assumption of irrationality. Only some of the statements need to be adapted. The most important change is that there is no longer a one-to-one correspondence between the points of the reciprocal lattice $\Sigma^*$ and its projection on $V$ defining the positions of the Bragg peaks. Furthermore, the projection of the lattice $\Sigma$ on the space $V_I$ forms a discrete set. The latter means the following. For an incommensurate modulation, the incommensurate structure, which is the intersection of a periodic structure with the hyperplane $\mathbf{r}_I = 0$, is also the intersection of the same periodic structure with a hyperplane $\mathbf{r}_I = \text{constant}$, where this constant is of the form

$$\sum_{i=1}^{3} h_i \mathbf{a}_{Ii} + \sum_{j=1}^{d} m_j \mathbf{a}_{I3+j}. \qquad (9.8.5.12)$$

Because for an incommensurate structure these vectors form a dense set in $V_I$, the phase of the modulation function with respect to the basic structure is not determined. For a commensurate modulation, however, the points (9.8.5.12) form a discrete set, even belong to a lattice, and the phase (or the phases) of the modulation are determined within vectors of this lattice. Notice that the grid of this lattice becomes finer as the denominators in the rational components become larger.

When $G_s$ is a $(3+d)$-dimensional superspace group, its elements, in general, do not leave the ordinary space $V$ invariant. The subgroup of all elements that do leave $V$ invariant, when restricted to $V$, is a group of distance-preserving transformations in three dimensions and thus a subgroup of $E(3)$, the three-dimensional Euclidean group. In general, this subgroup is not a three-dimensional space group. It is so when the modulation wavevectors all have rational components only, *i.e.* when $\sigma$ is a matrix with rational entries. Because the phase of the modulation function is now determined (within a given rational number smaller than 1), the space group depends in general on this phase.

As an example, consider a one-dimensional modulation of a basic structure with orthorhombic space group *Pcmn*. Suppose that the modulation wavevector is $\gamma\mathbf{c}^*$. Then the mirror $R = m_z$ perpendicular to the $c$ axis is combined with $R_I = \varepsilon = -1$. Suppose, furthermore, that the glide reflection perpendicular to the $a$ axis and the $b$ mirror are both combined with a phase shift $\frac{1}{2}$. In terms of the coordinates $x, y, z$ with respect to the $a, b$ and $c$ axes, and internal coordinate $t$, the generators of the $(3+1)$-dimensional superspace group $Pcmn(00\gamma)ss0$ act as

$$(x, y, z, t) \rightarrow (x+k, y+l, z+m, t-\gamma m+n), \quad k, l, m, n \text{ integers}, \qquad (9.8.5.13a)$$

$$(x, y, z, t) \rightarrow (-x+k+\tfrac{1}{2}, y+l, z+\tfrac{1}{2}+m, t-\gamma/2-\gamma m+\tfrac{1}{2}+n), \qquad (9.8.5.13b)$$

$$(x, y, z, t) \rightarrow (x+k, -y+l+\tfrac{1}{2}, z+m, t-\gamma m+\tfrac{1}{2}+n), \qquad (9.8.5.13c)$$

$$(x, y, z, t) \rightarrow (x+\tfrac{1}{2}+k, y+\tfrac{1}{2}+l, -z+\tfrac{1}{2}+m, -t-\gamma/2-\gamma m+n). \qquad (9.8.5.13d)$$

Note that these positions are referred to a split basis (*i.e.* of basis vectors lying either in $V$ or in $V_I$) and not to a basis of the lattice $\Sigma$. When the superstructure is the intersection of a periodic structure with the plane at $t = t_o$, its three-dimensional space group follows from equation (9.8.5.13) by the requirement $t' = t_o$. When $\gamma$ has the rational value $r/s$ with $r$ and $s$ relatively prime, the conditions for each of the generators to give an element of the three-dimensional space group are, respectively:

$$-rm + sn = 0 \qquad (9.8.5.14a)$$

$$-2rm + 2sn = r - s \qquad (9.8.5.14b)$$

$$-2rm + 2sn = -s \qquad (9.8.5.14c)$$

$$-2rm + 2sn = 4st, \qquad (9.8.5.14d)$$

for $m, n, r, s$ integers and $t$ real. These conditions are never satisfied simultaneously. It depends on the parity of both $r$ and $s$ which element occurs, and for the elements with $\varepsilon = -1$ it also depends on the value of the 'phase' $t$, or more precisely on the product $\tau = 4st$. The translation group is determined by the first condition as in (9.8.5.14*a*). Its generators are

