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rotation of the three axes which is not in the normalizer of $\mathcal{H}$ (or $\mathcal{G}$).

The number of supergroups of a space group $\mathcal{H}$ of a finite index is not always finite. This is the case of a space group $\mathcal{H}$ whose normalizer $\mathcal{N}(\mathcal{H})$ contains continuous translations in one, two or three independent directions (see *IT* A, Part 15). As typical examples one can consider the infinitely many centrosymmetric supergroups of the polar groups: there are no restrictions on the location of the additional inversion centre on the polar axis. For such group–supergroup pairs there could be up to three parameters *r*, *s* and *t* in the origin-shift column of the transformation matrix and in the translational part of the coset representatives. The parameters can have any value and each value corresponds to a different supergroup of the same space-group type.

1.7.3.2.2. The program CELLSUPER

The program *CELLSUPER* is an application similar to *CELLSUB* (*cf.* Section 1.7.3.1.4): in this case, the search is for the space-group types of supergroups $\mathcal{G}_s$ of $\mathcal{H}$ of a given maximum lattice index $[(i_L)_{\max}]$. The algorithm is similar to that of *CELLSUB*: using the data for the index and space-group types of minimal supergroups, the program constructs a tree of minimal supergroups starting from $\mathcal{H}$ and imposing the condition $[i_L] \le [(i_L)_{\max}]$. The input data of *CELLSUPER* coincide with those of *CELLSUB* with the only difference being that they are referred to the low-symmetry group $\mathcal{H}$. The output data include:

(i) The space-group types of the supergroups $\mathcal{G}_s$ of $\mathcal{H}$ with the corresponding indices $[i]$, $[i_P]$ and $[i_L]$. The supergroups are classified into *t*-supergroups, *k*-supergroups and *general* supergroups.

(ii) A link to the *SUPERGROUPS* module (*cf.* Section 1.7.3.2.1) enables the calculation of all different supergroups $(\mathcal{G}_s)_r$ of $\mathcal{H}$ of the space-group type $\mathcal{G}_s$ and index $[i]$. Each supergroup $(\mathcal{G}_s)_r$ is specified by the corresponding transformation matrix relating the conventional bases of the supergroup and the group, and the representatives of the coset decomposition $(\mathcal{G}_s)_r : \mathcal{H}$.

1.7.3.2.3. The program COMMONSUPER

The program *COMMONSUPER* calculates the space-group types of common supergroups $\mathcal{G}$ of two space groups $\mathcal{H}_1$ and $\mathcal{H}_2$ for a given maximal lattice index $[(i_L)_{\max}]$. The procedure used is analogous to the one implemented in the program *COMMONSUBS* (*cf.* Section 1.7.3.1.5). The two sets of supergroups of $\mathcal{H}_1$ and of $\mathcal{H}_2$ are determined by the program *CELLSUPER*. The intersection of the sets of supergroups gives the set of the space-group types of the common supergroups $\{\mathcal{G}\}$ of $\mathcal{H}_1$ and $\mathcal{H}_2$ with $[i_L] \le [(i_L)_{\max}]$. A relation between the indices $[i_1] = |\mathcal{G}|/|\mathcal{H}_1|$ and $[i_2] = |\mathcal{G}|/|\mathcal{H}_2|$ is obtained by imposing the structural requirement of equal numbers of formula units in the (primitive) unit cell of the common supergroup $\mathcal{G}$ obtained from the numbers of the formula units Z_1 and Z_2 of $\mathcal{H}_1$ and $\mathcal{H}_2$:

$$[i_2] = [i_1] \cdot \frac{Z_2}{Z_1} \cdot \frac{|\mathcal{P}_{\mathcal{H}_1}|}{|\mathcal{P}_{\mathcal{H}_2}|}. \qquad (1.7.3.2)$$

The program *COMMONSUPER* selects and lists those supergroups of the set $\{\mathcal{G}\}$ whose indices $[i_1] = |\mathcal{G}|/|\mathcal{H}_1|$ and $[i_2] = |\mathcal{G}|/|\mathcal{H}_2|$ satisfy the above condition.

