International Tables for Crystallography (2011). Vol. A1, Section 2.1.2.5.3, pp. 75–76.

There are seven maximal *t*-subgroups of *Pban*, No. 50, four of which are orthorhombic, $\mathcal{H} = Pba2$, $Pb2n$, $P2an$ and $P222$, and three of which are monoclinic, $\mathcal{H} = P112/n$, $P12/a1$ and $P2/b11$. In the orthorhombic subgroups, the centres of inversion of $\mathcal{G}$ are lost but at least one kind of twofold axis is retained. Therefore, no origin shift for $\mathcal{H}$ is necessary from the setting 'origin choice 1' of $\mathcal{G}(1)$, where the origin is placed at the intersection of the three twofold axes. For the column part of the transformation $(\boldsymbol{P}, \boldsymbol{p}_1)$, $\boldsymbol{p}_1 = \boldsymbol{o}$ holds. For the monoclinic maximal *t*-subgroups of *Pban* the origin is shifted from the intersection of the three twofold axes in $\mathcal{G}(1)$ to an inversion centre of $\mathcal{H}$.

On the other hand, the origin is situated on an inversion centre for origin choice 2 of $\mathcal{G}(2)$, as is the origin in the conventional description of the three monoclinic maximal *t*-subgroups. For them the origin shift is $\boldsymbol{p}_2 = \boldsymbol{o}$, while there is a nonzero column $\boldsymbol{p}_2$ for the orthorhombic subgroups.

(*b*) Both $\mathcal{G}$ and its subgroup $\mathcal{H} < \mathcal{G}$ are listed with two origins. Then the origin choice of $\mathcal{H}$ is the same as that of $\mathcal{G}$. This rule always applies to isomorphic subgroups as well as in some other cases.

Example 2.1.2.5.5

Maximal *k*-subgroups $\mathcal{H}$ = *Pnnn*, No. 48, of the space group $\mathcal{G}$ = *Pban*, No. 50. There are two such subgroups with the lattice relation $\mathbf{c}' = 2\mathbf{c}$. Both $\mathcal{G}$ and $\mathcal{H}$ are listed with two origins such that the origin choices of $\mathcal{G}$ and $\mathcal{H}$ are either the same or are strongly related.

(*c*) The group $\mathcal{G}$ is listed with one origin but the subgroup $\mathcal{H} < \mathcal{G}$ is listed with two origins. This situation is restricted to maximal *k*-subgroups with the only exception being $Ia\bar{3}d > I4_1/acd$, where there are three conjugate *t*-subgroups of index 3. In all cases the subgroup $\mathcal{H}$ is referred to origin choice 2. This rule is followed in the subgroup tables because it gives a better chance of retaining the origin of $\mathcal{G}$ in $\mathcal{H}$. If there are two origin choices for $\mathcal{H}$, then $\mathcal{H}$ has inversions and these are also elements of the supergroup $\mathcal{G}$. The (unique) origin of $\mathcal{G}$ is placed on one of the inversion centres. For origin choice 2 in $\mathcal{H}$, the origin of $\mathcal{H}$ may agree with that of $\mathcal{G}$, although this is not guaranteed. In addition, origin choice 2 is often preferred in structure determinations.

Example 2.1.2.5.6

Maximal *k*-subgroups of *Pccm*, No. 49. In the block
• Enlarged unit cell, [2] $\mathbf{a}' = 2\mathbf{a}$
one finds two subgroups *Pcna* (50, *Pban*). One of them has the origin of $\mathcal{G}$, the origin of the other subgroup is shifted by $\frac{1}{2}, 0, 0$ and is placed on one of the inversion centres of $\mathcal{G}$ that is removed from the first subgroup. The analogous situation is found in the block [2] $\mathbf{b}' = 2\mathbf{b}$, where the two subgroups of space-group type *Pncb* (50, *Pban*) show the analogous relation. In the next block, [2] $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, the four subgroups *Ccce* (68) behave similarly.

