

Magnetic Subperiodic Groups¹

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1. Introduction

The magnetic subperiodic groups, the 31 magnetic frieze group types, the 394 magnetic rod group types, and the 528 magnetic layer group types, are derived and given symbols based on the symbols for the non-magnetic subperiodic groups in Volume E of the *International Tables of Crystallography*. The symbols are constructed in analogy to the Opechowski-Guccione symbols for magnetic space groups. Tables are given which list one group from each type. Each group is specified not only by its symbol but also by explicitly listing the coset representatives of the coset decomposition of the group with respect to its translational subgroup. For magnetic subperiodic groups of the type \mathbf{M}_T and \mathbf{M}_R the subgroup of index two of unprimed elements is explicitly given.

The *subperiodic groups* in the title refer to the frieze groups, two-dimensional groups with one-dimensional translations, rod groups, three-dimensional groups with one-dimensional translations, and layer groups, three-dimensional groups with two-dimensional translations. There are 7, 75, and 80 non-magnetic frieze, rod, and layer group types, respectively (see, e.g. Shubnikov and Koptsik, 1974 or Vol. E of the *International Tables for Crystallography* (1999)). The magnetic frieze groups have been derived by Belov (1956) and the magnetic rod and layer groups by Neronova and Belov (1961) (see also the review by Zamorzaev and Palistrant (1980) and the monograph by Zamorzaev (1976)).

We have re-derived the magnetic subperiodic groups as an extension of the non-magnetic subperiodic groups, basing the symbols for the magnetic subperiodic

group types on the symbols of the non-magnetic subperiodic group types tabulated in Vol. E of the *International Tables for Crystallography* (1999). The form and meaning of the symbols is in analogy to the form and meaning of the Opechowski-Guccione symbols for magnetic space groups which differs, see Section 3.2 below, from form and meaning of the symbols used by Belov, Neronova, & Smirnova (1957).

In distinction from previous listings of only a symbol of each magnetic subperiodic group type, a specification of one group of each type is given. This consists of specifying the coordinate system used, and then relative to the coordinate system, the translational subgroup of the group and a set of coset representatives of the coset decomposition of the group with respect to its translational subgroup. The first part of the symbol of each magnetic subperiodic group specifies the coordinate system and the translational subgroup, see Figures 1. A set of coset representatives, called the *standard set of coset representatives*, is explicitly given for each group.

In Section 2, the concept of *magnetic superfamily* is reviewed. This concept provides for a sub-classification of magnetic subperiodic groups. This is followed, in Section 3, by a detailed explanation of the contents of the tables of the magnetic subperiodic groups.

2. Magnetic Superfamily of Groups

Let \mathbf{F} denote a crystallographic group type. The *magnetic superfamily* (Opechowski, 1986) of crystallographic groups of type \mathbf{F} consists of

- 1) Groups of type \mathbf{F} .
- 2) Groups of type $\mathbf{F}1'$, where "1'" denotes time inversion..
- 3) Groups of type $\mathbf{F}(\mathbf{D}) = \mathbf{D} + (\mathbf{F} - \mathbf{D})1'$ where \mathbf{D} is a subgroup of index two of \mathbf{F} . Groups of this type will also be denoted by \mathbf{M} .

The third set of groups is divided into two subdivisions:

- 3a) Groups \mathbf{M}_T , where \mathbf{D} is an equi-translational (*translationengleiche*) subgroup of \mathbf{F} .
- 3b) Groups \mathbf{M}_R , where \mathbf{D} is an equi-class (*klassengleiche*) subgroups of \mathbf{F} .

A survey of the crystallographic groups of the magnetic superfamily of crystallographic groups of type \mathbf{F} will consist of a listing of a set of coset representatives, of the decomposition of the group with respect to its translational subgroup, of one group from the groups of type \mathbf{F} and of one group from each of the types $\mathbf{F}1'$ and $\mathbf{F}(\mathbf{D})$. The symbol for each listed group is used to denote both the group and the group's type. Reference to *the group* \mathbf{F} , $\mathbf{F}1'$, or $\mathbf{F}(\mathbf{D})$ will refer to the listed group and to *the group type* \mathbf{F} , $\mathbf{F}1'$, or $\mathbf{F}(\mathbf{D})$ to that group's type. The numbers

of magnetic subperiodic group types **F**, **F1'**, and **F(D)** are:

| | F | F1' | F(D) | Total |
|---------------|----------|------------|-------------|-------|
| Frieze Groups | 7 | 7 | 17 | 31 |
| Rod Groups | 75 | 75 | 244 | 394 |
| Layer Groups | 80 | 80 | 368 | 528 |
| Grand Total | | | | 953 |

