5.1. TRANSFORMATIONS OF THE COORDINATE SYSTEM

Fig. 5.1.3.8. Hexagonal lattice projected along [001]. Primitive hexagonal cell \( P \) with \( a, b, c \) and the three triple hexagonal cells \( H \) with \( a_1, b_1, c_1; a_2, b_2, c_2; a_3, b_3, c_3 \). Origin for all cells is the same.

Fig. 5.1.3.9. Rhombohedral lattice with a triple hexagonal unit cell \( a, b, c \) in obverse setting (i.e. unit cell \( a_1, b_1, c_1 \) in Fig. 5.1.3.6d) and the three centred monoclinic cells. (a) C-centred cells \( C_1 \) with \( a_1, b_1, c_1; C_2 \) with \( a_2, b_2, c_2; \) and \( C_3 \) with \( a_3, b_3, c_3 \). The unique monoclinic axes are \( b_1, b_2 \) and \( b_3 \), respectively. Origin for all four cells is the same. (b) A-centred cells \( A_1 \) with \( a', b_1, c_1; A_2 \) with \( a', b_2, c_2; \) and \( A_3 \) with \( a', b_3, c_3 \). The unique monoclinic axes are \( c_1, c_2 \) and \( c_3 \), respectively. Origin for all four cells is the same.

The sequence of the corresponding inverse matrices \( P_i \) is reversed in the product

\[
P = P_n P_{n-1} \cdots P_1.
\]

The following items are also affected by a transformation:

(i) The metric matrix of direct lattice \( G \) [more exactly: the matrix of geometrical coefficients (metric tensor)] is transformed by the matrix \( P \) as follows:

\[
G' = P^t GP
\]

with \( P^t \) the transposed matrix of \( P \), i.e. rows and columns of \( P \) are interchanged. Specifically,

\[
G' = \begin{pmatrix}
   a' & a' & a' \\
   b' & b' & b' \\
   c' & c' & c'
\end{pmatrix}
= \begin{pmatrix}
   P_{11} & P_{21} & P_{31} \\
   P_{12} & P_{22} & P_{32} \\
   P_{13} & P_{23} & P_{33}
\end{pmatrix}
\begin{pmatrix}
   a & a & b & a & c \\
   b & a & b & b & c \\
   c & a & c & b & c
\end{pmatrix}
\times
\begin{pmatrix}
   P_{11} & P_{12} & P_{13} \\
   P_{21} & P_{22} & P_{23} \\
   P_{31} & P_{32} & P_{33}
\end{pmatrix}
\]

(ii) The metric matrix of reciprocal lattice \( G^* \) [more exactly: the matrix of geometrical coefficients (metric tensor)] is transformed by

\[
G'' = QG^*Q'.
\]

Here, the transposed matrix \( Q' \) is on the right-hand side of \( G^* \).

(iii) The volume of the unit cell \( V \) changes with the transformation. The volume of the new unit cell \( V' \) is obtained by

\[
V' = \det(P)V = \begin{vmatrix}
   P_{11} & P_{12} & P_{13} \\
   P_{21} & P_{22} & P_{23} \\
   P_{31} & P_{32} & P_{33}
\end{vmatrix}
V
\]

with \( \det(P) \) the determinant of the matrix \( P \). The corresponding equation for the volume of the unit cell in reciprocal space \( V^* \) is

\[
V'' = \det(Q)V^*.
\]

Matrices \( P \) and \( Q \) that frequently occur in crystallography are listed in Table 5.1.3.1.