The input data for *COMMONSUPER* include the specification of $\mathcal{H}_1$ and $\mathcal{H}_2$, the numbers of formula units per conventional unit cell, and the maximum lattice index $[(i_L)_{\max}]$. The output data of *COMMONSUPER* are:

(i) The space-group types of the common supergroups $\mathcal{G}$ of $\mathcal{H}_1$ and $\mathcal{H}_2$ with the indices $[i_1]$ and $[i_2]$, $[(i_L)_1]$ and $[(i_L)_2]$, and $[(i_P)_1]$ and $[(i_P)_2]$. Optional links to the programs *POINT* and *GENPOS* give access to data for the point group $\mathcal{P}_{\mathcal{G}}$ and the general positions of the supergroup $\mathcal{G}$.

(ii) A link to the *SUPERGROUPS* module (see Section 1.7.3.2.1) enables the calculation of all different supergroups $\mathcal{G}_r$ of $\mathcal{H}_1$ and $\mathcal{H}_2$ of a space-group type $\mathcal{G}$ and indices $[i_1]$ and $[i_2]$. Each supergroup $\mathcal{G}_r$ is specified by the corresponding transformation matrix relating the conventional bases of the supergroup and the group, and the representatives of the coset decomposition of $\mathcal{G}_r$ relative to $\mathcal{H}_1$ or $\mathcal{H}_2$.

Example 1.7.3.2.3

The program *COMMONSUPER* is useful in the search for structural relationships between structures whose symmetry groups $\mathcal{H}_1$ and $\mathcal{H}_2$ are not group–subgroup related. The derivation of the two structures as different distortions from a basic structure is a clear manifestation of such relationships. The symmetry group of the basic structure is a common supergroup of $\mathcal{H}_1$ and $\mathcal{H}_2$. Consider the ternary intermetallic compound CeAuGe. At 8.7 GPa a first-order phase transition is observed from a hexagonal arrangement (space group $P6_3mc$, No. 186, two formula units per unit cell, $Z_1 = 2$) into an orthorhombic high-pressure modification of symmetry *Pnma*, No. 62, $Z_2 = 4$ (Brouskov *et al.*, 2005). There is no group–subgroup relation between the symmetry groups of the high- and low-pressure structures. For $[(i_L)_{\max}] = 4$ the program finds two common supergroups of $\mathcal{H}_1 = P6_3mc$, $Z_1 = 2$ and $\mathcal{H}_2 = Pnma$, $Z_2 = 4$: (i) the group $P6_3/mmc$ with $[i_1] = 2$ and $[i_2] = 6$, and (ii) $P6/mmm$, with $[i_1] = 4$ and $[i_2] = 12$. The common basic structure of the AlB_2 type, proposed by Brouskov *et al.* (2005), corresponds to the common supergroup $P6/mmm$ found by *COMMONSUPER*.

1.7.4. Relations of Wyckoff positions for a group–subgroup pair of space groups

Consider two group–subgroup-related space groups $\mathcal{G} > \mathcal{H}$. Atoms that are symmetrically equivalent under $\mathcal{G}$, *i.e.* belong to the same orbit of $\mathcal{G}$, may become non-equivalent under $\mathcal{H}$, (*i.e.* the orbit splits) and/or their site symmetries may be reduced. The orbit relations induced by the symmetry reduction are the same for all orbits belonging to a Wyckoff position, so one can speak of Wyckoff-position relations or splitting of Wyckoff positions. Theoretical aspects of the relations of the Wyckoff positions for a group–subgroup pair of space groups $\mathcal{G} > \mathcal{H}$ have been treated in detail by Wondratschek (1993) (see also Section 1.5.3). A compilation of the Wyckoff-position splittings for all space groups and all their maximal subgroups is published as Part 3 of this volume. However, for certain applications it is easier to have the appropriate computer tools for the calculations of the Wyckoff-position splittings for $\mathcal{G} > \mathcal{H}$: for example, when $\mathcal{H}$ is not a maximal subgroup of $\mathcal{G}$, or when the space groups $\mathcal{G} > \mathcal{H}$ are related by transformation matrices different from those listed in the tables of Part 3. The program *WYCKSPLIT* (Kroumova, Perez-Mato & Aroyo, 1998) calculates the Wyckoff-position splittings for any group–subgroup pair. In addition, the program

