

3. ADVANCED TOPICS ON SPACE-GROUP SYMMETRY

Examples

From the list of maximal subgroups of the representative magnetic group of the type $Pb'a'm$ is the subgroup listed as

$$Pb'a'2 \quad 2 \quad (0, 0, 0; \mathbf{a}, \mathbf{b}, \mathbf{c}) \quad \{1|0\} \quad \{2_{001}|0\} \\ \{m_{010}|\frac{1}{2}, \frac{1}{2}, 0\}' \quad \{m_{100}|\frac{1}{2}, \frac{1}{2}, 0\}'$$

The first column gives the magnetic group type symbol of the subgroup. The second column gives the subgroup index of this subgroup as a subgroup of the representative group of type $Pb'a'm$. In the third column, the symbol $(O + \mathbf{p}; \mathbf{a}', \mathbf{b}', \mathbf{c}')$ gives the origin ' $O + \mathbf{p}$ ' and basis vectors \mathbf{a}' , \mathbf{b}' , \mathbf{c}' of the conventional unit cell of the non-primed subgroup, where \mathbf{p} , a translation of the origin of the coordinate system of the representative group $Pb'a'm$, and the conventional unit cell are such that the coset representatives listed are transformed into the standard cosets of the representative group of the subgroup type $Pb'a'2$. In this case, since the listed coset representatives are the standard cosets of the representative group of type $Pb'a'2$, no translation of origin is required, and consequently $O + \mathbf{p} = 0, 0, 0$. The conventional unit cell of the non-primed subgroup of the subgroup $Pb'a'2$ is the same as that of representative group of the type $Pb'a'2$ and consequently one finds $\mathbf{a}' = \mathbf{a}$, $\mathbf{b}' = \mathbf{b}$, $\mathbf{c}' = \mathbf{c}$.

That the listed coset representatives of the subgroup are the same as those of the representative group of that subgroup type is not always the case:

Example

A subgroup of type $P2/m$ of the representative group $Pb'a'm$ is listed as

$$P2/m \quad 2 \quad (0, 0, 0; \mathbf{b}, \mathbf{c}, \mathbf{a}) \quad \{1|0\} \quad \{2_{001}|0\} \quad \{\bar{1}|0\} \quad \{m_{001}|0\}$$

The standard set of coset representatives of the representative group $P2/m$ are

$$\{1|0\} \quad \{\bar{1}|0\} \quad \{2_{010}|0\} \quad \{m_{010}|0\}.$$

A change in setting to have the coset representatives of the subgroup be identical with the coset representatives of the representative group $P2/m$ is represented in the symbol $(0, 0, 0; \mathbf{b}, \mathbf{c}, \mathbf{a})$, *i.e.* changing the setting from $\mathbf{a}, \mathbf{b}, \mathbf{c}$ to $\mathbf{b}, \mathbf{c}, \mathbf{a}$.

Other cases may require a simultaneous change to both the origin and the setting of the conventional unit cell of the non-primed subgroup:

Example

A third subgroup of the representative group $Pb'a'm$ is the equi-class subgroup of the same type $Pb'a'm$:

$$Pb'a'm \quad 2 \quad (0, 0, \frac{1}{2}; \mathbf{a}, \mathbf{b}, 2\mathbf{c}) \quad \{1|0\} \quad \{2_{100}|\frac{1}{2}, \frac{1}{2}, 1\}' \\ \{2_{010}|\frac{1}{2}, \frac{1}{2}, 1\}' \quad \{2_{001}|0\} \\ \{\bar{1}|0, 0, 1\} \quad \{m_{100}|\frac{1}{2}, \frac{1}{2}, 0\}' \\ \{m_{010}|\frac{1}{2}, \frac{1}{2}, 0\}' \quad \{m_{001}|0, 0, 1\}$$

The listed coset representatives of this subgroup are not the same as the coset representatives of the representative group $Pb'a'm$, *i.e.* where the z component of the non-primitive translation associated with all coset representatives is zero. To have these listed coset representatives become identical with the coset representatives of the standard representative group of $Pb'a'm$, one must change the origin of the coordinate system. This information is provided in the symbol $(0, 0, \frac{1}{2}; \mathbf{a}, \mathbf{b}, 2\mathbf{c})$ where $O + \mathbf{p} = 0, 0, \frac{1}{2}$ denotes the translation under

which all the non-zero z components of the coset representatives are transformed to zero. Note also that the P in the subgroup symbol denotes a non-primed translational subgroup which is determined by $\mathbf{a}' = \mathbf{a}$, $\mathbf{b}' = \mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$, *i.e.* P denotes the translational group generated by the translations $\{1|1, 0, 0\}$, $\{1|0, 1, 0\}$ and $\{1|0, 0, 2\}$.

In the tabulations of the maximal subgroups of groups of the type $\mathcal{F}1'$ not all maximal subgroups are explicitly listed. The maximal subgroup \mathcal{F} of $\mathcal{F}1'$ is not listed. If \mathcal{G} is a maximal subgroup of \mathcal{F} , then $\mathcal{G}1'$ is a maximal subgroup of $\mathcal{F}1'$ and is also not explicitly listed. All maximal subgroups \mathcal{G} of \mathcal{F} are listed under \mathcal{F} , and consequently, all maximal subgroups $\mathcal{G}1'$ of $\mathcal{F}1'$ are then found from the list of all maximal subgroups \mathcal{G} of \mathcal{F} by multiplying each by $1'$. For each listed maximal subgroup, its non-primed subgroup type is explicitly given. For example, a listed subgroup of $Pma21'$ is

$$Pma'2' \quad Pm \quad 2 \quad (0, 0, 0; \mathbf{a}, \mathbf{b}, \mathbf{c}) \quad \{1|0\} \quad \{2_{001}|0\}' \\ \{m_{010}|\frac{1}{2}, 0, 0\}' \quad \{m_{100}|\frac{1}{2}, 0, 0\}$$

where the non-primed subgroup type Pm of $Pma'2'$ is given in the second column.

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