

1. SUBPERIODIC GROUP TABLES: FRIEZE-GROUP, ROD-GROUP AND LAYER-GROUP TYPES

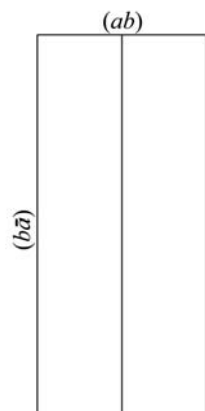


Fig. 1.2.6.18. The two settings for frieze groups. For the second setting, printed vertically, the page must be turned 90° clockwise or viewed from the right-hand side.

(2a + b ā + b c) setting for trigonal and hexagonal groups. These second tabulations aid in the correlation of Wyckoff positions of space groups and Wyckoff positions of rod groups. For example, the Wyckoff positions of the two space groups types $P3m1$ and $P31m$ can be easily correlated with, respectively, the Wyckoff positions of a rod group of the type R49 in the standard setting where the Hermann–Mauguin symbol is $\rho 3m1$ and in the second setting where the symbol is $\rho 31m$. In Table 1.2.6.3, we list the tetragonal, trigonal and hexagonal rod groups where in the different settings the two Hermann–Mauguin symbols are distinct.

(iii) Frieze groups

Two diagrams are given for each frieze group: a symmetry diagram and a general-position diagram. These diagrams are illustrated for the oblique and rectangular frieze groups in Figs. 1.2.6.16 and 1.2.6.17, respectively. We consider the two settings (ab) and (bā), see Fig. 1.2.6.18. In the frieze-group tables, Part 2, we replace the setting symbols with the corresponding Hermann–Mauguin symbols where a subindex is added to the lattice symbol to denote the direction of the translations. A listing of the frieze groups with the Hermann–Mauguin symbols of each group in the two settings is given in Table 1.2.6.4.

1.2.7. Origin

The origin has been chosen according to the following conventions:

(i) If the subperiodic group is centrosymmetric, then the inversion centre is chosen as the origin. For the three layer groups $p4/n$ (L52), $p4/nbm$ (L62) and $p4/nmm$ (L64), we give descriptions for two origins, at the inversion centre and at $(-\frac{1}{4}, -\frac{1}{4}, 0)$ from the inversion centre. This latter origin is at a position of high site symmetry and is consistent with having the origin on the fourfold axis, as is the case for all other tetragonal layer groups. The group symbols for the description with the origin at the inversion centre, e.g. $p4/n(\frac{1}{4}, \frac{1}{4}, 0)$, are followed by the shift $(\frac{1}{4}, \frac{1}{4}, 0)$ of the position of the origin used in the description having the origin on the fourfold axis.

(ii) For noncentrosymmetric subperiodic groups, the origin is at a point of highest site symmetry. If no symmetry is higher than 1, the origin is placed on a screw axis, a glide plane or at the intersection of several such symmetry elements.

Origin statement: In the line *Origin* immediately below the diagrams, the site symmetry of the origin is stated if different from the identity. A further symbol indicates all symmetry

Table 1.2.6.4. Distinct Hermann–Mauguin symbols for frieze groups in different settings

Frieze group	Setting symbol	
	(ab)	(bā)
	Hermann–Mauguin symbol	
F1	$\rho_a 1$	$\rho_b 1$
F2	$\rho_a 211$	$\rho_b 211$
F3	$\rho_a 1m1$	$\rho_b 11m$
F4	$\rho_a 11m$	$\rho_b 1m1$
F5	$\rho_a 11g$	$\rho_b 1g1$
F6	$\rho_a 2mm$	$\rho_b 2mm$
F7	$\rho_a 2mg$	$\rho_b 2gm$

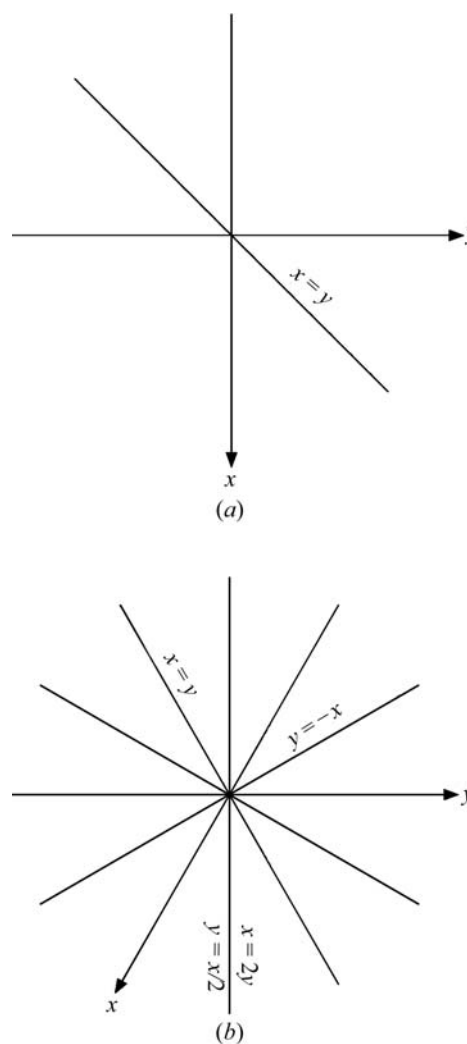


Fig. 1.2.8.1. Boundaries used to define the asymmetric unit for (a) tetragonal rod groups and (b) trigonal and hexagonal rod groups.

elements that pass through the origin. For the three layer groups $p4/n$ (L52), $p4/nbm$ (L62) and $p4/nmm$ (L64) where the origin is on the fourfold axis, the statement ‘at $-\frac{1}{4}, -\frac{1}{4}, 0$ from centre’ is given to denote the position of the origin with respect to an inversion centre.

1.2.8. Asymmetric unit

An asymmetric unit of a subperiodic group is a simply connected smallest part of space from which, by application of all symmetry operations of the subperiodic group, the whole space is filled exactly. For three-dimensional (two-dimensional) space groups,