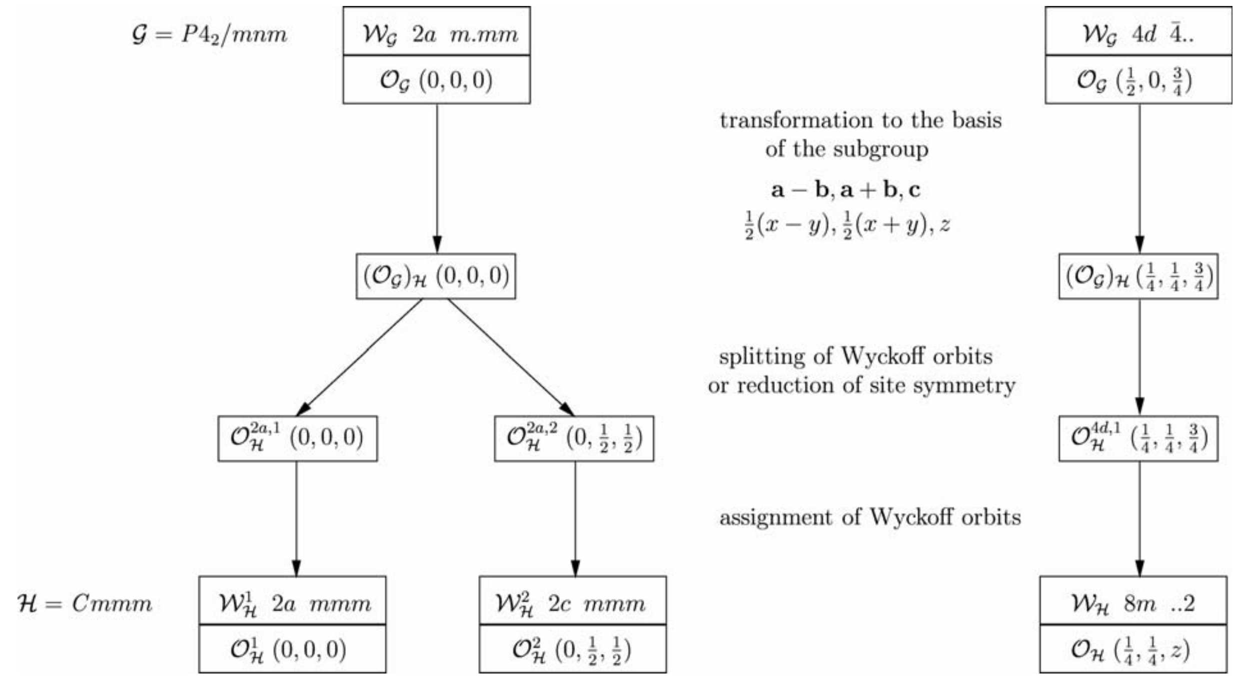

Fig. 1.7.4.1. Sequence of calculations of *WYCKSPLIT* for the splitting of the Wyckoff positions 2*a* *m.mm* (0, 0, 0) and 4*d* $\bar{4}$.. $(\frac{1}{2}, 0, \frac{3}{4})$ of $P4_2/mnm$, No. 136, with respect to its subgroup *Cmmm*, No. 65, of index 2. $(\mathcal{O}_\mathcal{G})_\mathcal{H}$ are the orbits of $P4_2/mnm$ in the basis of *Cmmm*.

provides further information on Wyckoff-position splittings that is not listed in Part 3, namely the relations between the representatives of the orbit of $\mathcal{G}$ and the corresponding representatives of the suborbits of $\mathcal{H}$.