3. Tables of Magnetic Subperiodic Groups

The tables of the frieze, rod, and layer groups are given in Tables 1, 2, and 3, respectively. The format of the tables is:

- 1) Serial number of the magnetic subperiodic group type.
- 2) Symbol of the magnetic subperiodic group and the group's type.
- 3) Symbol of the group type of the subgroup **D** of index two of **F** for magnetic subperiodic groups **F(D)**, and the position and orientation of the group **D** in the coordinate system of the group **F(D)** [which is the same as the coordinate system of **F**].
- 4) A set of coset representatives of the decomposition of the magnetic subperiodic group with respect to its translational subgroup.

3.1 Serial Number

A separate numbering system is used for the frieze, rod, and layer magnetic subperiodic group types. For each, a three part number $N_1.N_2.N_3$ is used. N_1 is a sequential number for the group type to which **F** belongs. It is the same numbering given in Vol. E of the *International Tables for Crystallography* (1999) for the subperiodic group types. N_2 is a sequential numbering of the magnetic subperiodic group types of the superfamily of **F**. Group types **F** always have the assigned number $N_1.1.N_3$, and group types **F1'** the assigned number $N_1.2.N_3$. N_3 is a global sequential numbering of magnetic subperiodic group types.

3.2 Magnetic Subperiodic Group Symbol

The symbol for a group **F** is that symbol for the group type **F** given in Volume E of the *International Tables of Crystallography* (1999). The group **F** is uniquely defined by its translational subgroup and the coset representatives of the coset decomposition of the group with respect to its translational subgroup. The coset representatives which we use to define the group are implied by the explicitly printed set of general equivalent positions given in Vol. E of the *International Tables for Crystallography* (1999). These coset representatives are also given in the tables, see Section 3.4 below. The symbol for a group **F1'** is that of the group type **F** followed by "1".

The symbol for a group $\mathbf{M}_T = \mathbf{F}(\mathbf{D}) = \mathbf{D} + (\mathbf{F} - \mathbf{D})1'$ is based on the symbol for the group **F**. As **D** is an equi-translational subgroup of **F**, i.e. the translational

subgroup $\mathbf{T}^{\mathbf{M}}_{\mathbf{T}}$ of the magnetic group $\mathbf{M}_{\mathbf{T}}$ is \mathbf{T} , the translational subgroup of \mathbf{F} . The translational part of the group symbol of a $\mathbf{M}_{\mathbf{T}}$ group is then the same as that of the corresponding group \mathbf{F} . If a number or letter in the rotational part of the symbol of \mathbf{F} is associated with an element of the group \mathbf{F} contained in the subgroup \mathbf{D} , it appears unchanged in the symbol for $\mathbf{M}_{\mathbf{T}}$, if not in \mathbf{D} , i.e. in $\mathbf{F} - \mathbf{D}$, it appears with a prime to denote that that element in $\mathbf{M}_{\mathbf{T}}$ is coupled with $1'$. For example, the magnetic layer group 285.171 is a group $\mathbf{M}_{\mathbf{T}}$ whose symbol is $\text{pm}2_1'b'$. In this case we have

$$\text{pm}2_1'b' = \text{pm}11 + (\text{pm}2_1b - \text{pm}11)1'$$

i.e. $\mathbf{F} = \text{pm}2_1b$ and $\mathbf{D} = \text{pm}11$. The letter "m" in the symbol for \mathbf{F} denotes the element $(m_x|000)$ which is contained in \mathbf{D} and consequently appears unprimed in the symbol for $\mathbf{M}_{\mathbf{T}}$. The symbols " 2_1 " and " b " denote the elements $(2_y|0\frac{1}{2}0)$ and $(m_z|0\frac{1}{2}0)$, respectively, are not contained in \mathbf{D} and consequently appear primed in the symbol for $\mathbf{M}_{\mathbf{T}}$.