$$\mathbf{a}, \mathbf{b}, \text{ and } s\mathbf{c},$$

where the last vector is the external part of the lattice vector $s(\mathbf{c}, -r/s) + r(0, 1)$. The other space-group elements can be derived in the same way. The possible space groups are:

| $\gamma = r/s$ | $\tau$ even integer | $\tau$ odd integer | otherwise |
|---|---|---|---|
| $r$ even, $s$ odd | $11\frac{2_1}{n}$ | $2_12_12_1$ | $112_1$ |
| $r$ odd, $s$ even | $1\frac{2_1}{c}1$ | $2_1cn$ | 1c1 |
| $r$ odd, $s$ odd | $\frac{2_1}{c}11$ | $c2_1n$ | $c11$ |

In general, the three-dimensional space groups compatible with a given $(3+d)$-dimensional superspace group can be determined using analogous equations.

As one can see from the table above, the orthorhombic $(3+d)$-dimensional superspace group leads in several cases to monoclinic three-dimensional space groups. The lattice of main reflections, however, still has orthorhombic point-group symmetry. Description in the conventional way by means of three-dimensional groups then neglects some of the structural features present. Even if the orthorhombic symmetry is slightly broken, the orthorhombic basic structure is a better characterization than a monoclinic one. Note that in that case the superspace-group symmetry is also only an approximation.

When the denominators of the wavevector components become small, additional symmetry operations become possible. Because the one-to-one correspondence between $\Sigma^*$ and $M^*$ is no longer present, there may occur symmetry elements with trivial action in $V$ but with nontrivial transformation in $V_I$. For $d = 1$, these possibilities have been enumerated. The corresponding Bravais classes are given in Table 9.8.3.2(*b*).

## APPENDIX *A*
## Glossary of symbols

$M^*$ Vector module in $m$-dimensional reciprocal space ($m = 1, 2, 3$; normally $m = 3$), isomorphic to $Z^n$ with $n \geq m$. The dimension of $M^*$ is $m$, its rank $n$.

$\mathbf{a}_i^*$ ($i = 1, \ldots, n$.) Basis of a vector module $M^*$ of rank $n$; if $n = 4$ and $\mathbf{q}$ is modulation wavevector (the $n = 4$ case is restricted in what follows to modulated crystals), the basis of $M^*$ is chosen as $\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*, \mathbf{q}$, with $\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$ a basis of the lattice of main reflections.

$\Lambda^*$ Lattice of main reflections, $m$-dimensional reciprocal lattice.

$\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$ (Conventional) basis of $\Lambda^*$ for $m = 3$.

$\Lambda$ Direct $m$-dimensional lattice, dual to $\Lambda^*$.

$V_s$ Superspace; Euclidean space of dimension $n = m + d$; $V_s = V \oplus V_I$.

$V$ Physical (or external) space of dimension $m$ ($m = 1, 2$ or 3), also indicated by $V_E$.

$V_I$ Internal (or additional) space of dimension $d$.

$\Sigma^*$ Reciprocal lattice in $n$-dimensional space, whose orthogonal projection on $V$ is $M^*$.

$\Sigma$ Lattice in $n$-dimensional superspace for which $\Sigma^*$ is the reciprocal one.

$a^*_{si}$ Lattice basis of $\Sigma^*$ in $V_s$ ($i = 1, \ldots, n$);
if $n = 4$, this basis can be chosen as $\{(\mathbf{a}^*, 0), (\mathbf{b}^*, 0), (\mathbf{c}^*, 0), (\mathbf{q}, 1)\}$ and is called standard. An equivalent notation is $(\mathbf{q}, 1) = (\mathbf{q}, \mathbf{d}^*)$;
for $n = 3 + d$, the general form of a standard basis is $(\mathbf{a}^*, 0)$, $(\mathbf{b}^*, 0)$, $(\mathbf{c}^*, 0)$, $(\mathbf{q}_1, \mathbf{d}^*_1), \ldots, (\mathbf{q}_j, \mathbf{d}^*_j), \ldots, (\mathbf{q}_d, \mathbf{d}^*_d)$.