1.7.4.1. *The program WYCKSPLIT*

To simplify the notation, we assume in the following that the group $\mathcal{G}$, its Wyckoff-position representatives and the points of the orbits are referred to the basis of the subgroup $\mathcal{H}$.

(1) *Splitting of the general position*. Consider the group–subgroup chain of space groups $\mathcal{G} > \mathcal{H}$ of an index [*i*]. The general-position orbits $\mathcal{O}_\mathcal{G}(X_0)$ have unique splitting schemes: they are split into [*i*] suborbits $\mathcal{O}_\mathcal{H}(X_{0,j})$ of the general position of the subgroup, *i.e.* they all are of the same multiplicity:

$$\mathcal{O}_\mathcal{G}(X_0) = \mathcal{O}_\mathcal{H}(X_{0,1}) \cup \ldots \cup \mathcal{O}_\mathcal{H}(X_{0,i}). \qquad (1.7.4.1)$$

This property is a direct corollary of the relation between the index [*i*] and the so-called reduction factors of the site-symmetry groups $\mathcal{S}_\mathcal{G}(X)$ and $\mathcal{S}_\mathcal{H}(X)$ of a point X in $\mathcal{G}$ and $\mathcal{H}$ (Wondratschek, 1993; see also Section 1.5.3).

The determination of the splitting of the general-position orbit $\mathcal{O}_\mathcal{G}(X_0)$ is then reduced to the selection of the [*i*] points $(X_{0,j})$ belonging to the [*i*] independent suborbits $\mathcal{O}_\mathcal{H}(X_{0,j})$ of $\mathcal{H}$, equation (1.7.4.1). Owing to the one-to-one mapping between the general-position points of $\mathcal{O}_\mathcal{G}(X_0)$ and the elements g of $\mathcal{G}$, the right cosets $\mathcal{H}g_j$ of the decomposition of $\mathcal{G}$ with respect to $\mathcal{H}$ (*cf.* Definition 1.2.4.2.1) correspond to the suborbits $\mathcal{O}_\mathcal{H}(X_{0,j})$. In this way, the representatives of these cosets can be chosen as the [*i*] points $X_{0,j}$ in the decomposition of $\mathcal{O}_\mathcal{G}(X_0)$.

(2) *Splitting of a special position*. The calculation of the splitting of a special Wyckoff position $\mathcal{W}_\mathcal{G}$ involves the following steps:

   (i) the determination of the suborbits $\mathcal{O}_\mathcal{H}(X_j)$ into which the special-Wyckoff-position orbit $\mathcal{O}_\mathcal{G}(X)$ has split;

   (ii) the assignment of the orbits $\mathcal{O}_\mathcal{H}(X_j)$ to the Wyckoff positions $\mathcal{W}_\mathcal{H}^l$ of $\mathcal{H}$;

   (iii) the determination of the correspondence between the points X_j^m of the suborbits $\mathcal{O}_\mathcal{H}(X_j)$ and the representatives of $\mathcal{W}_\mathcal{H}^l$.

The direct determination of the suborbits $\mathcal{O}_\mathcal{H}(X_j)$ is not an easy task. The restrictions on the site-symmetry groups $\mathcal{S}_\mathcal{H}(X_j)$ which follow from the reduction-factor lemma (*cf.* Section 1.5.3) are helpful but in many cases not sufficient for the determination of the suborbits. The solution used in our approach is based on the general-position decomposition, equation (1.7.4.1). It is important to note that each of the suborbits of the general position gives exactly one suborbit $\mathcal{O}_\mathcal{H}(X_j)$ when the variable parameters of $\mathcal{O}_\mathcal{H}(X_{0,j})$ are substituted by the corresponding parameters (fixed or variable) of the special position. The assignment of the suborbits to the Wyckoff positions of $\mathcal{H}$ is done by comparing the multiplicities of the orbits, the number of the variable parameters [the number of the variable parameters of $\mathcal{W}_\mathcal{H}^l$ is equal to or greater than that of $\mathcal{O}_\mathcal{H}(X_j)$] and the values of the fixed parameters. If there is more than one Wyckoff position

Table 1.7.4.1. *Wyckoff positions of Cmmm (No. 65) with multiplicities 2 and 8*

Each Wyckoff position is specified by its multiplicity and Wyckoff letter, site symmetry and a coordinate triplet of a representative element.

