

5. SCANNING OF SPACE GROUPS

the scanned group is hexagonal, the scanning group is orthorhombic with lattice type C. Because of the choice of bases, the lattice is denoted by the letter A in the Hermann–Mauguin symbols of the scanning groups.

We choose the vector \mathbf{c} of the hexagonal axis as the vector \mathbf{a}' for all orientations of these orbits. In addition we choose $\mathbf{b}' = \mathbf{a}$ and the scanning direction $\mathbf{d} = \mathbf{a} + 2\mathbf{b}$ for the orientation $(01\bar{1}0)$, while for the orientation $(2\bar{1}\bar{1}0)$, perpendicular to it, we choose $\mathbf{b}' = -(\mathbf{a} + 2\mathbf{b})$, $\mathbf{d} = \mathbf{a}$. Analogously, for the other pairs of mutually perpendicular orientations we choose: $\mathbf{b}' = \mathbf{b}$ and $\mathbf{d} = -(2\mathbf{a} + \mathbf{b})$ for the orientation $(\bar{1}010)$; $\mathbf{b}' = 2\mathbf{a} + \mathbf{b}$, $\mathbf{d} = \mathbf{b}$ for the orientation $(\bar{1}2\bar{1}0)$; $\mathbf{b}' = -(\mathbf{a} + \mathbf{b})$, $\mathbf{d} = (\mathbf{a} - \mathbf{b})$ for the orientation $(\bar{1}\bar{1}00)$; and $\mathbf{b}' = (\mathbf{b} - \mathbf{a})$, $\mathbf{d} = -(\mathbf{a} + \mathbf{b})$ for the orientation $(\bar{1}\bar{1}20)$. Hence the scanning groups for the pairs of orientations $(01\bar{1}0)/(2\bar{1}\bar{1}0)$, $(\bar{1}010)/(1\bar{2}10)$ and $(\bar{1}\bar{1}00)/(1\bar{1}20)$ are the same monoclinic or orthorhombic groups but the conventional basis vectors \mathbf{b}', \mathbf{d} of one of them are replaced by $-\mathbf{d}, \mathbf{b}'$, respectively, for the second one. Again there are cases when the locations of scanning groups are different for different pairs of orientations, in which case the corresponding row splits into three subrows. To compare the geometry of the bases, consult and compare Figs. 5.2.4.2 and 5.2.4.3.

Rhombohedral lattice. The resulting scanning groups are monoclinic of the I-centred type. The vectors of the rhombohedral basis $\mathbf{a}_r, \mathbf{b}_r, \mathbf{c}_r$ are related to vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ of the hexagonal basis as follows:

$$\begin{aligned}\mathbf{a}_r &= (2\mathbf{a} + \mathbf{b} + \mathbf{c})/3, & \mathbf{b}_r &= (-\mathbf{a} + \mathbf{b} + \mathbf{c})/3, \\ \mathbf{c}_r &= (-\mathbf{a} - 2\mathbf{b} + \mathbf{c})/3,\end{aligned}\quad (5.2.4.11)$$

as shown in Fig. 5.2.4.4, which corresponds to the obverse setting. In Figs. 5.2.4.5 and 5.2.4.6, we show the diagrams of the scanning groups in the plane of orientation $(1\bar{2}\bar{1}0)$ for the groups $R\bar{3}m, D_{3d}^5$ (No. 166) and $R\bar{3}c, D_{3d}^6$ (No. 167), projected orthogonally along the direction of \mathbf{b} . The vector $(\mathbf{a}_r + \mathbf{b}_r)$, whose projection is shown in both figures, is identical with the vector $(\mathbf{a} + \mathbf{b} + \mathbf{c})/2$ which is the I-centring vector of the monoclinic cell with conventional basis $\mathbf{a}' = \mathbf{c}, \mathbf{b}' = \mathbf{a}_r, \mathbf{d} = \mathbf{b}$. The vector \mathbf{b} plays the role of the scanning direction for orientation $(1\bar{2}\bar{1}0)$ to which it is perpendicular (this is the case of monoclinic/orthogonal scanning). For the orientation $(\bar{1}010)$, we choose the basis of the scanning group as $\mathbf{a} = \mathbf{c}, \mathbf{b}' = \mathbf{b}$ and $\mathbf{d} = -\mathbf{a}_r$, and we get a monoclinic/inclined scanning.

