subgroup is easily identified either as a *klassengleiche* or a *translationengleiche* subgroup.

1.3.4. Description of the checks

In order to avoid new errors being introduced in the typesetting process after the data have been checked and corrected, we carried out the computer checks directly on the LaTeX 2_ε sources used for the production of this volume. The tables have been typeset with specially designed LaTeX 2_ε macros, the primary purpose of which was to guarantee a homogeneous layout throughout the book. As a side effect, it was relatively easy to write a *GAP* program which parses the LaTeX 2_ε sources, recognizes the macros, extracts the data (the arguments of the macros), brings the data into a form suitable for further processing with routines from the *Cryst* package and finally performs the various checks. In this way, the checks could be done fully automatically, and could be repeated after every modification of the tabulated data.

In the following, we describe the checks that have been carried out. We first applied a number of tests individually to each of the tabulated maximal subgroups of low index: whether it is a subgroup, whether the index given is correct, whether the listed coordinate transformation maps the subgroup to the preferred setting of the given space-group type (and thus, whether the space-group type of the subgroup is correct) and whether the listed coordinate transformation maps the given generators of the subgroup to the standard generators of its space-group type, in the same order. Here, the preferred setting is the setting of the parent group, where applicable, and otherwise the preferred setting of the space-group type of the subgroup, if there is more than one setting in the tables.

In a second step, a complete set of maximal subgroups of low index (2, 3 or 4) is computed afresh with the routines from the *Cryst* package. These subgroups are then divided into conjugacy classes, and classified as *klassengleiche* or *translationengleiche* subgroups. This list is then compared with the tabulated list of maximal subgroups. It was verified that each maximal subgroup of a given index was listed exactly once, that the classification into conjugacy classes of subgroups was correct and that the subgroups were correctly identified as *klassengleiche* or as *translationengleiche* subgroups.

All the tests described above concern the maximal subgroups of low index. Unfortunately, similar automatic tests could not be performed on the series of isomorphic subgroups. The subgroups in these series contain variable parameters, and *Cryst* can only deal with fixed, concrete space groups without free parameters.

References

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