$a_{si}$ ($i = 1, \ldots, n$.) Lattice basis of $\Sigma$ in $V_s$ dual to $\{a^*_{si}\}$;
if $n = 4$, the standard basis is $(\mathbf{a}, -\mathbf{q}\cdot\mathbf{a}), (\mathbf{b}, -\mathbf{q}\cdot\mathbf{b}), (\mathbf{c}, -\mathbf{q}\cdot\mathbf{c}), (0, 1) = (0, \mathbf{d})$;
for $n = 3 + d$, a standard basis is dual to the standard one given above.

$\mathbf{q}_j$ Modulation wavevector(s) $\mathbf{q}_j = \sum_{i=1}^{3} \sigma_{ji}\mathbf{a}^*_i$;
if $n = 4$, $\mathbf{q} = \sum_{i=1}^{3} \sigma_i \mathbf{a}^*_i = \alpha\mathbf{a}^* + \beta\mathbf{b}^* + \gamma\mathbf{c}^*$;
$\sigma = (\alpha, \beta, \gamma)$;
if $n = 4$, $\mathbf{q} = \mathbf{q}^i + \mathbf{q}^r$, with $\mathbf{q}^i = (1/N)\sum_{R \text{ in } K} \varepsilon(R) R\mathbf{q}$, where $\varepsilon(R) = R_I$, and $N$ is the order of $K$.

$\mathbf{H}$ Bragg reflections: $\mathbf{H} = \sum_{i=1}^{n} h_i \mathbf{a}^*_i = (h_1, h_2, \ldots, h_n)$;
if $n = 4$, $\mathbf{H} = \sum_{i=1}^{4} h_i \mathbf{a}^*_i = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* + m\mathbf{q} = (h, k, l, m)$.

$H_s$ Embedding of $\mathbf{H}$ in $V_s$: for $\mathbf{H} = (h_1, \ldots, h_n) = \sum_{i=1}^{n} h_i \mathbf{a}^*_i$, one has correspondingly $H_s = (\mathbf{H}, \mathbf{H}_I) = \sum_{i=1}^{n} h_i a^*_{si}$.

$P_L$ Laue point group.

$O(m)$ Orthogonal group in $m$ dimensions.

$R$ Orthogonal point-group transformation, element of $O(m)$.

$K$ Point group, crystallographic subgroup of $O(m)$.

$R_s$ Superspace point-group element: $R_s = (R_E, R_I) = (R, R_I)$ element of $O(m) \times O(d)$ with $R_E = R$ external, and $R_I$ internal part of $R_s$, respectively;
if $n = 4$, superspace point-group element: $[R, \varepsilon(R)]$ with $\varepsilon(R) = \pm 1$, also written $(R, \varepsilon)$.

$K_s$ Point group, crystallographic subgroup of $O(m) \times O(d)$.

$K_E$ External part of $K_s$, crystallographic point group, subgroup of $O(m)$ with as elements the external part transformations of $K_s$.

$K_I$ Internal part of $K_s$, crystallographic point group, subgroup of $O(d)$ with as elements the internal part transformations of $K_s$.

$\mathbf{r}_o(\mathbf{n}, j)$ Atomic positions in the basic structure: $\mathbf{r}_o(\mathbf{n}, j) = \mathbf{n} + \mathbf{r}_j$ with $\mathbf{n} \in \Lambda$.

$\mathbf{r}(\mathbf{n}, j)$ Atomic positions in the displacively modulated structure;
($d = 1$): $\mathbf{r}(\mathbf{n}, j) = \mathbf{r}_o(\mathbf{n}, j) + \mathbf{u}_j[\mathbf{q}\cdot\mathbf{r}(\mathbf{n}, j) + \varphi_j]$. In general, however, different phases $\varphi_{j\alpha}$ may occur for different components $u_{j\alpha}$ along the crystallographic axes.

$\mathbf{u}_j(x)$ Modulation function for displacive modulation with $\mathbf{u}_j(x + 1) = \mathbf{u}_j(x)$.

