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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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