For $\mathcal{G}$ = *Pmma*, No. 51, the same holds for the two subgroups of the type *Pmmn* (59) in the block [2] $\mathbf{b}' = 2\mathbf{b}$.

On the other hand, for $\mathcal{G}$ = *Immm*, No. 71, in the block 'Loss of centring translations' three subgroups of type *Pmmn* (59) and one of type *Pnnn* (48) are listed. All of them need an origin shift of $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ because they have lost the inversion centres of the origin of $\mathcal{G}$.

2.1.2.5.3. Space groups with a rhombohedral lattice

The seven trigonal space groups with a rhombohedral lattice are often called *rhombohedral space groups*. Their HM symbols begin with the lattice letter *R* and they are listed with both hexagonal axes and rhombohedral axes.

Rules

(*a*) A rhombohedral subgroup $\mathcal{H}$ of a rhombohedral space group $\mathcal{G}$ is listed in the same setting as $\mathcal{G}$: if $\mathcal{G}$ is referred to hexagonal axes, so is $\mathcal{H}$; if $\mathcal{G}$ is referred to rhombohedral axes, so is $\mathcal{H}$.

(*b*) If $\mathcal{G}$ is a non-rhombohedral trigonal or a cubic space group, then a rhombohedral subgroup $\mathcal{H} < \mathcal{G}$ is always referred to hexagonal axes.

(*c*) A non-rhombohedral subgroup $\mathcal{H}$ of a rhombohedral space group $\mathcal{G}$ is referred to its conventional setting.

Remarks

Rule (*a*) provides a clear definition, in particular for the axes of isomorphic subgroups.

Rule (*b*) has been followed in the subgroup tables because the rhombohedral setting is rarely used in crystallography.

Rule (*c*) implies that monoclinic subgroups of rhombohedral space groups are referred to the setting 'unique axis *b*'.

There is a peculiarity caused by the two settings of the rhombohedral space groups. The rhombohedral lattice appears to be centred in the hexagonal axes setting, whereas it is primitive in the rhombohedral axes setting. Therefore, there are trigonal subgroups of a rhombohedral space group $\mathcal{G}$ which are listed in the block 'Loss of centring translations' for the hexagonal axes setting of $\mathcal{G}$ but are listed in the block 'Enlarged unit cell' when $\mathcal{G}$ is referred to rhombohedral axes. Although unnecessary and not done for other space groups with primitive lattices, the line

• Loss of centring translations none

is listed for the rhombohedral axes setting.

Example 2.1.2.5.7

$\mathcal{G} = R3$, No. 146. Maximal *klassengleiche* subgroups of index 2 and 3. Comparison of the data for the settings 'hexagonal axes' and 'rhombohedral axes'. The data for the general position and the generators are omitted.

HEXAGONAL AXES

	• Loss of centring translations		
[3]	$P3_2$ (145)		0, 1/3, 0
[3]	$P3_1$ (144)		1/3, 1/3, 0
[3]	$P3$ (143)		
	• Enlarged unit cell		
[2]	$\mathbf{a}' = -\mathbf{b}, \mathbf{b}' = \mathbf{a} + \mathbf{b}, \mathbf{c}' = 2\mathbf{c}$		
	$R3$ (146)	$-\mathbf{b}, \mathbf{a} + \mathbf{b}, 2\mathbf{c}$	
...			

