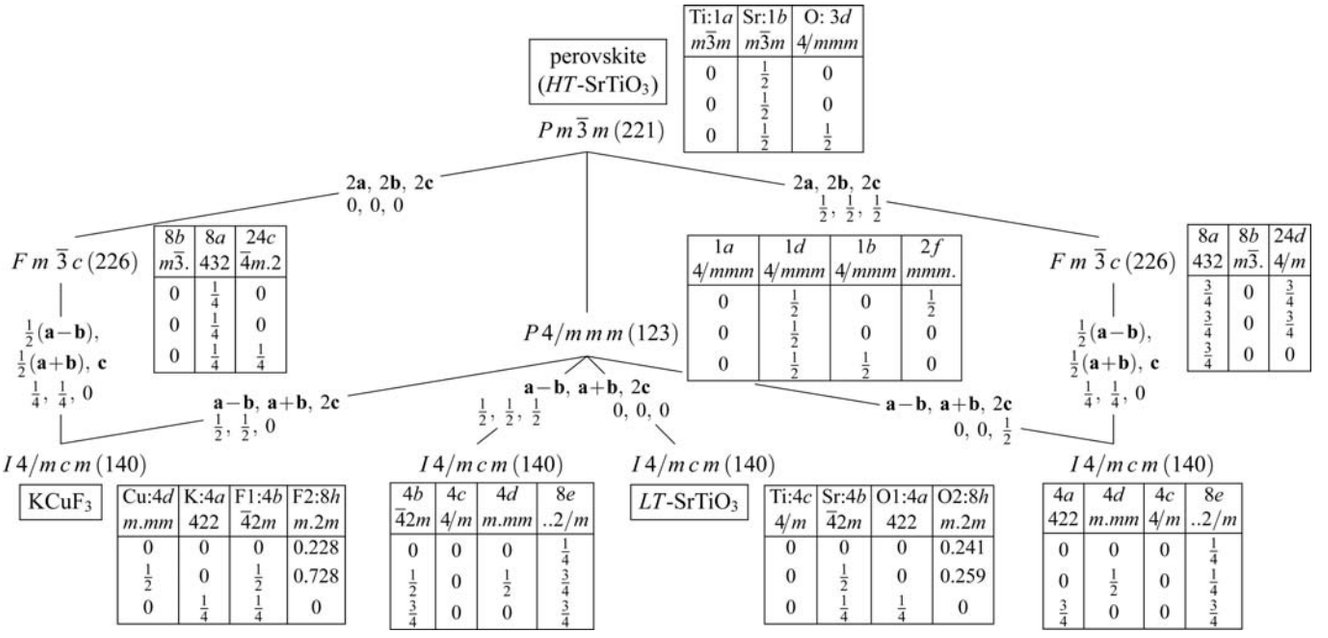

Fig. 2.1.8.4. Complete graph of the group–subgroup chains from perovskite, $Pm\bar{3}m$, here high-temperature $SrTiO_3$, to the four subgroups of type $I4/mcm$ with their tetragonal axes in the **c** direction. Two of them correspond to $KCuF_3$ and low-temperature $SrTiO_3$. The transformations and origin shifts given in the connecting lines specify the basis vectors and origins of the maximal subgroups in terms of the bases of the preceding space groups (Bärnighausen tree as explained in Section 1.6.3).

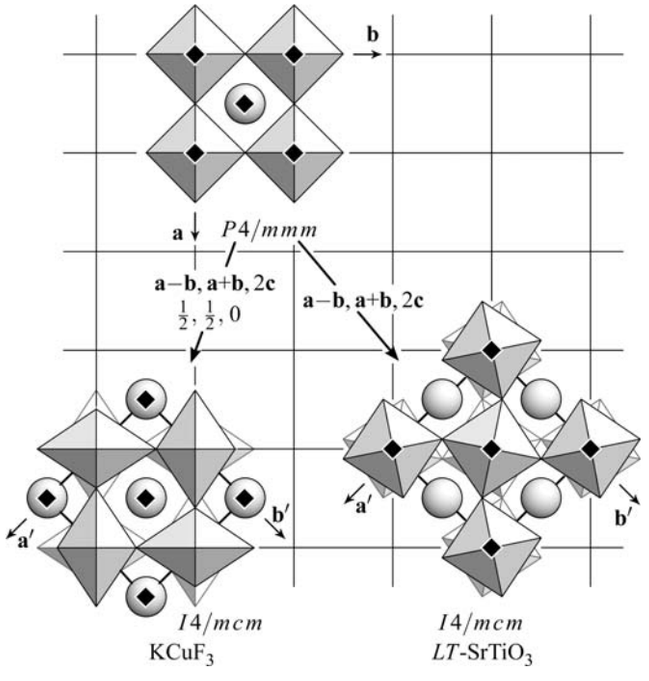

Fig. 2.1.8.5. Two different subgroups of $P4/mmm$, both of type $I4/mcm$, correspond to two kinds of distortions of the coordination octahedra of the perovskite structure. The difference is due to the origin shift by $\frac{1}{2}, \frac{1}{2}, 0$ on the left side, resulting in a different selection of the fourfold rotation axes that are retained in the subgroups.

symmetry of cubic perovskites. The other space groups are *t*-subgroups of $Pm\bar{3}m$. They would be taken if for some reason the site symmetries of the orbits would contradict the site symmetries of $Pm\bar{3}m$. Similarly, the true symmetry of these tetragonal perovskite derivatives would be $P4/mmm$ with the original (only tetragonally distorted) lattice and not $I4/mcm$.[9] For the two (empty) subgroups $I4/mcm$ a distorted variant of the perovskite structure does not exist. Other special positions or the general position of the original cubic space group have to be occupied if the space group $I4/mcm$ shall be realized. This example shows clearly the difference between the subgroup graphs of group theory and the Bärnighausen trees of crystal chemistry.

[9] The restriction to *t*-subgroups in the space-group tables of *Strukturbericht* 1 is probably a consequence of the fact that only these subgroups of space groups were known in 1931. No tetragonal perovskites are described in that volume. In the later volumes, *Strukturbericht* 2 *ff.*, the listing of the space-group tables has been discontinued.

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