

1.6. RELATING CRYSTAL STRUCTURES BY GROUP-SUBGROUP RELATIONS

In addition, by experience we know that setting up trees of group-subgroup relations is susceptible to pitfalls. Some sources of errors are: not taking into account necessary origin shifts; wrong origin shifts; wrong basis and/or coordinate transformations; unnecessary basis transformations just for the sake of clinging on to standard space-group settings; lack of distinction between space groups and space-group types; lack of keeping track of the development of the atomic positions from group to subgroup; using different space-group or coordinate settings for like structures. If the group-subgroup relations are correct, but origin shifts or basis transformations have not been stated, this can cause subsequent errors and misunderstandings.

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