

5. SCANNING OF SPACE GROUPS

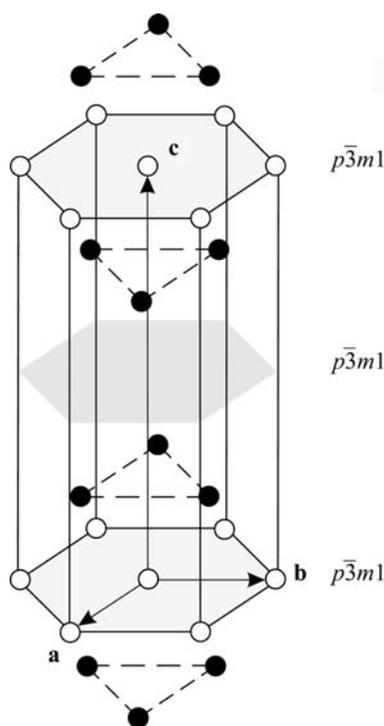


Fig. 5.2.5.1. The structure of cadmium iodide, CdI_2 . The section planes of two orbits in special positions are distinguished by shading. The figure is drastically elongated in the c direction to exhibit the layer symmetries.

horizontal lines in the tables of orientation orbits and auxiliary bases. The orbit contains six orientations in groups of the Laue class $m\bar{3}(T_h)$ and 12 orientations in groups of the Laue class $m\bar{3}m(O_h)$. The orbit turns into a special orbit with fixed parameters for the special values $m = 1, n = 0$ in groups of both the Laue classes $m\bar{3}(T_h)$ and $m\bar{3}m(O_h)$. The scanning changes from monoclinic/inclined to orthorhombic in the Laue class $m\bar{3}(T_h)$, to tetragonal in the Laue class $m\bar{3}m(O_h)$. The symmetry of the orientation also increases to orthorhombic for special values $m = 1, n = 1$ in groups of the Laue class $m\bar{3}m(O_h)$.

The choice of bases for the three subsets is the same as in orthorhombic groups, where the orientations of subsets are separated into three different orbits and the auxiliary bases are expressed in terms of vectors of the conventional cubic basis for the centring types P and I . For the centring type F , the Miller indices differ in the original and auxiliary basis. In this case, we express the Miller indices with reference to the original basis as (hkl) and relate them to Miller indices $(mn0)$ with reference to the auxiliary bases. These relations are the same as in the case of F -centring in orthorhombic groups, see relations (5.2.4.2) and (5.2.4.3).

Orientation orbit (hhl) : The orbit contains 12 orientations which divide into three subsets corresponding to the three main cubic axes. In each of the subsets, one of the vectors of the conventional cubic basis is chosen as the vector $\hat{\mathbf{b}}$ of the auxiliary basis. The orientations of the subsets are separated by horizontal lines across the table. The first subset corresponds to the vector \mathbf{c} of the cubic basis and the orientations in this subset are the same as in the (hhl) orbit for tetragonal groups of the Laue class $4/mmm(D_{4h})$. The orientations within each subset are further divided into two pairs of orientations to which correspond two different unique axes of the monoclinic scanning group. These subsets are again separated by horizontal lines across the last two columns. For the centring types P and I and for the first subset of orientations, the description of orientations and bases coincides with the description of the orbit (hhl) in tetragonal groups of the Laue class $4/mmm(D_{4h})$ and centring types P and I , including the choice of auxiliary and conventional bases of scanning groups and relations between Miller indices h, l and m, n . For the other

subsets of orientations, the data in tables are obtained by the cyclic permutation of vectors \mathbf{a}, \mathbf{b} and \mathbf{c} .

For the centring type F , orientation (hhl) , we choose the auxiliary basis of the scanning group with the unique axis vectors $\hat{\mathbf{c}} = (\mathbf{a} - \mathbf{b})/2, \hat{\mathbf{b}} = \mathbf{c}$ and $\hat{\mathbf{a}} = (\mathbf{a} + \mathbf{b})/2$, while for the orientation $(\bar{h}hl)$, we choose $\hat{\mathbf{c}} = (\mathbf{a} + \mathbf{b})/2, \hat{\mathbf{b}} = \mathbf{c}$ and $\hat{\mathbf{a}} = (\mathbf{a} - \mathbf{b})/2$. The bases for the remaining orientations are again obtained by the cyclic permutation of vectors of the conventional cubic basis.

