal space and denoted by V_I. The embedding is uniquely defined by the relations

$$a_{si}^* = (\mathbf{a}_i^*, \mathbf{a}_{Ii}^*), \quad i = 1, \ldots, n, \qquad (9.8.4.9)$$

where $\{a_{si}^*\}$ is a basis of Σ^* and $\{\mathbf{a}_i^*\}$ a basis of M^*. The vectors $\mathbf{a}_{Ii}^*$ span V_I.

The crystal density ρ in V can also be embedded as ρ_s in V_s by identifying the Fourier coefficients $\hat{\rho}$ at points of M^* and of Σ^* having correspondingly the same components.

$$\hat{\rho}_s(h_1, \ldots, h_n) \equiv \hat{\rho}(h_1, \ldots, h_n). \qquad (9.8.4.10)$$

Then ρ_s is invariant with respect to translations of the lattice Σ with basis

references