

1.2. GUIDE TO THE USE OF THE SUBPERIODIC GROUP TABLES

Table 1.2.6.2. Distinct Hermann–Mauguin symbols for monoclinic and orthorhombic rod groups in different settings

Rod group	Setting symbol					
	(abc)	(bāc)	(c̄ba)	(bca)	(ācb)	(c̄āb)
Rod group	Hermann–Mauguin symbol					
R3	$\neq_c 211$	$\neq_c 121$	$\neq_a 112$	$\neq_b 112$	$\neq_b 211$	$\neq_a 121$
R4	$\neq_c m11$	$\neq_c 1m1$	$\neq_a 11m$	$\neq_b 11m$	$\neq_b m11$	$\neq_a 1m1$
R5	$\neq_c c11$	$\neq_c 1c1$	$\neq_a 11a$	$\neq_b 11b$	$\neq_b b11$	$\neq_a 1a1$
R6	$\neq_c 2/m11$	$\neq_c 12/m1$	$\neq_a 112/m$	$\neq_b 112/m$	$\neq_b 2/m11$	$\neq_a 12/m1$
R7	$\neq_c 2/c11$	$\neq_c 12/c1$	$\neq_a 112/a$	$\neq_b 112/b$	$\neq_b 2/b11$	$\neq_a 12/a1$
R8	$\neq_c 112$	$\neq_c 112$	$\neq_a 211$	$\neq_b 121$	$\neq_b 121$	$\neq_a 211$
R9	$\neq_c 112_1$	$\neq_c 112_1$	$\neq_a 2_111$	$\neq_b 12_11$	$\neq_b 12_11$	$\neq_a 2_111$
R10	$\neq_c 11m$	$\neq_c 11m$	$\neq_a m11$	$\neq_b 1m1$	$\neq_b 1m1$	$\neq_a m11$
R11	$\neq_c 112/m$	$\neq_c 112/m$	$\neq_a 2/m11$	$\neq_b 12/m1$	$\neq_b 12/m1$	$\neq_a 2/m11$
R12	$\neq_c 112_1/m$	$\neq_c 112_1/m$	$\neq_a 2_1/m11$	$\neq_b 12_1/m1$	$\neq_b 12_1/m1$	$\neq_a 2_1/m11$
R13	$\neq_c 222$	$\neq_c 222$	$\neq_a 222$	$\neq_b 222$	$\neq_b 222$	$\neq_a 222$
R14	$\neq_c 222_1$	$\neq_c 222_1$	$\neq_a 2_122$	$\neq_b 22_12$	$\neq_b 22_12$	$\neq_a 2_122$
R15	$\neq_c mm2$	$\neq_c mm2$	$\neq_a 2mm$	$\neq_b m2m$	$\neq_b m2m$	$\neq_a 2mm$
R16	$\neq_c cc2$	$\neq_c cc2$	$\neq_a 2aa$	$\neq_b b2b$	$\neq_b b2b$	$\neq_a 2aa$
R17	$\neq_c mc2_1$	$\neq_c cm2_1$	$\neq_a 2_1am$	$\neq_b b2_1m$	$\neq_b m2_1b$	$\neq_a 2_1ma$
R18	$\neq_c 2mm$	$\neq_c m2m$	$\neq_a mm2$	$\neq_b mm2$	$\neq_b 2mm$	$\neq_a m2m$
R19	$\neq_c 2cm$	$\neq_c c2m$	$\neq_a ma2$	$\neq_b bm2$	$\neq_b 2mb$	$\neq_a m2a$
R20	$\neq_c mmm$	$\neq_c mmm$	$\neq_a mmm$	$\neq_b mmm$	$\neq_b mmm$	$\neq_a mmm$
R21	$\neq_c ccm$	$\neq_c ccm$	$\neq_a maa$	$\neq_b bmb$	$\neq_b bmb$	$\neq_a maa$
R22	$\neq_c mcm$	$\neq_c cmm$	$\neq_a mam$	$\neq_b bmm$	$\neq_b mmb$	$\neq_a mma$

