(4) Tetragonal space groups:

(i) $\mathbf{c}' = 3\mathbf{c}$.

(5) Trigonal space groups:

(*a*) Trigonal space groups with hexagonal *P* lattice:

(i) $\mathbf{c}' = 3\mathbf{c}$,

(ii) $\mathbf{a}' = 3\mathbf{a},\ \mathbf{b}' = 3\mathbf{b}$, *H*-centring,

(iii) $\mathbf{a}' = \mathbf{a} - \mathbf{b},\ \mathbf{b}' = \mathbf{a} + 2\mathbf{b},\ \mathbf{c}' = 3\mathbf{c}$, *R* lattice,

(iv) $\mathbf{a}' = 2\mathbf{a} + \mathbf{b}, \mathbf{b}' = -\mathbf{a} + \mathbf{b},\ \mathbf{c}' = 3\mathbf{c}$, *R* lattice,

(v) $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b}$.

(*b*) Trigonal space groups with rhombohedral *R* lattice and hexagonal axes:

(i) $\mathbf{a}' = -2\mathbf{b},\ \mathbf{b}' = 2\mathbf{a} + 2\mathbf{b}$.

(*c*) Trigonal space groups with rhombohedral *R* lattice and rhombohedral axes:

(i) $\mathbf{a}' = \mathbf{a} - \mathbf{b},\ \mathbf{b}' = \mathbf{b} - \mathbf{c},\ \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c}$,

(ii) $\mathbf{a}' = \mathbf{a} - \mathbf{b} + \mathbf{c},\ \mathbf{b}' = \mathbf{a} + \mathbf{b} - \mathbf{c},\ \mathbf{c}' = -\mathbf{a} + \mathbf{b} + \mathbf{c}$.

(6) Hexagonal space groups:

(i) $\mathbf{c}' = 3\mathbf{c}$,

(ii) $\mathbf{a}' = 3\mathbf{a},\ \mathbf{b}' = 3\mathbf{b}$, *H*-centring,

(iii) $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b}$.

(7) Cubic space groups with *P* lattice:

(i) $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b},\ \mathbf{c}' = 2\mathbf{c}$, *I* lattice.

2.1.5. Series of maximal isomorphic subgroups

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2.1.5.1. *General description*

Maximal subgroups of index higher than 4 have index p, p^2 or p^3, where p is prime, are necessarily isomorphic subgroups and are infinite in number. Only a few of them are listed in *IT* A in the block 'Maximal isomorphic subgroups of lowest index IIc'. Because of their infinite number, they cannot be listed individually, but are listed in this volume as members of series under the heading 'Series of maximal isomorphic subgroups'. In most of the series, the HM symbol for each isomorphic subgroup $\mathcal{H} < \mathcal{G}$ will be the same as that of $\mathcal{G}$. However, if $\mathcal{G}$ is an enantiomorphic space group, the HM symbol of $\mathcal{H}$ will be either that of $\mathcal{G}$ or that of its enantiomorphic partner.

Example 2.1.5.1.1.

Two of the four series of isomorphic subgroups of the space group $P4_1$, No. 76, are (the data on the generators are omitted):

[p]	$\mathbf{c}' = p\mathbf{c}$		
	$P4_3$ (78)	$p > 2;\ p \equiv 3$ (mod 4)	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$
		no conjugate subgroups	
	$P4_1$ (76)	$p > 4;\ p \equiv 1$ (mod 4)	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$
		no conjugate subgroups	

On the other hand, the corresponding data for $P4_3$, No. 78, are

[p]	$\mathbf{c}' = p\mathbf{c}$		
	$P4_3$ (78)	$p > 4;\ p \equiv 1$ (mod 4)	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$
		no conjugate subgroups	
	$P4_1$ (76)	$p > 2;\ p \equiv 3$ (mod 4)	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$
		no conjugate subgroups	

Note that in both tables the subgroups of the type $P4_3$, No. 78, are listed first because of the rules on the sequence of the subgroups.

If an isomorphic maximal subgroup of index $i \leq 4$ is a member of a series, then it is listed twice: as a member of its series *and* individually under the heading 'Enlarged unit cell'.

Most isomorphic subgroups of index 3 are the first members of series but those of index 2 or 4 are rarely so. An example is the space group $P4_2$, No. 77, with isomorphic subgroups of index 2 (not in any series) and 3 (in a series); an exception is found in space group $P4$, No. 75, where the isomorphic subgroup for $\mathbf{c}' = 2\mathbf{c}$ is the first member of the series [p] $\mathbf{c}' = p\mathbf{c}$.

2.1.5.2. *Basis transformation*

The conventional basis of the unit cell of each isomorphic subgroup in the series has to be defined relative to the basis of the original space group. For this definition the prime p is frequently sufficient as a parameter.

Example 2.1.5.2.1.

The isomorphic subgroups of the space group $P4_222$, No. 93, can be described by two series with the bases of their members:

[p]	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$
[p^2]	$p\mathbf{a},\ p\mathbf{b},\ \mathbf{c}$.

In other cases, one or two positive integers, here called q and r, define the series and often the value of the prime p.

Example 2.1.5.2.2.

In space group $P\overline{6}$, No. 174, the series $q\mathbf{a} - r\mathbf{b},\ r\mathbf{a} + (q+r)\mathbf{b},\ \mathbf{c}$ is listed. The values of q and r have to be chosen such that while $q > 0,\ r > 0,\ p = q^2 + r^2 + qr$ and p is prime.

Example 2.1.5.2.3.

In the space group $P112_1/m$, No. 11, unique axis c, the series $p\mathbf{a},\ -q\mathbf{a} + \mathbf{b},\ \mathbf{c}$ is listed. Here p and q are independent and q may take the p values $0 \leq q < p$ for each value of p.

2.1.5.3. *Origin shift*

Each of the sublattices discussed in Section 2.1.4.3.2 is common to a conjugacy class or belongs to a normal subgroup of a given series. The subgroups in a conjugacy class differ by the positions of their conventional origins relative to the origin of the space group $\mathcal{G}$. To define the origin of the conventional unit cell of each subgroup in a conjugacy class, one, two or three integers, called u, v or w in these tables, are necessary. For a series of subgroups of index p, p^2 or p^3 there are p, p^2 or p^3 conjugate subgroups, respectively. The positions of their origins are defined by the p or p^2 or p^3 permitted values of u or u, v or u, v, w, respectively.

Example 2.1.5.3.1.

The space group $\mathcal{G}$, $P\overline{4}2c$, No. 112, has two series of maximal isomorphic subgroups $\mathcal{H}$. For one of them the lattice relations are [p^2] $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}$, listed as $p\mathbf{a}, p\mathbf{b}, \mathbf{c}$ for the transformation matrix. The index is p^2. For each value of p there exist exactly p^2 conjugate subgroups with origins in the points $u,\ v,\ 0$, where the parameters u and v run independently: $0 \leq u < p$ and $0 \leq v < p$.

In another type of series there is exactly one (normal) subgroup $\mathcal{H}$ for each index p; the location of its origin is always chosen at the origin $0, 0, 0$ of $\mathcal{G}$ and is thus not indicated as an origin shift.

Example 2.1.5.3.2.

Consider the space group $Pca2_1$, No. 29. Only one subgroup exists for each value of p in the series $\mathbf{a}, \mathbf{b}, p\mathbf{c}$. This is indicated in the tables by the statement 'no conjugate subgroups'.

references