decimal value indicates that the coordinate is not fixed by symmetry). Simultaneously, the site symmetry of the metal atom is reduced from 4/*mmm* to 4*mm* and the $z$ coordinate becomes independent. In fact, the W atom is shifted from $z = 0$ to $z = 0.066$, *i.e.* it is not situated in the centre of the octahedron of the surrounding O atoms. This shift is the cause of the symmetry reduction. There is no splitting of the Wyckoff positions in this step of symmetry reduction, but a decrease of the site symmetries of all atoms.

When cooled, at 1170 K *HT*-$WO_3$ is transformed to $\alpha$-$WO_3$. This involves mutual rotations of the coordination octahedra along **c** and requires another step of symmetry reduction. Again, the Wyckoff positions do not split in this step of symmetry reduction, but the site symmetries of all atoms are further decreased.

Upon further cooling, $WO_3$ undergoes several other phase transitions that involve additional distortions and, in each case, an additional symmetry reduction to another subgroup (not shown in Fig. 1.7.2.2). For more details see Müller (2013), Section 11.6, and references therein.

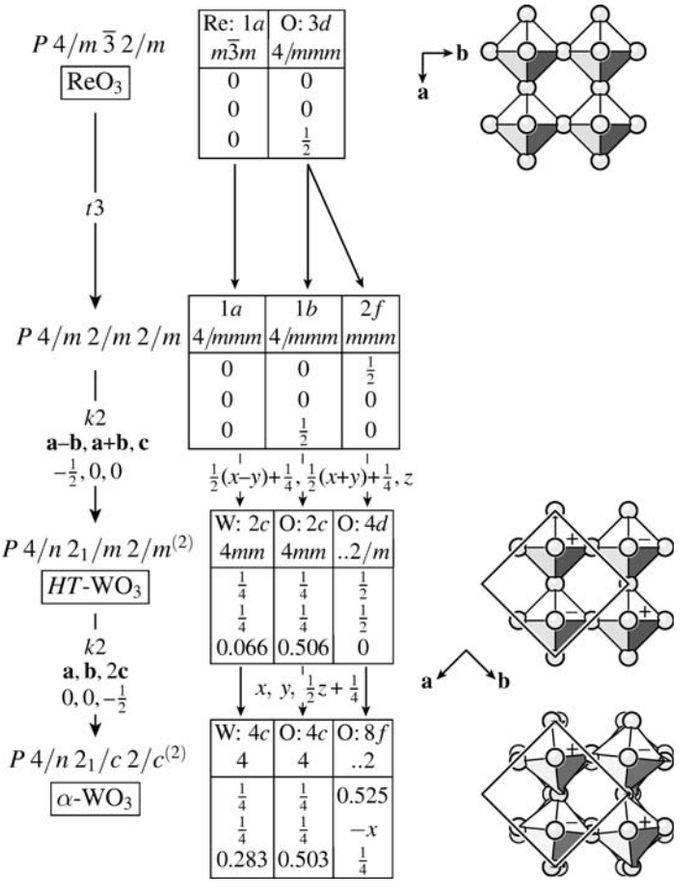


**Figure 1.7.2.2**
Group–subgroup relations (Bärnighausen tree) from the $ReO_3$ type to two polymorphic forms of $WO_3$. The superscript (2) after the space-group symbols states the origin choice. + and − in the images of high-temperature $WO_3$ and $\alpha$-$WO_3$ indicate the direction of the $z$ shifts of the W atoms from the octahedron centres. Structural data for $WO_3$ are taken from Locherer *et al.* (1999).

### 1.7.2.4. Domain structures

In the case of phase transitions and of topotactic reactions[3] that involve a symmetry reduction, the kind of group–subgroup relation determines how many kinds of domains and what domain states can be formed. If the lower-symmetry product results from a *translationengleiche* group–subgroup relation, twinned crystals are to be expected. A *klassengleiche* group–subgroup relation will cause antiphase domains. The number of different kinds of twin or antiphase domains corresponds to the index of the symmetry reduction. For example, the phase transition from *HT*-$WO_3$ to $\alpha$-$WO_3$ involves a *klassengleiche* group–subgroup relation of index 2 (*k*2 in Fig. 1.7.2.2); no twins will be formed, but two kinds of antiphase domains can be expected.

### 1.7.2.5. Presentation of the relations between the Wyckoff positions among group–subgroup-related space groups

Group–subgroup relations as outlined in the preceding sections can only be correct if all atomic positions of the hettotypes result directly from those of the aristotype.

Every group–subgroup relation between space groups entails specific relations between their Wyckoff positions. If the index of symmetry reduction is 2, a Wyckoff position either splits into two symmetry-independent positions that keep the site symmetry, or there is no splitting and the site symmetry is reduced. If the index is 3 or higher, a Wyckoff position either splits, or its site symmetry is reduced, or both happen. Given the relative settings and origin choices of a space group and its subgroup, there exist unique relations between their Wyckoff positions. Laws governing these relations are considered in Chapter 1.5 of the second edition of *IT* A1.

Volume A1, Part 3, *Relations between the Wyckoff positions*, contains tables for all space groups. For every one of them, all maximal subgroups are listed, including the corresponding coordinate transformations. For all Wyckoff positions of a space group the relations to the Wyckoff positions of the subgroups are given. This includes the infinitely many maximal isomorphic subgroups, for which general formulae are given. Isomorphic subgroups are a special kind of *klassengleiche* subgroup that belong to the same or the enantiomorphic space-group type, *i.e.* group and subgroup have the same or the enantiomorphic space-group symbol; the unit cell of the subgroup is increased by some integral factor, which is $p$, $p^2$ or $p^3$ ($p$ = prime number) in the case of maximal isomorphic subgroups.

[3] A topotactic reaction is a chemical reaction in the solid state where the orientation of the product crystal is determined by the orientation of the educt crystal.

## 1.7.3. Relationships between space groups and subperiodic groups

By D. B. Litvin and V. Kopský

The present volume in the series *International Tables for Crystallography* (Volume A: *Space-Group Symmetry*) treats one-, two- and three-dimensional space groups. Volume E in the series, *Subperiodic Groups* (2010), treats two- and three-dimensional subperiodic groups: frieze groups (groups in two-dimensional space with translations in a one-dimensional subspace), rod groups (groups in three-dimensional space with translations in a one-dimensional subspace) and layer groups (groups in three-dimensional space with translations in a two-dimensional subspace). In the same way in which three-dimensional space groups are used to classify the atomic structure of three-dimensional crystals, the subperiodic groups are used to classify the atomic structure of other crystalline structures, such as liquid crystals, domain interfaces, twins and thin films.