One standard scanning table is given for each of the seven group types with a rhombohedral lattice because neither the bases of scanning groups nor their symbols change with the change from hexagonal to rhombohedral basis. None of the entries in the scanning tables needs to be changed with the exception of Bravais–Miller indices $(hkil)$, which are replaced by corresponding Miller indices (hkl) as follows: (0001) is replaced

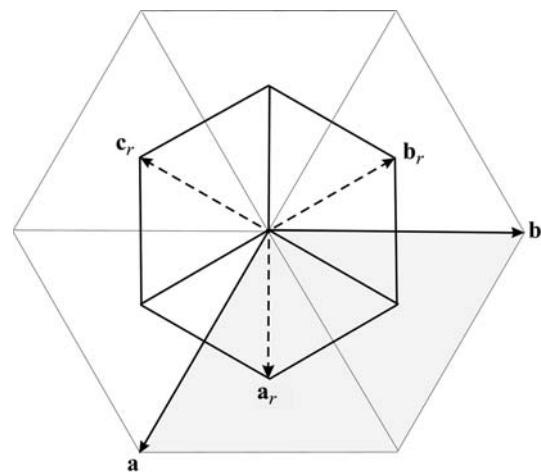


Fig. 5.2.4.4. The relationship between hexagonal and rhombohedral bases in the obverse setting.

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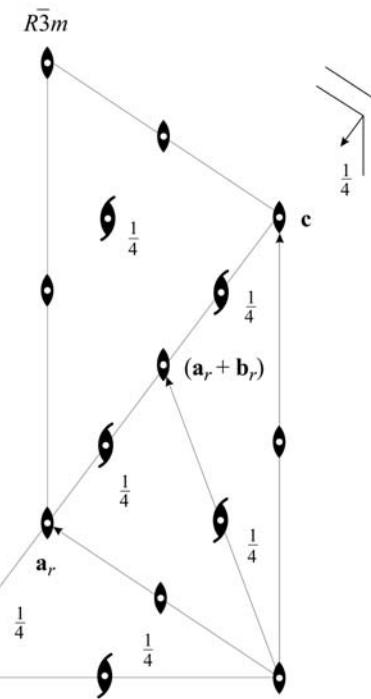


Fig. 5.2.4.5. The diagram of the scanning group $R\bar{3}m$ in the plane of orientation $(1\bar{2}\bar{1}0)$ projected orthogonally along \mathbf{b} .

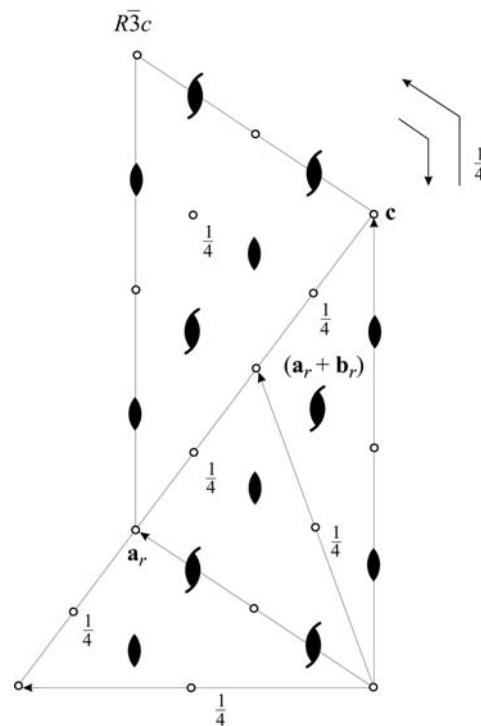


Fig. 5.2.4.6. The diagram of the scanning group $R\bar{3}c$ in the plane of orientation $(1\bar{2}\bar{1}0)$ projected orthogonally along \mathbf{b} .

by $(111)_2$ the set $(01\bar{1}0), (\bar{1}010), (\bar{1}\bar{1}00)$ by $(1\bar{1}\bar{1}), (\bar{1}11), (\bar{1}\bar{1}1)$ and the set $(12\bar{1}0), (\bar{1}\bar{1}20), (2\bar{1}\bar{1}0)$ by $(01\bar{1}), (\bar{1}01), (\bar{1}\bar{1}0)$. The indices are given in parallel in the two columns for the designation of orientation orbits. To abbreviate expressions for vectors of the conventional bases $(\mathbf{a}', \mathbf{b}', \mathbf{d})$ of scanning groups, we express these vectors in terms of vectors of hexagonal basis $(\mathbf{a}, \mathbf{b}, \mathbf{c})$ and of vectors of rhombohedral basis $(\mathbf{a}_r, \mathbf{b}_r, \mathbf{c}_r)$. To obtain the bases $(\mathbf{a}', \mathbf{b}', \mathbf{d})$ in terms of vectors of the hexagonal basis, we substitute for vectors of the rhombohedral bases the combinations (5.2.4.11), to obtain them in terms of vectors of rhombohedral bases, we substitute for vectors of hexagonal bases the combinations