RHOMBOHEDRAL AXES

	• Loss of centring translations		none
	• Enlarged unit cell		
[2]	$\mathbf{a}' = \mathbf{a} + \mathbf{c}, \mathbf{b}' = \mathbf{a} + \mathbf{b}, \mathbf{c}' = \mathbf{b} + \mathbf{c}$		
	$R3$ (146)	$\mathbf{a} + \mathbf{c}, \mathbf{a} + \mathbf{b}, \mathbf{b} + \mathbf{c}$	
[3]	$\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{b} - \mathbf{c}, \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c}$		
	$P3_2$ (145)	$\mathbf{a} - \mathbf{b}, \mathbf{b} - \mathbf{c}, \mathbf{a} + \mathbf{b} + \mathbf{c}$	0, 1/3, −1/3
	$P3_1$ (144)	$\mathbf{a} - \mathbf{b}, \mathbf{b} - \mathbf{c}, \mathbf{a} + \mathbf{b} + \mathbf{c}$	1/3, 0, −1/3
	$P3$ (143)	$\mathbf{a} - \mathbf{b}, \mathbf{b} - \mathbf{c}, \mathbf{a} + \mathbf{b} + \mathbf{c}$	

The sequence of the blocks has priority over the classification by increasing index. Therefore, in the setting 'hexagonal axes', the subgroups of index 3 precede the subgroup of index 2.
In the tables, the lattice relations are simpler for the setting 'hexagonal axes'.
The complete general position is listed for the maximal k-subgroups of index 3 in the setting 'hexagonal axes'; only the generator is listed for rhombohedral axes.

2.1.3. I Maximal *translationengleiche* subgroups (t-subgroups)

2.1.3.1. Introduction

In this block, all maximal t-subgroups $\mathcal{H}$ of the plane groups and the space groups $\mathcal{G}$ are listed individually. Maximal t-sugroups are always non-isomorphic.

For the sequence of the subgroups, see Section 2.1.2.4. There are no lattice relations for t-subgroups because the lattice is retained. Therefore, the sequence is determined only by the rising value of the index and by the decreasing space-group number.

2.1.3.2. A description in close analogy with IT A

The listing is similar to that of *IT* A and presents on one line the following information for each subgroup $\mathcal{H}$:

[*i*] HMS1 (No., HMS2) sequence matrix shift

Conjugate subgroups are listed together and are connected by a left brace.

The symbols have the following meaning:

[*i*]	index of $\mathcal{H}$ in $\mathcal{G}$;
HMS1	HM symbol of $\mathcal{H}$ referred to the coordinate system and setting of $\mathcal{G}$. This symbol may be nonconventional;
No.	space-group No. of $\mathcal{H}$;
HMS2	conventional HM symbol of $\mathcal{H}$ if HMS1 is not a conventional HM symbol;
sequence	sequence of numbers; the numbers refer to those coordinate triplets of the general position of $\mathcal{G}$ that are retained in $\mathcal{H}$, *cf. Remarks*; for general position *cf.* Section 2.1.2.2.2;
matrix	matrix part of the transformation to the conventional setting corresponding to HMS2, *cf.* Section 2.1.3.3;
shift	column part of the transformation to the conventional setting corresponding to HMS2, *cf.* Section 2.1.3.3.

Remarks

In the sequence column for space groups with centred lattices, the abbreviation '(numbers)+' means that the coordinate triplets specified by 'numbers' are to be taken plus those obtained by adding each of the centring translations, see the comments following Examples 2.1.3.2.2 and 2.1.3.2.3.

The symbol HMS2 is omitted if HMS1 is a conventional HM symbol.

The following deviations from the listing of *IT* A are introduced in these tables:

No.: the space-group No. of $\mathcal{H}$ is added.
HMS2: In order to specify the setting clearly, the *full* HM symbol is listed for monoclinic subgroups, not the standard (short) HM symbol as in *IT* A.
matrix, shift: These entries contain information on the transformation of $\mathcal{H}$ from the setting of $\mathcal{G}$ to the standard setting of $\mathcal{H}$. They are explained in Section 2.1.3.3.

In general, the numbers in the list 'Sequence' of $\mathcal{H}$ follow the order of the numbers in the group $\mathcal{G}$, *i.e.* they rise monotonically. Sometimes this sequence is modified because those entries which have the same additional translations are joined together, see, *e.g.* the maximal k-subgroups of $Fm\overline{3}m$ with 'Loss of centring translations'. In addition, in a class of conjugate subgroups, the monotonically rising order may be obeyed only for the first member of the conjugacy class. The order of the other members is then determined by the conjugation of the first member. (In *IT* A the monotonically rising order of the numbers is kept in all conjugate subgroups.)