The symbol for a group $\mathbf{M}_{\mathbf{R}} = \mathbf{F}(\mathbf{D}) = \mathbf{D} + (\mathbf{F} - \mathbf{D})1'$ is also based on the symbol for the group \mathbf{F} . (This is in contradistinction to the "BNS" symbols of $\mathbf{M}_{\mathbf{R}}$ groups (Belov, Neronova, & Smirnova (1957)) where the symbol for a $\mathbf{M}_{\mathbf{R}}$ group is based on the symbol for the group \mathbf{D} .) As this is an equi-class magnetic group, half the translations of \mathbf{F} are now coupled with $1'$ in $\mathbf{M}_{\mathbf{R}}$ and half the translations remain unprimed in $\mathbf{M}_{\mathbf{R}}$. The unprimed translations constitute the translational subgroup $\mathbf{T}^{\mathbf{D}}$ of \mathbf{D} . We can write the coset decomposition of the translational subgroup \mathbf{T} of \mathbf{F} with respect to the translational subgroup $\mathbf{T}^{\mathbf{D}}$ of \mathbf{D} as

$$\mathbf{T} = \mathbf{T}^{\mathbf{D}} + \mathbf{t}_{\alpha} \mathbf{T}^{\mathbf{D}}$$

where \mathbf{t}_α is a translation of \mathbf{F} which appears primed (coupled with 1') in \mathbf{M}_R . The translational subgroup of \mathbf{M}_R can then be written as

$$\mathbf{T}_R^M = \mathbf{T}^D + \mathbf{t}_\alpha' \mathbf{T}^D$$

Symbols for the translational groups \mathbf{T} , the translational subgroups \mathbf{T}^D of \mathbf{T} used in the symbol for \mathbf{M}_R groups, and the choice of the translations \mathbf{t}_α are given in Figures 1.

The symbol for a magnetic group $\mathbf{M}_R = \mathbf{F}(\mathbf{D})$ is based on the symbol of the group \mathbf{F} , and is also a symbol for the subgroup \mathbf{D} of unprimed elements. The translational part of the symbol of \mathbf{F} is replaced by the symbol for the translational subgroup \mathbf{T}^D of \mathbf{D} . If a coset representative $(R|\tau(R))$ of \mathbf{T} in \mathbf{F} appears as the coset representative $(R|\tau(R)+\mathbf{t}_\alpha)$ of \mathbf{T}^D in \mathbf{D} , then the number or letter corresponding to $(R|\tau(R))$ in the symbol for \mathbf{F} is primed. If $(R|\tau(R))$ appears unchanged as a coset representative of \mathbf{T}^D in \mathbf{D} , then the number or letter corresponding to $(R|\tau(R))$ in the symbol for \mathbf{F} is unchanged. The resulting symbol is a symbol for \mathbf{D} based on the symbol for \mathbf{F} and is also a symbol for the magnetic subperiodic group $\mathbf{M}_R = \mathbf{F}(\mathbf{D})$. The symbol specifies not only \mathbf{D} but also \mathbf{F} : By deleting the subindex on the translational part of the symbol and the primes on the rotational part one obtains the symbol specifying \mathbf{F} . Having specified \mathbf{D} and \mathbf{F} one has specified the group $\mathbf{M}_R = \mathbf{F}(\mathbf{D})$. For example: Consider the group 19.1.104, $\mathbf{F} = p222$:

$$\mathbf{F} = \mathbf{T} + (2_x|000)\mathbf{T} + (2_y|000)\mathbf{T} + (2_z|000)\mathbf{T}$$

The symbol for the $\mathbf{M}_R = \mathbf{F}(\mathbf{D})$ group 19.5.108 is $p_{2a}2'2'2$ and is based on the symbol for \mathbf{F} . The translational subgroup \mathbf{T}^D of \mathbf{D} is given by the symbol p_{2a} where $\mathbf{t}_\alpha = \mathbf{a}$.