Wyckoff multiplicity and letter	Site symmetry	Representative element
2*d*	*mmm*	$(0, 0, \frac{1}{2})$
2*c*	*mmm*	$(\frac{1}{2}, 0, \frac{1}{2})$
2*b*	*mmm*	$(\frac{1}{2}, 0, 0)$
2*a*	*mmm*	(0, 0, 0)
8*q*	..*m*	$(x, y, \frac{1}{2})$
8*p*	..*m*	$(x, y, 0)$
8*o*	.*m*.	$(x, 0, z)$
8*n*	*m*..	$(0, y, z)$
8*m*	..2	$(\frac{1}{4}, \frac{1}{4}, z)$

of $\mathcal{H}$ satisfying these conditions, then the assignment is done by a direct comparison of the points of the suborbit $\mathcal{O}_{\mathcal{H}}(X_j)$ with those of a special $\mathcal{W}^l_{\mathcal{H}}$ orbit obtained by substitution of the variable parameters by arbitrary numbers. The determination of the explicit correspondences between the points of $\mathcal{O}_{\mathcal{H}}(X_j)$ and the representatives of $\mathcal{W}^l_{\mathcal{H}}$ is done by comparing the values of the fixed parameters and the variable-parameter relations in both sets.

The program *WYCKSPLIT* calculates the splitting of the Wyckoff positions for a group–subgroup pair $\mathcal{G} > \mathcal{H}$ given the corresponding transformation relating the coordinate systems of $\mathcal{G}$ and $\mathcal{H}$.

Input to *WYCKSPLIT*:

The program needs as input the following information:

(i) The specification of the space-group types $\mathcal{G}$ and $\mathcal{H}$ by their *IT* A numbers.

(ii) The transformation matrix–column pair $(\boldsymbol{P}, \boldsymbol{p})$ that relates the basis of $\mathcal{G}$ to that of $\mathcal{H}$. The user can input a specific transformation or follow a link to the *IT* A1 database for the maximal subgroups of $\mathcal{G}$. In the case of a non-maximal subgroup, the program *SUBGROUPGRAPH* provides the transformation matrix (or matrices) for a specified index of $\mathcal{H}$ in $\mathcal{G}$. The transformations are checked for consistency with the default settings of $\mathcal{G}$ and $\mathcal{H}$ used by the program.

The Wyckoff positions $\mathcal{W}_{\mathcal{G}}$ to be split can be selected from a list. In addition, it is possible to calculate the splitting of any orbit $O_{\mathcal{G}}(X)$ specified by the coordinate triplet of one of its points.

Output of *WYCKSPLIT*:

(i) Splittings of the selected Wyckoff positions $\mathcal{W}_{\mathcal{G}}$ into Wyckoff positions $\mathcal{W}^l_{\mathcal{H}}$ of the subgroup, specified by their multiplicities and Wyckoff letters.

(ii) The correspondence between the representatives of the Wyckoff position and the representatives of its suborbits is presented in a table where the coordinate triplets of the representatives of $\mathcal{W}_{\mathcal{G}}$ are referred to the bases of the group and of the subgroup.

WYCKSPLIT can treat group or subgroup data in unconventional settings if the transformation matrices to the corresponding conventional settings are given.