Transformation of Miller indices: The straight line in which a plane (hhl) intersects with the plane $(1\bar{1}0)$ has the direction of a vector $(\mathbf{a} + \mathbf{b})/2h - \mathbf{c}/l$ or of the vector $\mathbf{b}' = n\hat{\mathbf{a}} - m\hat{\mathbf{c}} = n(\mathbf{a} + \mathbf{b})/2 - m\mathbf{c}$. As these two vectors can differ only by a numerical factor, the pair $(2m, n)$ must be proportional to the pair (h, l) and we obtain the relations

$$h \text{ odd} \Rightarrow m = h, n = 2l; \quad h \text{ even} \Rightarrow m = h/2, n = l,$$

recorded at the bottom row of the orientation-orbit table for the centring type F .

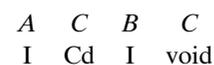
For the special values $h = 1, l = 0$, this orbit turns into an orbit (110) with fixed parameters and an orthorhombic scanning group.

5.2.5. Applications

5.2.5.1. Layer symmetries in crystal structures

The following two examples show the use of layer symmetries in the description of crystal structures.

Example 1: Fig. 5.2.5.1 shows the crystal structure of cadmium iodide, CdI_2 . The space group of this crystal is $P\bar{3}m1, D_{3d}^3$ (No. 164). The anions form a hexagonal close packing of spheres and the cations occupy half of the octahedral holes, filling one of the alternate layers. In close-packing notation, the CdI_2 structure is:



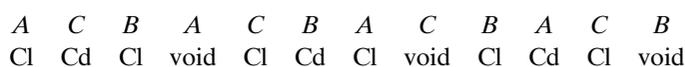
From the scanning tables, we obtain for planes with the (0001) orientation and at heights $0\mathbf{c}$ or $\frac{1}{2}\mathbf{c}$ a sectional layer symmetry $p\bar{3}m1$ (L72), and for planes of this orientation at any other height a sectional layer symmetry $p3m1$ (L69).

The plane at height $0\mathbf{c}$ contains cadmium ions. This plane defines the orbit of planes of orientation (0001) located at points $P + n\mathbf{c}$, where $n \in Z$ (Z is the set of all integers). All these planes contain cadmium ions in the same arrangement (C layer filled with Cd).

The plane at height $\frac{1}{2}\mathbf{c}$ defines the orbit of planes of orientation (0001) located at points $P + (n + \frac{1}{2})\mathbf{c}$, where $n \in Z$. All these planes lie midway between A and B layers of iodine ions with the B layer below, the A layer above the plane. They contain only voids.

The planes at levels $\frac{1}{4}\mathbf{c}$ and $\frac{3}{4}\mathbf{c}$ contain B and A layers of iodine ions, respectively. These planes and all planes produced by translations $n\mathbf{c}$ from them belong to the same orbit because the operations $\bar{3}$ exchange the A and B layers.

Example 2: The space group of cadmium chloride, CdCl_2 , is $R\bar{3}m, D_{3d}^5$ (No. 166). Fig. 5.2.5.2 shows the structure of CdCl_2 in its triple hexagonal cell. The anions form a cubic close packing of spheres and the cations occupy half of the octahedral holes of each alternate layer. In close-packing notation, the CdCl_2 structure is:



We choose the origin at a cadmium ion and the hexagonal basis vectors \mathbf{a}, \mathbf{b} as shown in Fig. 5.2.5.2. This corresponds to the obverse setting for which the scanning table is given in Part 6. The planes with the (0001) orientation at the heights $0\mathbf{c}, \frac{1}{6}\mathbf{c}, \frac{1}{3}\mathbf{c}, \frac{1}{2}\mathbf{c}, \frac{2}{3}\mathbf{c}$ and $\frac{5}{6}\mathbf{c}$ have a sectional layer group of the type $p\bar{3}m1$ (L72) and at any other height have a sectional layer group of the type $p3m1$ (L69).