Table 1.2.6.3. Distinct Hermann–Mauguin symbols for tetragonal, trigonal and hexagonal rod groups in different settings

Rod group	Setting symbol	
	(abc)	(a ± b b ∓ a c)
Rod group	Hermann–Mauguin symbol	
R35	$\neq_4 2cm$	$\neq_4 2mc$
R37	$\neq_4 \bar{2}m$	$\neq_4 \bar{2}m2$
R38	$\neq_4 \bar{2}c$	$\neq_4 \bar{2}c2$
R41	$\neq_4 2/mmc$	$\neq_4 2/mcm$

Rod group	Setting symbol	
	(abc)	(±2a ± b ∓ a ± b c) (±a ± 2b ∓ 2a ∓ b c) (∓a ± b ∓ a ∓ 2b c)
Rod group	Hermann–Mauguin symbol	
R46	$\neq_3 12$	$\neq_3 21$
R47	$\neq_3 1_12$	$\neq_3 1_121$
R48	$\neq_3 2_12$	$\neq_3 2_121$
R49	$\neq_3 m1$	$\neq_3 1m$
R50	$\neq_3 c1$	$\neq_3 1c$
R51	$\neq_3 \bar{1}m$	$\neq_3 \bar{1}m1$
R52	$\neq_3 \bar{1}c$	$\neq_3 \bar{1}c1$
R70	$\neq_6 3mc$	$\neq_6 3cm$
R71	$\neq_6 \bar{3}m2$	$\neq_6 \bar{3}2m$
R72	$\neq_6 \bar{3}c2$	$\neq_6 \bar{3}2c$
R75	$\neq_6 3/mmc$	$\neq_6 3/mcm$

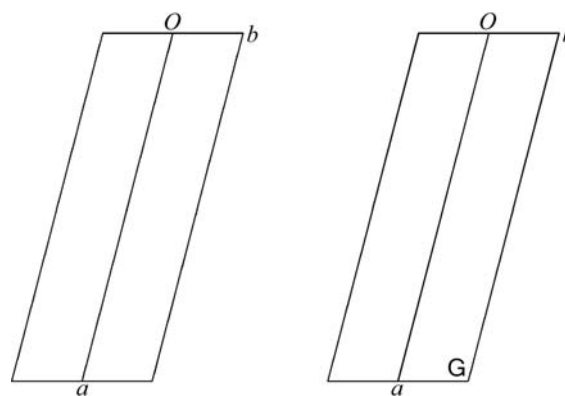


Fig. 1.2.6.16. Diagrams for oblique frieze groups.

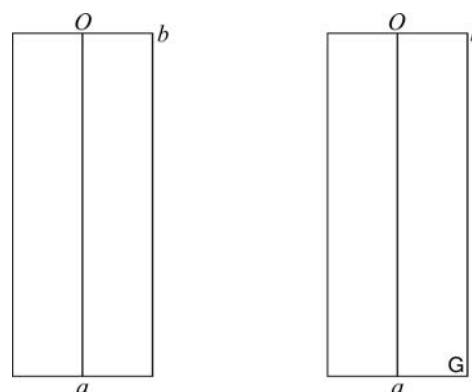


Fig. 1.2.6.17. Diagrams for rectangular frieze groups.

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.

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

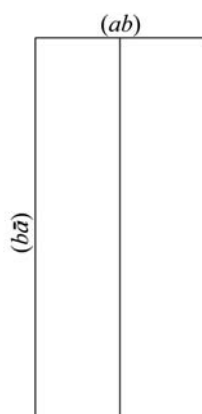


Fig. 1.2.6.18. The two settings for frieze groups. For the second setting, printed vertically, the page must be turned 90° clockwise or viewed from the right-hand side.

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 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, because they contain three-dimensional (two-dimensional) translational symmetry, the asymmetric unit is a finite part of space [see Section 2.8 of *IT A* (1983)]. For subperiodic groups, because the translational symmetry is of a lower dimension than that of the space, the asymmetric unit is infinite in size. We define the asymmetric unit for subperiodic groups by setting the limits on the coordinates of points contained in the asymmetric unit.