The two "2"s in $p_{2a}2'2'2$ denote that the coset representatives $(2_x|000)$ and $(2_y|000)$ of \mathbf{T} in \mathbf{F} appear as the coset representatives $(2_x|100)$ and $(2_y|100)$ of \mathbf{T}^D in \mathbf{D} . As the third "2" is unprimed, the coset representative $(2_z|000)$ remains unchanged. We have then the subgroup:

$$\mathbf{D} = \mathbf{T}^D + (2_x|100)\mathbf{T}^D + (2_y|100)\mathbf{T}^D + (2_z|000)\mathbf{T}^D$$

We note that these same coset representatives of \mathbf{T}^D in \mathbf{D} are also the coset representatives of \mathbf{T}_R^M in \mathbf{M}_R .

$$\mathbf{M}_R = \mathbf{T}_R^M + (2_x|100)\mathbf{T}_R^M + (2_y|100)\mathbf{T}_R^M + (2_z|000)\mathbf{T}_R^M$$

Since $\mathbf{T}_R^M = \mathbf{T}^D + \mathbf{t}_\alpha' \mathbf{T}^D$ it follows that:

$$\mathbf{M}_R = \mathbf{D} + (\mathbf{F}-\mathbf{D})1'$$

$$\begin{aligned} \mathbf{M}_R = & \mathbf{T}^D + (2_x|100)\mathbf{T}^D + (2_y|100)\mathbf{T}^D + (2_z|000)\mathbf{T}^D + \\ & + (1|100)\mathbf{T}^D + (2_x|000)\mathbf{T}^D + (2_y|000)\mathbf{T}^D + (2_z|100)\mathbf{T}^D \end{aligned}$$

Consequently, a primed number or letter in the symbol for \mathbf{M}_R (which is a symbol for \mathbf{D}) denotes that the corresponding element appears in \mathbf{D} coupled with \mathbf{t}_α and primed in $(\mathbf{F}-\mathbf{D})1'$, e.g. $(2_x|100)$ is in \mathbf{D} and $(2_x|000)'$ in $(\mathbf{F}-\mathbf{D})1'$. An unprimed number or letter in the symbol for \mathbf{M}_R (which is a symbol for \mathbf{D}) denotes that the corresponding element appears unchanged in \mathbf{D} and coupled with \mathbf{t}_α and primed in $(\mathbf{F}-\mathbf{D})1'$, e.g. $(2_z|000)$ is in \mathbf{D} and $(2_z|100)'$ in $(\mathbf{F}-\mathbf{D})1'$.

3.3 Symbol of the subgroup \mathbf{D}

The third column contains the group type symbol of the subgroup **D** of index two of the magnetic group **M** = **F(D)**.

a) For **M_T** groups, **D** is defined by the translational subgroup **T** of **F** and the unprimed coset representatives listed in the fourth column.

b) For **M_R** groups, **D** is defined by the translational subgroup **T^D** and the set of all coset representatives listed in the fourth column.

While the group type symbol of **D** is given, the coset representatives of the subgroup **D** of **M_T** or **M_R** defined in a) or b), respectively, may not be identical with the coset representatives of the group **D** found in the listing of the magnetic subperiodic groups. Consequently, to show the relationship between this group **D** and the group of type **D** listed in the tables, additional information is provided to define a new coordinate system in which the coset representatives of this subgroup of type **D** are identical with the coset representatives listed for the group **D**.

Let (**O**; **a**, **b**, **c**) be the coordinate system in which the group **F** is defined. "**O**" is the origin of the coordinate system, and **a**, **b**, and **c** are the basis vectors of the coordinate system. **a**, **b**, and **c** represent a set of basis vectors for a primitive cell for primitive lattices and for a conventional cell for centered lattices. A second coordinate system is defined by (**O**+**t**; **a'**, **b'**, **c'**). The origin is translated from **O** to **O**+**t**, and then the basis vectors **a**, **b**, and **c** are changed to **a'**, **b'** and **c'**.

Immediately following the group type symbol for the subgroup **D** of **F** we give a coordinate system (**O**+**t**; **a'**, **b'**, **c'**) [In the tables, for typographical simplicity, the symbols "**O**+" are omitted.] in which the coset representatives of the subgroup **D** of

F are identical with the coset representatives of the group **D** found in the listing of the magnetic subperiodic groups. **t**, **a'**, **b'**, and **c'** are given in terms of the basis vectors of the coordinate system (**O**;**a**,**b**,**c**) of the group **F**.