Example 2.1.3.2.1

$\mathcal{G} = Pm\overline{3}m$, No. 221, tetragonal t-subgroups
I Maximal *translationengleiche* subgroups

$$\left\{\begin{array}{ll} [3]\ P4/m12/m\ (123,\ P4/mmm) & 1;\ 2;\ 3;\ 4;\ 13;\ 14;\ 15;\ 16;\ \ldots \\ [3]\ P4/m12/m\ (123,\ P4/mmm) & 1;\ 4;\ 2;\ 3;\ 18;\ 19;\ 17;\ 20;\ \ldots \\ [3]\ P4/m12/m\ (123,\ P4/mmm) & 1;\ 3;\ 4;\ 2;\ 22;\ 24;\ 23;\ 21;\ \ldots \end{array}\right.$$

Comments:
If $\boldsymbol{W}_1, \boldsymbol{W}_2, \boldsymbol{W}_3, \ldots$ is the order of the first sequence, then the second sequence follows the order $\boldsymbol{C}^{-1}\boldsymbol{W}_1\boldsymbol{C}$, $\boldsymbol{C}^{-1}\boldsymbol{W}_2\boldsymbol{C}$, $\boldsymbol{C}^{-1}\boldsymbol{W}_3\boldsymbol{C}, \ldots$. Here the $\boldsymbol{C}$ means a threefold rotation and is the conjugating element; for the second subgroup $\boldsymbol{C} = (9)\ y, z, x$ of the general position of $Pm\overline{3}m$; for the third subgroup $\boldsymbol{C} = (5)\ z, x, y$. In this example the columns $\boldsymbol{w}$ of the symmetry operations (and thus of the conjugating elements) are the zero columns $\boldsymbol{o}$ and could be omitted.

The description of the subgroups can be explained by the following four examples.

Example 2.1.3.2.2

$\mathcal{G} = C1m1$, No. 8, UNIQUE AXIS b
I Maximal *translationengleiche* subgroups
[2] $C1$ (1, $P1$) 1+
Comments:
HMS1: $C1$ is not a conventional HM symbol. Therefore, the conventional symbol $P1$ is added as HMS2 after the space-group number 1 of $\mathcal{H}$.
sequence: '1+' means x, y, z; $x + \frac{1}{2}, y + \frac{1}{2}, z$.

Example 2.1.3.2.3

$\mathcal{G} = Fdd2$, No. 43
I Maximal *translationengleiche* subgroups
...
[2] $F112$ (5, $A112$) (1; 2)+
Comments:
HMS1: $F112$ is not a conventional HM symbol; therefore, the conventional symbol $A112$ is added to the space-group No. 5 as HMS2. The setting unique axis c is inherited from $\mathcal{G}$.
sequence: (1, 2)+ means:

$$\begin{array}{llll} x, y, z; & x, y+\frac{1}{2}, z+\frac{1}{2}; & x+\frac{1}{2}, y, z+\frac{1}{2}; & x+\frac{1}{2}, y+\frac{1}{2}, z; \\ \bar{x}, \bar{y}, z; & \bar{x}, \bar{y}+\frac{1}{2}, z+\frac{1}{2}; & \bar{x}+\frac{1}{2}, \bar{y}, z+\frac{1}{2}; & \bar{x}+\frac{1}{2}, \bar{y}+\frac{1}{2}, z; \end{array}$$

Example 2.1.3.2.4

$\mathcal{G} = P4_2/nmc = P4_2/n2_1/m2/c$, No. 137, ORIGIN CHOICE 2
I Maximal *translationengleiche* subgroups
...
[2] $P2/n\ 2_1/m\ 1$ (59, $Pmmn$) 1; 2; 5; 6; 9; 10; 13; 14

references