Example 1.7.4.1.1

To illustrate the calculation of the Wyckoff-position splitting we consider the group–subgroup pair $P4_2/mnm$ (No. 136) > *Cmmm* (No. 65) of index 2, see Fig. 1.7.4.1. The relation between the conventional bases $(\mathbf{a}, \mathbf{b}, \mathbf{c})$ of the group and of the subgroup $(\mathbf{a}', \mathbf{b}', \mathbf{c}')$ is retrieved by the program *MAXSUB* and is given by $\mathbf{a}' = \mathbf{a} - \mathbf{b}$, $\mathbf{b}' = \mathbf{a} + \mathbf{b}$, $\mathbf{c}' = \mathbf{c}$. The general position of $P4_2/mnm$ splits into two suborbits of the general position of *Cmmm*:

$$16k\ 1\ (x, y, z) \rightarrow 16r\ 1\ (x_1, y_1, z_1) \cup 16r\ 1\ (x_2, y_2, z_2).$$

This splitting is directly related to the coset decomposition of $P4_2/mnm$ with respect to *Cmmm*. As coset representatives, *i.e.* as points which determine the splitting of the general position, one can choose $X_{0,1} = (x_1, y_1, z_1)$ and $X_{0,2} = (x_2, y_2, z_2) = (y, x + \frac{1}{2}, z + \frac{1}{2}))$ (referred to the basis of the subgroup).

The splitting of any special Wyckoff position is obtained from the splitting of the general position. The consecutive steps of the splittings of the special positions $4d\ \bar{4}..\ (\frac{1}{2}, 0, \frac{3}{4})$ and $2a\ m.mm\ (0, 0, 0)$ are shown in Fig. 1.7.4.1. First it is necessary to transform the representatives of $\mathcal{W}_{\mathcal{G}}$ to the basis of $\mathcal{H}$, which gives the orbits $(\mathcal{O}_{\mathcal{G}})_{\mathcal{H}}(0, 0, 0)$ and $(\mathcal{O}_{\mathcal{G}})_{\mathcal{H}}(\frac{1}{4}, \frac{1}{4}, \frac{3}{4})$. The substitution of the values $x = 0$, $y = 0$, $z = 0$ in the coordinate triplets of the decomposed general position of $\mathcal{G}$ (*cf.* the corresponding output of *WYCKSPLIT*) gives two suborbits of multiplicity 2 for the $2a$ position: $\mathcal{O}^{2a,1}_{\mathcal{H}}(0, 0, 0)$ and $\mathcal{O}^{2a,2}_{\mathcal{H}}(0, \frac{1}{2}, \frac{1}{2})$. The assignment of the suborbits $\mathcal{O}^{2a,j}_{\mathcal{H}}$ to the Wyckoff positions of $\mathcal{H}$ (*cf.* Table 1.7.4.1) is straightforward. Summarizing: the Wyckoff position $2a\ m.mm\ (0, 0, 0)$ splits into two independent positions of *Cmmm* with no site-symmetry reduction:

$$2a\ m.mm\ (0, 0, 0) \rightarrow 2a\ mmm\ (0, 0, 0) \cup 2c\ mmm\ (0, \tfrac{1}{2}, \tfrac{1}{2}).$$

No splitting occurs for the case of the special $4d$ position orbit: the result is one orbit of multiplicity 8, $\mathcal{O}^{4d,1}_{\mathcal{H}}(\frac{1}{4}, \frac{1}{4}, \frac{3}{4})$. The assignment of $\mathcal{O}^{4d,1}_{\mathcal{H}}(\frac{1}{4}, \frac{1}{4}, \frac{3}{4})$ is also obvious: there are five Wyckoff positions of *Cmmm* of multiplicity 8 but four of them are discarded as they have fixed parameters 0 or $\frac{1}{2}$ (Table 1.7.4.1). The orbit $\mathcal{O}^{4d,1}_{\mathcal{H}}$ belongs to the Wyckoff position $8m\ ..2\ (\frac{1}{4}, \frac{1}{4}, z)$.

As expected, the sum of the site-symmetry reduction factors equals the index of *Cmmm* in $P4_2/mnm$ for both cases (*cf.* Section 1.5.3). The loss of the fourfold inversion axis results in the appearance of an additional degree of freedom corresponding to the variable parameter of $8m\ ..2\ (\frac{1}{4}, \frac{1}{4}, z)$.

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