

13.1. ISOMORPHIC SUBGROUPS

Table 13.1.2.2. Isomorphic subgroups of the space groups (cont.)

ORTHORHOMBIC SYSTEM

$\mathbf{O}_1 = \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & S_{22} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}$			
Conditions: $S_{11} > 0, S_{22} > 0, S_{33} > 0, S_{11}S_{22}S_{33} > 1$			
	S_{11}	S_{22}	S_{33}
\mathbf{O}_1^a	n_1	n_2	n_3
\mathbf{O}_1^b	n_1	n_2	$2n_3 + 1$
\mathbf{O}_1^c	$2n_1 + 1$	$2n_2 + 1$	n_3
\mathbf{O}_1^d	$2n_1 + 1$	$2n_2 + 1$	$2n_3 + 1$
\mathbf{O}_1^e	$2n_1$	$2n_2$	$2n_3 + 1$
\mathbf{O}_1^f	$2n_1$	$2n_2$	n_3
\mathbf{O}_1^g	$2n_1$	$2n_2$	$2n_3$
\mathbf{O}_1^h	$2n_1 + 1$	n_2	n_3
\mathbf{O}_1^i	$2n_1 + 1$	n_2	$2n_3 + 1$
\mathbf{O}_1^j	n_1	$2n_2 + 1$	$2n_3 + 1$
\mathbf{O}_1^k	n_1	$2n_2$	$2n_3$
\mathbf{O}_1^l	$2n_1 + 1$	$2n_2$	$2n_3$
$\mathbf{O}_4 = \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & 0 & S_{23} \\ 0 & S_{32} & 0 \end{pmatrix}$			
Conditions: $S_{11} = 2n_1 > 0, S_{23} = -n_2 < 0, S_{32} = 2n_3 > 0$			
$\mathbf{O}_5 = \begin{pmatrix} 0 & 0 & S_{13} \\ 0 & S_{22} & 0 \\ S_{31} & 0 & 0 \end{pmatrix}$			
Conditions: $S_{13} = -n_1 < 0, S_{22} = 2n_2 > 0, S_{31} = 2n_3 > 0$			
$\mathbf{O}_6 = \begin{pmatrix} 0 & S_{12} & 0 \\ S_{21} & 0 & 0 \\ 0 & 0 & S_{33} \end{pmatrix}$			
Conditions: $S_{12} = 2n_1 > 0, S_{21} = -n_2 < 0, S_{33} = 2n_3 > 0$			

The following general rule exists: only those matrices \mathbf{O}_i are permissible for which, if the non-zero coefficients are replaced by 1, the corresponding transformation of the axes conserves the Hermann–Mauguin symbol.

Examples

- (1) When the three letters of the Hermann–Mauguin symbol are the same, as in $P222, Pmmm, Pnnn$ etc., the Hermann–Mauguin symbol does not change and all six matrices are valid.
- (2) When the z axis plays a privileged role and when the x and y axes are equivalent, only \mathbf{O}_1 and \mathbf{O}_6 apply. Examples are $P222_1, Pbam$ and $Ccca$. In $Pmma$, the x and y axes are not equivalent because the interchange leads to $Pmmb$ (the non-equivalence of the x and y axes can also be recognized by inspection of the full symbol $P2_1/m 2/m 2/a$).
- (3) Matrix \mathbf{O}_1 always applies.

13.1.2.3. Triclinic system

As stated above, $P1$ has only isomorphic subgroups and the general nature of the matrix \mathbf{S} [equation (13.1.1.3)] requires the use of special techniques (cf. Chapter 13.2, Derivative lattices); they apply also to $P\bar{1}$.

Table 13.1.2.2. Isomorphic subgroups of the space groups (cont.)

TETRAGONAL SYSTEM

$\mathbf{T}_1 = \begin{pmatrix} S_{11} & -S_{21} & 0 \\ S_{21} & S_{11} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}$			
Conditions: $S_{11} > 0, S_{21} \geq 0, S_{33} > 0, (S_{11}^2 + S_{21}^2)S_{33} > 1$			
	S_{11}	S_{21}	S_{33}
\mathbf{T}_1^a	n_1	n_2	n_3
\mathbf{T}_1^b	n_1	n_2	$4n_3 + 1$
\mathbf{T}_1^c	n_1	n_2	$4n_3 + 3$
\mathbf{T}_1^d	n_1	n_2	$2n_3 + 1$
\mathbf{T}_1^e	$2n_1 + 1$	$2n_2$	$2n_3 + 1$
\mathbf{T}_1^f	$2n_1$	$2n_2 + 1$	$2n_3 + 1$
\mathbf{T}_1^g	$2n_1 + 1$	$2n_2 + 1$	$2n_3$
\mathbf{T}_1^h	$2n_1$	$2n_2$	$2n_3$
\mathbf{T}_1^i	$2n_1 + 1$	$2n_2$	n_3
\mathbf{T}_1^j	$2n_1$	$2n_2 + 1$	n_3
$\mathbf{T}_2 = \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & S_{11} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}$			
Conditions: $S_{11} > 0, S_{33} > 0, S_{11}S_{33} > 1$			
	S_{11}		S_{33}
\mathbf{T}_2^a	n_1		n_2
\mathbf{T}_2^b	$2n_1 + 1$		n_2
\mathbf{T}_2^c	n_1		$4n_2 + 1$
\mathbf{T}_2^d	n_1		$4n_2 + 3$
\mathbf{T}_2^e	$2n_1 + 1$		$4n_2 + 1$
\mathbf{T}_2^f	$2n_1 + 1$		$4n_2 + 3$
\mathbf{T}_2^g	n_1		$2n_2 + 1$
\mathbf{T}_2^h	$2n_1 + 1$		$2n_2 + 1$
\mathbf{T}_2^i	$2n_1$		$2n_2$
$\mathbf{T}_3 = \begin{pmatrix} S_{11} & -S_{11} & 0 \\ S_{11} & S_{11} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}$			
Conditions: $S_{11} > 0, S_{33} > 0$			
$\mathbf{T}_3^a: S_{33} = n_1; \mathbf{T}_3^b: S_{33} = 4n_1 + 1; \mathbf{T}_3^c: S_{33} = 4n_1 + 1;$			
$\mathbf{T}_3^d: S_{33} = 2n_1 + 1; \mathbf{T}_3^e: S_{33} = 2n_1$			

13.1.2.4. Parity conditions

In equation (13.1.1.2b), there occurs the choice of the origin by means of s , the nature of the lattice by means of t_G and the nature of the symmetry operations by means of the column matrices \mathbf{w} and \mathbf{w}' . The three factors, origin, lattice type, screw and glide components, impose parity conditions on the coefficients of the matrix \mathbf{S} . Only a few examples are given here.

When (\mathbf{W}, \mathbf{w}) and $(\mathbf{W}', \mathbf{w}')$ are operators of lattice translations of \mathcal{H} , say (\mathbf{I}, t_G) and $(\mathbf{I}, t_{\mathcal{H}})$, equation (13.1.1.2b) reduces to

$$\mathbf{S} \cdot t_{\mathcal{H}} = t_G. \tag{13.1.1.4}$$

Example

In a tetragonal I lattice, t_G is either an integral or a fractional translation. If $t_{\mathcal{H}}$ is $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ and the matrix \mathbf{S} is replaced by \mathbf{T}_1 , one obtains