Example 1: For the **M_T** magnetic layer group 14.3.68 = p2/m'11 one finds in the tables:

$$p211 (000;\mathbf{a},\mathbf{b},\mathbf{c}) \quad (1|000) \quad (2_x|000) \quad (\overline{1}|000)' \quad (m_x|000)'$$

The translational subgroup of **D** is generated by the translations (1|100) and (1|010) and the coset representatives of this group are (1|000) and (2_x|000), the unprimed coset representatives on the right. This subgroup **D** is of type p211. In the tables, listed for the group 8.1.34 p211, one finds the identical two coset representatives. Consequently, there is no change the coordinate system, i.e. **t**=(000) and **a'**=**a**, **b'**=**b**, and **c'**=**c**. In the coordinate system of the magnetic group p2/m'11, the coset representatives of its subgroup **D**, of the type p211, are identical with the coset representatives of the group p211 found in the tables.

Example 2: For the **M_R** magnetic layer group 19.5.108 p_{2a}2'2'2 one finds in the tables:

$$p2_122 (000;2\mathbf{a},\mathbf{b},\mathbf{c}) \quad (1|000) \quad (2_x|100) \quad (2_y|100) \quad (2_z|000)$$

The translational subgroup of **D** is generated by the translations (1|200) and (1|010) and the coset representatives of this group are all those coset representatives on the right. This subgroup **D** is of type p2₁22. In the tables, listed for the group 20.1.111 p2₁22 one finds a different set of coset representatives:

$$(1|000) \quad (2_x|\frac{1}{2}00) \quad (2_y|\frac{1}{2}00) \quad (2_z|000)$$

Consequently, to show the relationship between the subgroup **D** of type p2₁22 and the listed group p2₁22, we change the coordinate system in which **D** is defined to (**O**+000;2**a**,**b**,**c**). In this new coordinate system the coset representatives of **D** are identical with the coset representatives of the representative group p2₁22.

Example 3: For the **M_T** magnetic layer group 20.4.114 p2₁22' one finds in the tables:

$$p211 \left(\frac{1}{4}0 \ 0; \mathbf{b}, \overline{\mathbf{a}}, \mathbf{c} \right) \quad (1|000) \quad (2_x|\frac{1}{2}00)' \quad (2_y|\frac{1}{2}00) \quad (2_z|000)'$$

The translational subgroup of **D** is generated by the translations (1|100) and (1|010) and the coset representatives of this group are (1|000) and (2_y|\frac{1}{2}00), the unprimed coset representatives on the right. The group **D** is of type p211. In the tables, for the group p211 one finds a different set of coset representatives, (1|000) and (2_x|000). Consequently, to show the relationship between the subgroup **D** of type p211 and the listed group p211, we change the coordinate system in which **D** is defined to (**O**+ $\frac{1}{4}$ 0 0;**b**, $\overline{\mathbf{a}}$,**c**) . The origin is first translated from **O** to **O**+**t** , where **t**=($\frac{1}{4}$ 00) and the a new set of basis vectors, **a'**=**b**, **b'**= $\overline{\mathbf{a}}$, and **c'**=**c** are defined. In this new coordinate system the coset representatives of **D** are identical with the coset representatives of the group p211.

3.4 Coset Representatives

The groups listed are defined by their translational subgroups and a set of coset representatives of the coset decomposition of each group with respect to its respective translational subgroup. The defining coset representatives are listed on the right hand side of the tables.

A group **F** is defined by its translational subgroup and the set of coset representatives implied by the coordinates of the set of equivalent positions explicitly listed under the group type in Vol. E of *International Tables for Crystallography* (1999). For example, The group **F** = p2₁22 has a primitive translational subgroup generated by (1|100) and (1|010). The coordinates of the set of equivalent positions listed in Vol. E under the group type p2₁22 are:

$$x, y, z; \quad x + \frac{1}{2}, \bar{y}, \bar{z}; \quad \bar{x} + \frac{1}{2}, y, \bar{z}; \quad \bar{x}, \bar{y}, z$$

Corresponding to these are the symmetry elements

$$(1|000); \quad (2_x|\frac{1}{2}00); \quad (2_y|\frac{1}{2}00); \quad (2_z|000),$$

respectively, which are taken as the coset representatives.

