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* also occurs for $R32$ 6*c* and $R\bar{3}$ 6*c*. Again, neither subgroup allows 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 differently deformed, 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 $6x$ around the points of the R lattice are split into two oppositely oriented triangles $3x$, which may have different size. In $R\bar{3}$ and in $R3m$, the hexagons may be differently deformed.

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 differently deformed.

3.4.4.5. 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.	x,x,x	..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 3.4.3.3:

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

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

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

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

3.4.4.6. 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 3.4.4.2 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).

3.4.4.7. Weissenberg complexes

In general, each lattice complex involves point configurations that cannot be related to any crystal structure because the shortest distances between the atoms in a corresponding arrangement would become too small. Only the 67 Weissenberg complexes (*cf.* Section 3.4.1.5.2) form an exception from this rule. Assuming that the metrical parameters are chosen adequately, each point configuration stemming from a Weissenberg complex may, in principle, refer to the arrangement of some atoms in a crystal structure. In case of the 36 invariant lattice complexes this property is immediately evident. The further 31 Weissenberg complexes have one or more degrees of freedom (*cf.* Section 3.4.1.5.2 and Table 3.4.1.1). Nevertheless, varying the corresponding free coordinate parameters never results in point configurations with infinitesimally small distances.

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