1.2.8.1. Frieze groups

For all frieze groups, a limit is set on the x coordinate of the asymmetric unit by the inequality

$$0 \leq x \leq \text{upper limit on } x.$$

For the y coordinate, either there is no limit and nothing further is written, or there is the lower limit of zero, *i.e.* $0 \leq y$.

Example: The frieze group $\mu 2mm$ (F6)

Asymmetric unit $0 \leq x \leq 1/2; 0 \leq y$.

1.2.8.2. Rod groups

For all rod groups, a limit is set on the z coordinate of the asymmetric unit by the inequality

$$0 \leq z \leq \text{upper limit on } z.$$

For each of the x and y coordinates, either there is no limit and nothing further is written, or there is the lower limit of zero.

For tetragonal, trigonal and hexagonal rod groups, additional limits are required to define the asymmetric unit. These limits are given by additional inequalities, such as $x \leq y$ and $y \leq x/2$. Fig. 1.2.8.1 schematically shows the boundaries represented by such inequalities.

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

Frieze group	Setting symbol	
	(ab)	($b\bar{a}$)
	Hermann–Mauguin symbol	
F1	$\mu_a 1$	$\mu_b 1$
F2	$\mu_a 211$	$\mu_b 211$
F3	$\mu_a 1m1$	$\mu_b 11m$
F4	$\mu_a 11m$	$\mu_b 1m1$
F5	$\mu_a 11g$	$\mu_b 1g1$
F6	$\mu_a 2mm$	$\mu_b 2mm$
F7	$\mu_a 2mg$	$\mu_b 2gm$

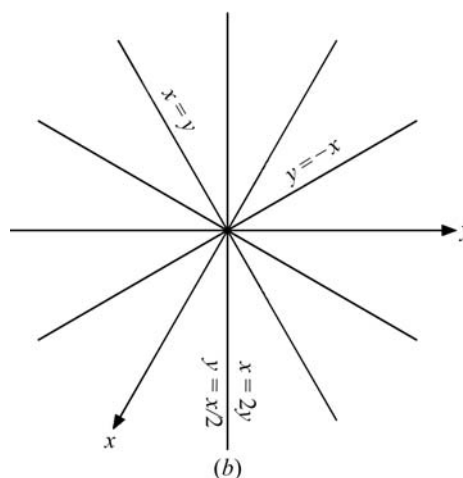
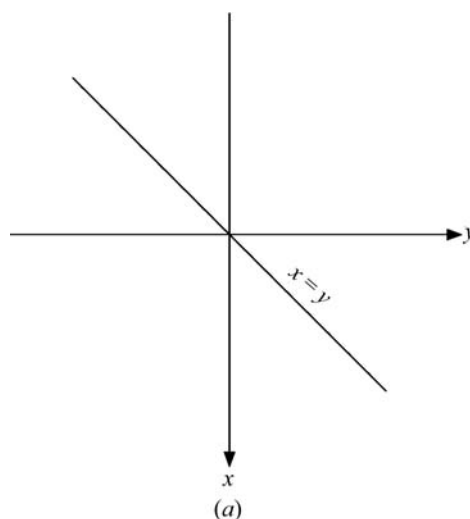


Fig. 1.2.8.1. Boundaries used to define the asymmetric unit for (a) tetragonal rod groups and (b) trigonal and hexagonal rod groups.

Example: The rod group $\mu 6_3mc$ (R70)

Asymmetric unit $0 \leq x; 0 \leq y; 0 \leq z \leq 1; y \leq x/2$.

1.2.8.3. Layer groups

For all layer groups, limits are set on the x coordinate and y coordinate of the asymmetric unit by the inequalities

$$0 \leq x \leq \text{upper limit on } x$$

$$0 \leq y \leq \text{upper limit on } y.$$

For the z coordinate, either there is no limit and nothing further is written, or there is the lower limit of zero.

references