that may arise from special choices of the coordinates can be read from the central part of the symbol (*e.g.* $P4/nmm\ c$: $0\frac{1}{2}0$ ..2 $CI1z$ indicates that, by special choice of z, either hkl: $h+k=2n$ or hkl: $h+k+l=2n$ may be produced).

14.3.4. Phase transitions

If a crystal undergoes a phase transition from a high- to a low-symmetry modification, the transition may be connected with a group–subgroup degradation. In such a case, the comparison of the lattice complexes corresponding to the Wyckoff positions of the original space group on the one hand and of its various subgroups on the other hand very often shows which of these subgroups are suitable for the low-symmetry modification.

This kind of procedure will be demonstrated with the aid of a space group $R\bar{3}m$ and its three translation-equivalent subgroups with index 2, namely $R32$, $R\bar{3}$ and $R3m$. In the course of the subgroup degradation, the Wyckoff positions of $R\bar{3}m$ behave differently:

The descriptive symbols R and $00\frac{1}{2}$ R refer to Wyckoff positions $R\bar{3}m$ 3*a* and 3*b* as well as to Wyckoff positions $R32$ 3*a* and 3*b* and $R\bar{3}$ 3*a* and 3*b*. Therefore, all corresponding point configurations and atomic arrangements remain unchanged in these subgroups. In subgroup $R3m$, however, the respective Wyckoff position is 3*a* with descriptive symbol $R[z]$, *i.e.* a shift parallel to [001] of the entire point configuration is allowed.

The descriptive symbol $R2z$ for $R\bar{3}m$ 6*c* occurs also for $R32$ 6*c* and $R\bar{3}$ 6*c*. Again both subgroups do not allow any deformations of the corresponding point configurations or atomic arrangements. Symmetry reduction to $R3m$, however, yields a splitting of each $R2z$ configuration into two $R[z]$ configurations. The two z parameters may be chosen independently.

As M and $00\frac{1}{2}$ M are the descriptive symbols not only of $R\bar{3}m$ 9*e* and 9*d* but also of $R\bar{3}$ 9*e* and 9*d*, $R\bar{3}$ does not enable any deformation of the corresponding atomic arrangements. In $R32$ and in $R3m$, however, the respective point configurations may be deformed differently, as the descriptive symbols show: $R3x$ and $00\frac{1}{2}$ $R3x$ ($R32$ 9*d* and 9*e*), $R3x\bar{x}[z]$ ($R3m$ 9*b*).

Wyckoff positions $R\bar{3}m$ 18*f* and 18*g* ($R6x$ and $00\frac{1}{2}$ $R6x$) correspond to $R32$ 9*d* and 9*e* ($R3x$ and $00\frac{1}{2}$ $R3x$), to $R\bar{3}$ 18*f* ($R6xyz$), and to $R3m$ 18*c* ($R3x\bar{x}2y[z]$). In $R32$, the hexagons 6*x* around the points of the *R* lattice are split into two oppositely oriented triangles 3*x*, which may have different size. In $R\bar{3}$ and in $R3m$, the hexagons may be deformed differently.

Wyckoff position $R\bar{3}m$ 18*h* ($R6x\bar{x}z$) corresponds to sets of trigonal antiprisms around the points of an *R* lattice. These antiprisms may be distorted in $R32$ 18*f* ($R3x2yz$) or rotated in $R\bar{3}$ 18*f* ($R6xyz$). In $R3m$ 9*b* ($R3x\bar{x}[z]$), each antiprism is split into two parallel triangles that may differ in size.

In each of the three subgroups, any point configuration belonging to the general position $R\bar{3}m$ 36*i* splits into two parts. Each of these parts may be deformed differently.

14.3.5. Incorrect space-group assignment

In the literature, some crystal structures are still described within space groups that are only subgroups of the correct symmetry groups. Many such mistakes (but not all of them) could be avoided by simply looking at the lattice complexes (and their descriptive symbols) that correspond to the Wyckoff positions of the different kinds of atoms. Whenever the same (or an analogous) lattice-complex description of a crystal structure is also possible within a supergroup, then the crystal structure has at least that symmetry.

Examples

(1) The crystal structure of β-$LiRhO_2$ has been refined in space group $F4_132$ (*cf.* Hobbie & Hoppe, 1986).

Rh	16*c*	.32	$\frac{1}{8}\frac{1}{8}\frac{1}{8}$	T
Li	16*d*	.32	$\frac{5}{8}\frac{5}{8}\frac{5}{8}$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ T
O	32*e*	.3.	xxx	..2 $D4xxx$

The same atomic arrangement is possible in the supergroup $Fd\bar{3}m$ of $F4_132$, as can easily be read from Table 14.2.3.2:

Rh	16*c*	$.\bar{3}m$	$\frac{1}{8}\frac{1}{8}\frac{1}{8}$	T
Li	16*d*	$.\bar{3}m$	$\frac{5}{8}\frac{5}{8}\frac{5}{8}$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ T
O	32*e*	.3*m*	xxx	..2 $D4xxx$

Therefore, β-$LiRhO_2$ should be described in $Fd\bar{3}m$.

(2) $KIAs_4O_6$ (Pertlik, 1988) has been described with symmetry $P622$.

I	1*a*	622	000	P
K	1*b*	622	$00\frac{1}{2}$	$00\frac{1}{2}$ P
As	4*h*	3..	$\frac{1}{3}\frac{2}{3}z$	$G2z$
O	6*i*	2..	$\frac{1}{2}0z$	$N2z$

Space group $P6/mmm$ allows the same atomic arrangement:

I	1*a*	$6/mmm$	000	P
K	1*b*	$6/mmm$	$00\frac{1}{2}$	$00\frac{1}{2}$ P
As	4*h*	3*m*.	$\frac{1}{3}\frac{2}{3}z$	$G2z$
O	6*i*	2*mm*	$\frac{1}{2}0z$	$N2z$

Therefore, $KIAs_4O_6$ should be described in $P6/mmm$.

14.3.6. Application of descriptive lattice-complex symbols

Descriptive symbols of lattice complexes – at least those of the invariant lattice complexes – have been used for the description of crystal structures (*cf.* Section 14.3.2 and the literature cited there), for the nomenclature of three-periodic surfaces (von Schnering & Nesper, 1987) and in connection with orbifolds of space groups (Johnson *et al.*, 2001).

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references