14.3. Applications of the lattice-complex concept

BY W. FISCHER AND E. KOCH

14.3.1. Geometrical properties of point configurations

To study the geometrical properties of all point configurations in three-dimensional space, it is not necessary to consider all Wyckoff positions of the space groups or all 1128 types of Wyckoff set. Instead, one may restrict the investigations to the characteristic Wyckoff positions of the 402 lattice complexes. The results can then be transferred to all noncharacteristic Wyckoff positions of the lattice complexes, as listed in Tables 14.2.3.1 and 14.2.3.2.

The determination of all types of sphere packings with cubic or tetragonal symmetry forms an example for this kind of procedure (Fischer, 1973, 1974, 1991*a*,*b*, 1993). The cubic lattice complex *I*4*xxx*, for example, allows two types of sphere packings within its characteristic Wyckoff position $I\bar{4}3m$ 8*c* *xxx* .3*m*, namely $9/3/c2$ for $x = 3/16$ and $6/4/c1$ for $3/16 < x < \frac{1}{4}$ (*cf.* Fischer, 1973). Ag_3PO_4 crystallizes with symmetry $P\bar{4}3n$ (Deschizeaux-Cheruy *et al.*, 1982) and the oxygen atoms occupy Wyckoff position 8*e* *xxx* .3., which also belongs to *I*4*xxx*. Comparison of the coordinate parameter $x = 0.1491$ for the oxygen atoms with the sphere-packing parameters listed for $I\bar{4}3m$ *c* shows directly that the oxygen arrangement in this crystal structure does not form a sphere packing.

Other examples for this approach are the derivation of crystal potentials (Naor, 1958), of coordinate restrictions in crystal structures (Smirnova, 1962), of Patterson diagrams (Koch & Hellner, 1971), of Dirichlet domains (Koch, 1973, 1984) and of sphere packings for subperiodic groups (Koch & Fischer, 1978).

The 30 lattice complexes in two-dimensional space correspond uniquely to the 'henomeric types of dot pattern' introduced by Grünbaum and Shephard (*cf. e.g.* Grünbaum & Shephard, 1981; Grünbaum, 1983).

14.3.2. Relations between crystal structures

Frequently, different crystal structures show the same geometrical arrangement for some of their atoms, even though their space groups do not belong to the same type. In these cases, the corresponding Wyckoff positions either belong to the same lattice complex or there exist close relationships between them, *e.g.* limiting-complex relations.

Examples

(1) The Fe atoms in pyrite FeS_2 occupy Wyckoff position 4*a* 000 .$\bar{3}$. of $Pa\bar{3}$ (descriptive symbol *F*) that belongs to the invariant lattice complex $Fm\bar{3}m$ *a*. Accordingly, the Fe atoms in pyrite form a face-centred cubic lattice as do the Cu atoms in the element structure of copper.

(2) Cuprite Cu_2O crystallizes with symmetry $Pn\bar{3}m$. The oxygen atoms occupy Wyckoff position 2*a* 000 $\bar{4}3m$ (descriptive symbol *I*) and the copper atoms position 4*b* $\frac{1}{4}\frac{1}{4}\frac{1}{4}$.$\bar{3}m$ (descriptive symbol $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ *F*). Position 2*a* belongs to lattice complex $Im\bar{3}m$ *a* and position 4*b* to $Fm\bar{3}m$ *a*. Therefore, the O atoms form a body-centred cubic lattice like the W atoms in the structure of tungsten, and the copper atoms form a face-centred cubic lattice. The tungsten configuration is shifted by $(\frac{1}{4}\frac{1}{4}\frac{1}{4})$ with respect to the copper configuration.

(3) K_2NaAlF_6 (elpasolite, *cf.* Morss, 1974) and $K_2PbNi(NO_2)_6$ (*cf.* Takagi *et al.*, 1975) crystallize with symmetry $Fm\bar{3}m$ and $Fm\bar{3}$, respectively.

K_2NaAlF_6

Al	4*a*	$m\bar{3}m$	000	*F*
Na	4*b*	$m\bar{3}m$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}F$
K	8*c*	$\bar{4}3m$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}P_2$
F	24*e*	4*m*.*m*	*x*00	*F*6*z*
			$x = 0.219$	

$K_2PbNi(NO_2)_6$

Ni	4*a*	$m\bar{3}$.	000	*F*
Pb	4*b*	$m\bar{3}$.	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}F$
K	8*c*	23.	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}P_2$
N	24*e*	*mm*2..	*x*00	*F*6*z*
			$x = 0.1966$	
O	48*h*	*m*..	0*yz*	*F*6*z*2*x*

As the descriptive lattice-complex symbols for the various atomic positions show immediately, the two crystal structures are very similar. The only difference originates from the replacement of the fluorine atoms in elpasolite by NO_2 groups in $K_2PbNi(NO_2)_6$, which causes the symmetry reduction from $Fm\bar{3}m$ to $Fm\bar{3}$.

(4) The crystal structure of CoU (Baenziger *et al.*, 1950) may be interpreted as a slightly distorted CsCl (or β-brass, CuZn)-type structure. CsCl corresponds to Wyckoff positions 1*a* and 1*b* of $Pm\bar{3}m$ with descriptive symbol *P* and $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*, respectively; Co and U both occupy Wyckoff position 8*a* .3. *xxx* of $I2_13$ with $x = 0.0347$ for U and $x = 0.294$ for Co. As the descriptive symbol 2_12_1.. P_2Y^*1xxx shows, this Wyckoff position belongs to a Weissenberg complex with two invariant limiting complexes, namely *P* ($Pm\bar{3}m$ *a*) and Y^* ($I4_132$ *a*). $x = 0$ corresponds to P_2, $x = \frac{1}{4}$ to $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2, $x = \frac{1}{8}$ to ${}^+Y^*$ and $x = \frac{7}{8}$ to ${}^-Y^*$. Consequently, the uranium and cobalt atoms form approximately a P_2 and a $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2 configuration, respectively.

Publications by Hellner (1965, 1976*a*,*b*,*c*, 1977, 1979), Loeb (1970), Smirnova & Vasserman (1971), Sakamoto & Takahasi (1971), Niggli (1971), Fischer & Koch (1974), Hellner *et al.* (1981) and Hellner & Sowa (1985) refer to this aspect.

14.3.3. Reflection conditions

Wyckoff positions belonging to the same lattice complex show analogous reflection conditions. Therefore, lattice complexes have also been used to check the reflection conditions for all Wyckoff positions in the space-group tables of this volume.

The descriptive symbols may supply information on the reflection conditions. If the symbol does not contain any distribution-symmetry part, the reflection conditions of the Wyckoff position are indicated by the symbol of the invariant lattice complex in the central part (*e.g.* $P4/nmm$ *g*: *C*4*xx* shows that the reflection condition is that of a *C* lattice, $hkl: h + k = 2n$). In the case that the site set consists of only one point, *i.e.* the Wyckoff position belongs to a Weissenberg complex, all conditions for general reflections *hkl*

references