$h$, $k$ and $l$ in all rhombohedral space groups, described with 'rhombohedral axes', and of $h$ and $k$ in some tetragonal space groups are not stated;

(vii) in the 'hexagonal-axes' descriptions of trigonal and hexagonal space groups, Bravais–Miller indices $hkil$ are used. They obey two conditions:

($a$) $h + k + i = 0$, *i.e.* $i = -(h + k)$;

($b$) the indices $h$, $k$, $i$ are cyclically permutable; this is not stated. Further details can be found in textbooks of crystallography.

Note that the integral reflection conditions for a rhombohedral lattice, described with 'hexagonal axes', permit the presence of only one member of the pair $hkil$ and $\bar{h}\bar{k}il$ for $l \neq 3n$ (*cf.* Table 2.2.13.1). This applies also to the zonal reflections $h\bar{h}0l$ and $\bar{h}h0l$, which for the rhombohedral space groups must be considered separately.

*Example*

For a monoclinic crystal ($b$ unique), the following reflection conditions have been observed:

(1) $hkl$: $h + k = 2n$;

(2) $0kl$: $k = 2n$; $h0l$: $h, l = 2n$; $hk0$: $h + k = 2n$;

(3) $h00$: $h = 2n$; $0k0$: $k = 2n$; $00l$: $l = 2n$.

Line (1) states that the cell used for the description of the space group is $C$ centred. In line (2), the conditions $0kl$ with $k = 2n$, $h0l$ with $h = 2n$ and $hk0$ with $h + k = 2n$ are a consequence of the integral condition (1), leaving only $h0l$ with $l = 2n$ as a new condition. This indicates a glide plane $c$. Line (3) presents no new condition, since $h00$ with $h = 2n$ and $0k0$ with $k = 2n$ follow from the integral condition (1), whereas $00l$ with $l = 2n$ is a consequence of a zonal condition (2). Accordingly, there need not be a twofold screw axis along [010]. Space groups obeying the conditions are $Cc$ (9, $b$ unique, cell choice 1) and $C2/c$ (15, $b$ unique, cell choice 1). On the basis of diffraction symmetry and reflection conditions, no choice between the two space groups can be made (*cf.* Part 3).

For a different choice of the basis vectors, the reflection conditions would appear in a different form owing to the transformation of the reflection indices (*cf.* cell choices 2 and 3 for space groups $Cc$ and $C2/c$ in Part 7).

### 2.2.13.2. *Special or 'extra' reflection conditions*

These apply either to the integral reflections $hkl$ or to particular sets of zonal or serial reflections. In the space-group tables, the minimal special conditions are listed that, on combination with the general conditions, are sufficient to generate the complete set of conditions. This will be apparent from the examples below.

*Examples*

(1) $P4_222$ (93)

General position $8p$: $00l$: $l = 2n$, due to $4_2$; the projection on [001] of any crystal structure with this space group has periodicity $\frac{1}{2}c$.

Special position $4i$: $hkl$: $h + k + l = 2n$; any set of symmetrically equivalent atoms in this position displays additional $I$ centring.

Special position $4n$: $0kl$: $l = 2n$; any set of equivalent atoms in this position displays a glide plane $c \perp [100]$. Projection of this set along [100] results in a halving of the original $c$ axis, whence the special condition. Analogously for $h0l$: $l = 2n$.

(2) $C12/c1$ (15, unique axis $b$, cell choice 1)

General position $8f$: $hkl$: $h + k = 2n$, due to the $C$-centred cell.

Special position $4d$: $hkl$: $k + l = 2n$, due to additional $A$ and $B$ centring for atoms in this position. Combination with the general condition results in $hkl$: $h + k, h + l, k + l = 2n$ or $hkl$ all odd or all even; this corresponds to an $F$-centred arrangement of atoms in this position.

Special position $4b$: $hkl$: $l = 2n$, due to additional halving of the $c$ axis for atoms in this position. Combination with the general condition results in $hkl$: $h + k, l = 2n$; this corresponds to a $C$-centred arrangement in a cell with half the original $c$ axis. No further condition results from the combination.

(3) $I12/a1$ (15, unique axis $b$, cell choice 3)

For the description of space group No. 15 with cell choice 3 (see Section 2.2.16 and space-group tables), the reflection conditions appear as follows:

General position $8f$: $hkl$: $h + k + l = 2n$, due to the $I$-centred cell.

Special position $4b$: $hkl$: $h = 2n$, due to additional halving of the $a$ axis. Combination gives $hkl$: $h, k + l = 2n$, *i.e.* an $A$-centred arrangement of atoms in a cell with half the original $a$ axis.

An analogous result is obtained for position $4d$.

(4) $Fmm2$ (42)

General position $16e$: $hkl$: $h + k, h + l, k + l = 2n$, due to the $F$-centred cell.

Special position $8b$: $hkl$: $h = 2n$, due to additional halving of the $a$ axis. Combination results in $hkl$: $h, k, l = 2n$, *i.e.* all indices even; the atoms in this position are arranged in a primitive lattice with axes $\frac{1}{2}a$, $\frac{1}{2}b$ and $\frac{1}{2}c$.

For the cases where the special reflection conditions are described by means of combinations of 'OR' and 'AND' instructions, the 'AND' condition always has to be evaluated with priority, as shown by the following example.

*Example*: $P\bar{4}3n$ (218)

Special position $6d$: $hkl$: $h + k + l = 2n$ or $h = 2n + 1$, $k = 4n$ and $l = 4n + 2$.

This expression contains the following two conditions:

($a$) $hkl$: $h + k + l = 2n$;

($b$) $h = 2n + 1$ and $k = 4n$ and $l = 4n + 2$.

A reflection is 'present' (occurring) if either condition ($a$) is satisfied or if a permutation of the three conditions in ($b$) are simultaneously fulfilled.

### 2.2.13.3. *Structural or non-space-group absences*

Note that in addition *non-space-group absences* may occur that are not due to the symmetry of the space group (*i.e.* centred cells, glide planes or screw axes). Atoms in general or special positions may cause additional systematic absences if their coordinates assume special values [*e.g.* 'noncharacteristic orbits' (Engel *et al.*, 1984)]. Non-space-group absences may also occur for special arrangements of atoms ('false symmetry') in a crystal structure (*cf.* Templeton, 1956; Sadanaga *et al.*, 1978). Non-space-group absences may occur also for polytypic structures; this is briefly discussed by Durovič in Section 9.2.2.2.5 of *International Tables for Crystallography* (2004), Vol. C. Even though all these 'structural absences' are fortuitous and due to the special arrangements of atoms in a particular crystal structure, they have the appearance of space-group absences. Occurrence of structural absences thus may lead to an *incorrect assignment of the space group*. Accordingly, the reflection conditions in the space-group tables must be considered as a minimal set of conditions.

The use of reflection conditions and of the symmetry of reflection intensities for space-group determination is described in Part 3.





references