The coset representatives of groups **F1'** are not explicitly given. These are taken as the coset representatives of **F** plus each of these coset representatives multiplied by 1'. For example, the coset representatives of **F** = p2₁22 are given above. The coset representatives of **F1'** = p2₁221' are

$$\begin{array}{llll} (1|000); & (2_x|\frac{1}{2}00); & (2_y|\frac{1}{2}00); & (2_z|000); \\ (1|000)'; & (2_x|\frac{1}{2}00)'; & (2_y|\frac{1}{2}00)'; & (2_z|000)'. \end{array}$$

The coset representatives of groups $\mathbf{M}_T = \mathbf{F}(\mathbf{D})$ are derived from the coset representatives of \mathbf{F} . Each coset representative of \mathbf{F} appears unchanged or primed as a coset representative of \mathbf{M}_T . For example, The coset representatives of $\mathbf{F} = p2_122$ are

$$(1|000); \quad (2_x|\frac{1}{2}00); \quad (2_y|\frac{1}{2}00); \quad (2_z|000).$$

The coset representatives of $\mathbf{M}_T = p2_1'22'$ are:

$$(1|000); \quad (2_x|\frac{1}{2}00)'; \quad (2_y|\frac{1}{2}00); \quad (2_z|000)'.$$

The coset representatives of groups $\mathbf{M}_R = \mathbf{F}(\mathbf{D})$ are also derived from the coset representatives of \mathbf{F} . They are also chosen such that they are coset representatives of \mathbf{D} with respect to its subgroup \mathbf{T}^D . Each coset representative of \mathbf{F} appears either unchanged or multiplied by \mathbf{t}_α . For example: The coset representatives of $\mathbf{F} = p2_122$ are

$$(1|000); \quad (2_x|\frac{1}{2}00); \quad (2_y|\frac{1}{2}00); \quad (2_z|000).$$

The coset representatives of $\mathbf{M}_R = p_{2b}2_1'2'2$, where $\mathbf{t}_\alpha = (010)$, are:

$$(1|000); \quad (2_x|\frac{1}{2}10); \quad (2_y|\frac{1}{2}10); \quad (2_z|000).$$

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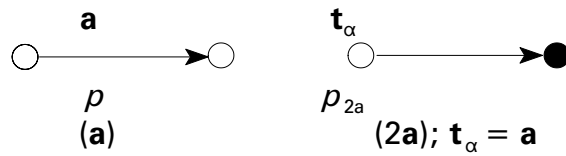
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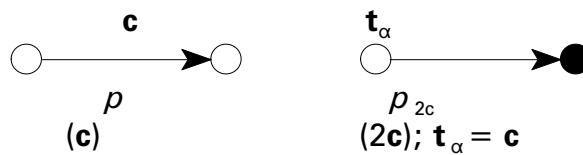
Zamorzaev, A.M. & Palistrant, A.P. (1980). *Zeit. fur Krist.* **151** 231-248.

Figures 1: Diagrams of translational groups. Below each diagram is given the symbol for the group and generators, or for the unprimed subgroup, its generators, and the definition of the translation \mathbf{t}_α .

Frieze Groups:

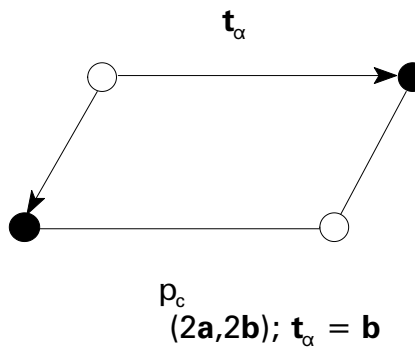
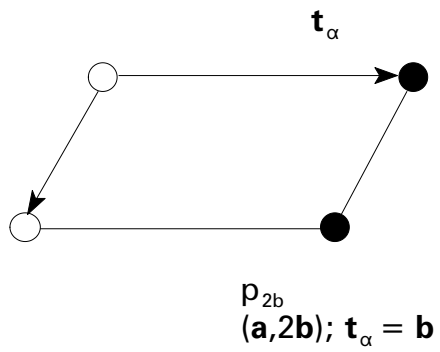
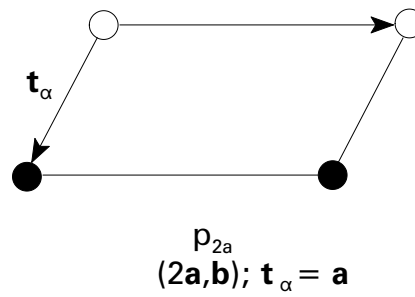
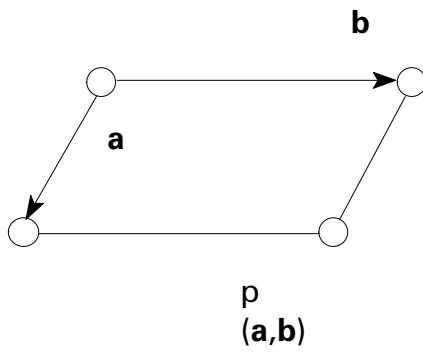


