20.2-03 DECEITFUL TREES OF SUBGROUPS, RETURN TO THE HERMANN THEOREM.

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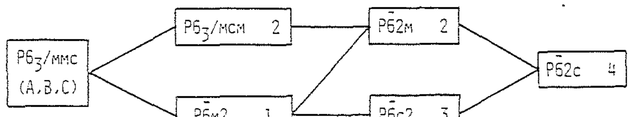
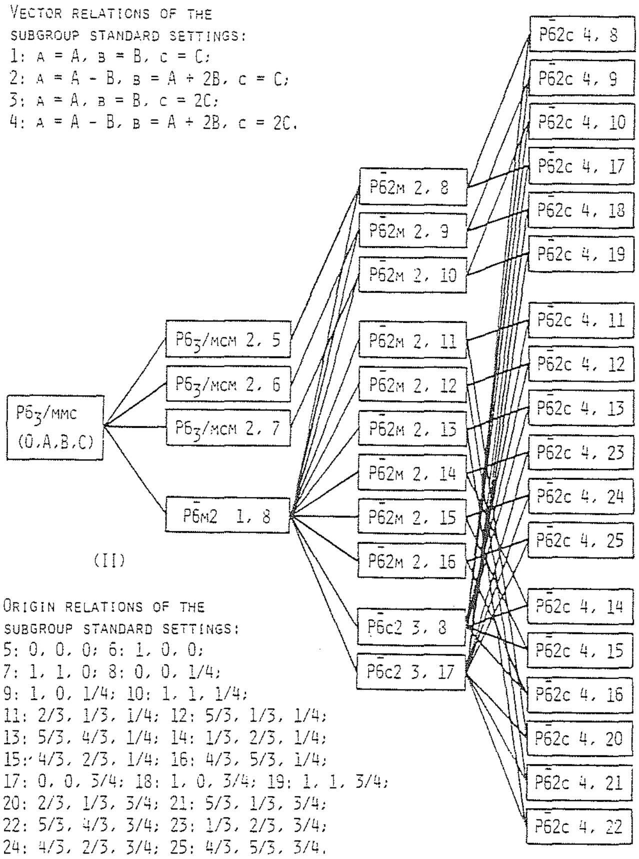
The most part of existing tables of maximal subgroups of space groups list only the type not the subgroups themselves in the case of "klassengleich" (k-) subgroups, while "translationengleich" (t-) subgroups are extensively listed. As a consequence, the subgroup trees which are obtained from these tables are often very condensed and risk to be false. For instance, let us consider the so-built tree (I) of maximal subgroups leading to the subgroup P$\bar{6}$2c (a = A - B, b = A + 2B, c = 2C) of the space group P6$_3$/mmc (A, B, C). The number of intermediate subgroups of this tree is 4. To go from P6$_3$/mmc to P$\bar{6}$2c there appears 3 possible ways: (1) P6$_3$/mmc—P6$_3$/mcm—P$\bar{6}$2m—P$\bar{6}$2c, (2) P6$_3$/mmc—P$\bar{6}$m2—P$\bar{6}$2m—P$\bar{6}$2c and (3) P6$_3$/mmc—P$\bar{6}$m2—P$\bar{6}$c2—P$\bar{6}$2c. In reality, this inference is not true. Indeed the authentic tree of subgroups is more complicated (II), there are 18 subgroups P$\bar{6}$2c (A - B, A + 2B, 2C) with non-congruent origins and 15 intermediate subgroups. The 18 subgroups P$\bar{6}$2c are divided into 3 conjugation classes. Indeed, to go to the 1st-class subgroups, the 3 types of way are possible. On the contrary, to go to the 2nd- and 3rd-class subgroups, only 2 types of way [(2), (3)] are possible. This fact is to be connected to the Hermann Theorem: "Each space subgroup g of a space group G is a k-subgroup of a given t-subgroup g° of G (g°: Hermann subgroup of g)". For example, the Hermann subgroup of any subgroup P$\bar{6}$2c (A - B, A + 2B, 2C) is the subgroup P$\bar{6}$m2 (A, B, C; 0, 0, 1/4). But the "reciprocal" statement of the Hermann Theorem is not true: each space subgroup is not necessarily a t-subgroup of a k-subgroup of G. For instance, only 3 subgroups P$\bar{6}$2m (A - B, A + 2B, C) are at the same time k-subgroups of a t-subgroup (P$\bar{6}$m2) and t-subgroups of a k-subgroup (P6$_3$/mcm) of P6$_3$/mmc. Let us notice that the type of way (1) is a k-t-k type of way; thus the 1st-class subgroups P$\bar{6}$2c are not t-subgroups of a k-subgroup of P6$_3$/mmc.



(I)



(II)

Vector relations of the subgroup standard settings:
1: a = A, b = B, c = C;
2: a = A - B, b = A + 2B, c = C;
3: a = A, b = B, c = 2C;
4: a = A - B, b = A + 2B, c = 2C.

Origin relations of the subgroup standard settings:
5: 0, 0, 0; 6: 1, 0, 0;
7: 1, 1, 0; 8: 0, 0, 1/4;
9: 1, 0, 1/4; 10: 1, 1, 1/4;
11: 2/3, 1/3, 1/4; 12: 5/3, 1/3, 1/4;
13: 5/3, 4/3, 1/4; 14: 1/3, 2/3, 1/4;
15: 4/3, 2/3, 1/4; 16: 4/3, 5/3, 1/4;
17: 0, 0, 3/4; 18: 1, 0, 3/4; 19: 1, 1, 3/4;
20: 2/3, 1/3, 3/4; 21: 5/3, 1/3, 3/4;
22: 5/3, 4/3, 3/4; 23: 1/3, 2/3, 3/4;
24: 4/3, 2/3, 3/4; 25: 4/3, 5/3, 3/4.