$p_j(x)$ Modulation function for occupation modulation with $p_j(x + 1) = p_j(x)$.

$g$ Euclidean transformation in $m$ dimensions; $g = \{R|\mathbf{v}\}$ element of the space group $G$ with rotational part $R$ and translational part $\mathbf{v}$.

$\mathbf{v}^o$ Intrinsic translation part (origin independent).

$g_s$ Superspace group transformation ($d = 1$):
$g_s = \{(R, \varepsilon)|(\mathbf{v}, \Delta)\} = (\{R|\mathbf{v}\}, \{\varepsilon|\Delta\}) = \{R_s|\upsilon_s\}$
element of the superspace group $G_s$.
In the $(3 + d)$-dimensional case:
$g_s = \{(R, R_I)|(\mathbf{v}, \mathbf{v}_I)\} = (\{R|\mathbf{v}\}, \{R_I|\mathbf{v}_I\})$.

$\upsilon_I$ Internal shift ($d = 1$): $\upsilon_I = \Delta = \delta - \mathbf{q}\cdot\mathbf{v}$.

$\tau$ Intrinsic internal shift ($d = 1$): $\tau = \delta - \mathbf{q}^r\cdot\mathbf{v}$.

$\Gamma^*(R)$ Point-group transformation $R$ with respect to a basis of $M^*$ and at the same time superspace point-group transformation $R_s$ with respect to a corresponding basis of $\Sigma^*$.

$\Gamma(R)$ Superspace point-group transformation with respect to a lattice basis of $\Sigma$ dual to that of $\Sigma^*$ leading to $\Gamma^*(R)$. The mutual relation is then $\Gamma^*(R) = \tilde{\Gamma}(R^{-1})$ with the tilde denoting transposition.

$\Gamma_E(R)$, $\Gamma_I(R)$, $\Gamma_M(R)$: external, internal, and mixed blocks of $\Gamma(R)$, respectively.

$\Gamma^*_E(R)$, $\Gamma^*_I(R)$, $\Gamma^*_M(R)$: external, internal, and mixed blocks of $\Gamma^*(R)$, respectively.

$S_{\mathbf{H}}$ Structure factor:

$$S_{\mathbf{H}} = \sum_{\mathbf{n}} \sum_{j} f_j(\mathbf{H}) \exp[2\pi i \mathbf{H}\cdot\mathbf{r}(\mathbf{n}, j)].$$

$f_j(\mathbf{H})$ Atomic scattering factor for atom $j$.

## APPENDIX *B*
## Basic definitions

In the following, we give a short definition of the most important notions appearing in the theory and of the equivalence relations used in the tables. The latter are especially adapted to the case of modulated crystal phases.

[i] *Vector module*. A set of all integral linear combinations of a finite number of vectors. The *dimension* of the vector module is the dimension ($m$) of the space $V$ (also indicated as $V_E$ and called external) generated by it over the real numbers. Its *rank* ($n$) is the minimal number of rationally independent vectors that generate the vector module. If this rank is equal to the dimension, the vector module is also a lattice. In general, a vector module of rank $n$ and dimension $m$ is the orthogonal projection on the $m$-dimensional space $V$ of an $n$-dimensional lattice. We shall restrict ourselves mainly to the case $m = 3$ and $n = 4$, but the following definitions are valid for modulated phases of arbitrary dimension and rank. The *dimension of the modulation* ($d$) is $n - m$. The modulation phases span a $d$-dimensional space $V_I$ (called internal or additional).

[ii] *Superspace*. $V_s$ is an $n$-dimensional Euclidean space that is the direct sum of an $m$-dimensional *external* space $V$ (of the crystal) and a $d$-dimensional *internal* space $V_I$ (for the additional degrees of freedom). $V$ is sometimes denoted by $V_E$.

[iii] *Split basis*. For the space $V_s = V \oplus V_I$, this is a basis with $m$ basis vectors in $V$ and $d = n - m$ basis vectors in $V_I$.

[iv] *Standard basis*. For the $(m + d)$-dimensional space $V_s = V \oplus V_I$, a standard basis in direct space is one having the last $d$ basis vectors lying in $V_I$ ($d$ = dimension of $V_I$ = dimension of the modulation). A standard basis in



references