Rod Groups

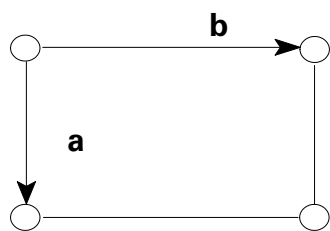


Layer Groups:

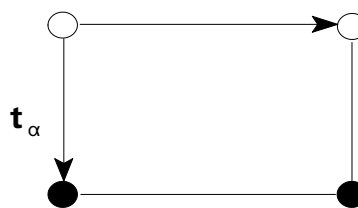
Triclinic/Oblique System, Monoclinic/Oblique System



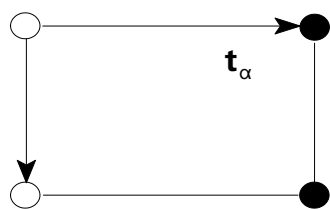
Monoclinic/Rectangular System, Orthorhombic/Rectangular System



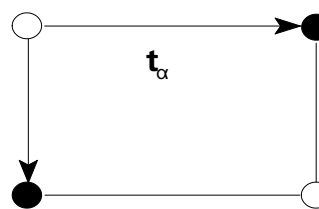
p
 (a,b)



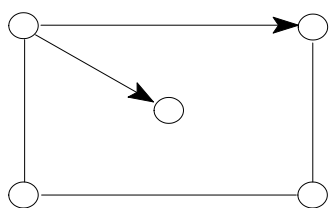
p_{2a}
 $(2a,b); t_{\alpha} = a$



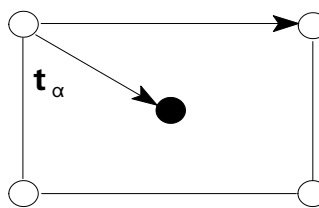
p_{2b}
 $(a,2b); t_{\alpha} = b$



p_c
 $(2a,2b); t_{\alpha} = b$

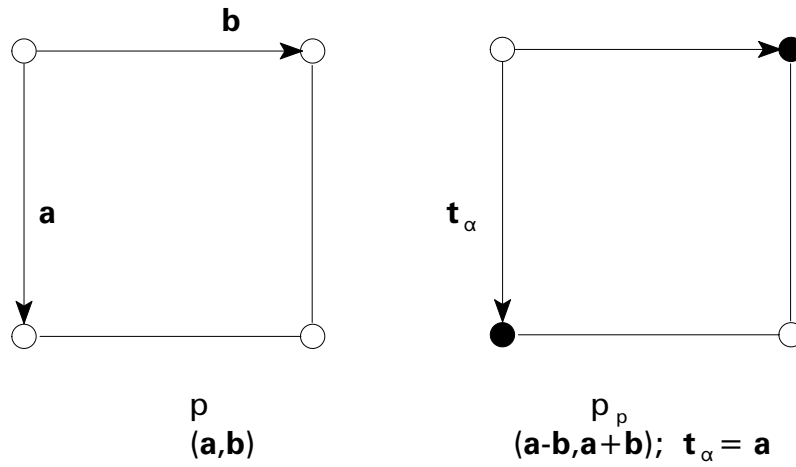


c
 $((a+b)/2, (a-b)/2)$



c_p
 $(a,b); t_{\alpha} = (a+b)/2$

Tetragonal/Square System



Trigonal/Hexagonal System, Hexagonal/Hexagonal System