20.2-04 SUBGROUPS OF ORTHORHOMBIC AND TETRAGONAL SPACE GROUPS.

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In a previous paper (Acta Cryst. (1977) A33, 985-986) we have derived space subgroups of triclinic and monoclinic space groups. Tables of subgroups of orthorhombic and tetragonal space groups are now available. Here are given for example the subgroup settings (vectors a, b, c and co-ordinates X°, Y°, Z° of origin o) with reference to the setting (O, A, B, C) of supergroup P222$_1$ ($n_{ij} \in \mathbb{Z}$).

P1: $a = n_{11}A + n_{21}B + n_{31}C$; $b = n_{12}A + n_{22}B + n_{32}C$; $c = n_{13}A + n_{23}B + n_{33}C$; X°, Y°, Z° $\in \mathbb{R}$.

P112: 1/ $a = n_{11}A + n_{31}C$; $b = n_{12}A + n_{32}C$; $c = n_{23}B$; 2X° $\in \mathbb{Z}$; Y° $\in \mathbb{R}$; 4Z° odd.

2/ $a = n_{21}B + n_{31}C$; $b = n_{22}B + n_{31}C$; $c = n_{13}A$; X° $\in \mathbb{R}$; 2Y°, 2Z° $\in \mathbb{Z}$.

P112$_1$: 1/ $a = n_{11}A + n_{21}B$; $b = n_{12}A + n_{22}B$; $c = (2n_{33} + 1)C$; 2X°, 2Y° $\in \mathbb{Z}$; Z° $\in \mathbb{R}$.

2/ $a = n_{11}A + n_{31}C$; $b = n_{12}A + n_{32}C$; $c = 2n_{23}B$; 2X° $\in \mathbb{Z}$; Y° $\in \mathbb{R}$; 4Z° odd.

3/ $a = n_{21}B + n_{31}C$; $b = n_{22}B + n_{32}C$; $c = 2n_{13}A$; X° $\in \mathbb{R}$; 2Y°, 2Z° $\in \mathbb{Z}$.

B112: 1/ $a = 2n_{11}A + 2n_{31}C$; $b = n_{12}A + n_{32}C$; $c = 2n_{23}B$; 2X° $\in \mathbb{Z}$; Y° $\in \mathbb{R}$; 4Z° odd.

2/ $a = 2n_{21}B + 2n_{31}C$; $b = n_{22}B + n_{31}C$; $c = 2n_{13}A$; 2X°, 2Y° $\in \mathbb{Z}$; Z° $\in \mathbb{R}$.

P222$_1$: 1/ $a = n_{11}A$; $b = n_{22}B$; $c = (2n_{33} + 1)C$; 2X°, 2Y°, 2Z° $\in \mathbb{Z}$.

2/ $a = n_{21}B$; $b = n_{12}A$; $c = (2n_{33} + 1)C$; 2X°, 2Y° $\in \mathbb{Z}$; 4Z° odd.

P2$_1$2$_1$2: 1/ $a = (2n_{31} + 1)C$; $b = 2n_{12}A$; $c = n_{23}B$; 2X°, 2Y° $\in \mathbb{Z}$; 4Z° odd.

2/ $a = 2n_{21}B$; $b = (2n_{32} + 1)C$; $c = n_{13}A$; 2X°, 2Y°, 2Z° $\in \mathbb{Z}$.

3/ $a = 2n_{11}A$; $b = (2n_{32} + 1)C$; $c = n_{23}B$; 2X°, 2Y° $\in \mathbb{Z}$; 4Z° odd.

4/ $a = (2n_{31} + 1)C$; $b = 2n_{22}B$; $c = n_{13}A$; 2X°, 2Y°, 2Z° $\in \mathbb{Z}$.

P2$_1$2$_1$2$_1$: 1/ $a = 2n_{11}A$; $b = 2n_{22}B$; $c = (2n_{33} + 1)C$; 2X°, 2Y°, 2Z° $\in \mathbb{Z}$.

2/ $a = (2n_{31} + 1)C$; $b = 2n_{12}A$; $c = 2n_{23}B$; 2X°, 2Y°, 2Z° $\in \mathbb{Z}$.

3/ $a = 2n_{21}B$; $b = (2n_{32} + 1)C$; $c = 2n_{13}A$; 2X°, 2Y°, 2Z° $\in \mathbb{Z}$.

4/ $a = 2n_{11}A$; $b = (2n_{32} + 1)C$; $c = 2n_{23}B$; 2X°, 2Y° $\in \mathbb{Z}$; 4Z° odd.

5/ $a = (2n_{31} + 1)C$; $b = 2n_{22}B$; $c = 2n_{13}A$; 2X°, 2Y° $\in \mathbb{Z}$; 4Z° odd.

6/ $a = 2n_{21}B$; $b = 2n_{12}A$; $c = (2n_{33} + 1)C$; 2X°, 2Y° $\in \mathbb{Z}$; 4Z° odd.

C222$_1$: 1/ $a = 2n_{11}A$; $b = 2n_{22}B$; $c = (2n_{31} + 1)C$; 2X°, 2Y°, 2Z° $\in \mathbb{Z}$.

2/ $a = 2n_{21}B$; $b = 2n_{12}A$; $c = (2n_{31} + 1)C$; 2X°, 2Y° $\in \mathbb{Z}$; 4Z° odd.