

## 13. ISOMORPHIC SUBGROUPS OF SPACE GROUPS

$$\mathbf{a}' = \mathbf{a}, \quad \mathbf{b}' = \mathbf{b}, \quad \mathbf{c}' = 2\mathbf{c}.$$

This transformation is permitted for  $P4/mmm$  but not for  $P4/mcc$  where the parity rules require  $S_{33} = 2n + 1$ . Thus, the lowest value of  $S_{11}^2 S_{33}$  for a subgroup of space group  $P4/mcc$  is 3 and the axis transformation is

$$\mathbf{a}' = \mathbf{a}, \quad \mathbf{b}' = \mathbf{b}, \quad \mathbf{c}' = 3\mathbf{c}.$$

## 13.1.2.5. Plane groups

There is no difficulty in reducing the preceding considerations to plane groups, where  $\mathbf{S}$  is a  $(2 \times 2)$  matrix and  $\mathbf{s}$  a  $(2 \times 1)$  matrix.

## 13.1.2.6. Tables of matrices for isomorphic subgroups

The matrices and the restrictions on the coefficients are listed for the plane groups in Table 13.1.2.1 and for the space groups in Table 13.1.2.2.

For the triclinic and monoclinic systems, there is an infinite choice of matrices for each index, owing to the infinite number of equivalent unit cells. For the other space groups, several different (but finitely many) choices of matrix occur. In all cases, we have restricted this choice to *one* matrix for each group–subgroup relation so that *each subgroup is listed exactly once* (apart from origin choice).

## Example

No. 178,  $P6_122$ , has the matrix  $\mathbf{H}_2^k$  for all isomorphic and isosymbolic subgroups  $P6_122$ , having the lattices  $n_{11}\mathbf{a}$ ,  $n_{11}\mathbf{b}$ ,  $(6n_{33} + 1)\mathbf{c}$  ( $n_{11} \geq 1, n_{33} \geq 0$ ), whilst  $\mathbf{H}_3^o$  is used for all isomorphic and isosymbolic subgroups with the lattices  $n_{11}(2\mathbf{a} + \mathbf{b})$ ,  $n_{11}(-\mathbf{a} + \mathbf{b})$ ,  $(6n_{33} + 1)\mathbf{c}$  ( $n_{11} \geq 1, n_{33} \geq 0$ ). These two kinds of subgroups are obviously different, having different translation lattices. The same group,  $P6_122$ , has the matrix  $\mathbf{H}_2^l$  for the isomorphic and enantiomorphic subgroups  $P6_522$  of lattices  $n_{11}\mathbf{a}$ ,  $n_{11}\mathbf{b}$ ,  $(6n_{33} + 5)\mathbf{c}$  whilst  $\mathbf{H}_3^c$  is used for the isomorphic and enantiomorphic subgroups  $P6_522$  of lattices  $n_{11}(2\mathbf{a} + \mathbf{b})$ ,  $n_{11}(-\mathbf{a} + \mathbf{b})$ ,  $(6n_{33} + 5)\mathbf{c}$ .

In the tables, each system is preceded by the appropriate general form of the matrix, which is also given in this chapter, followed by the more specialized matrices such as  $\mathbf{T}_2, \mathbf{T}_3$ . Under *Conditions*, we have listed the nonredundant inequalities and parity conditions\* that ensure the uniqueness of the matrix for each subgroup. Also, we have used rules in order to avoid repetition of equivalent unit cells. For instance, for trigonal and hexagonal groups (rhombohedral groups excepted), we have restricted  $\mathbf{a}'$  to lie between  $\mathbf{a}$  and  $\mathbf{a} + \mathbf{b}$  excluding this last vector from the sector of  $60^\circ$  because there is a repetition after a  $60^\circ$  rotation of the unit cell.

\* More exactly 'congruence modulo  $\mathbb{Z}$  conditions'.