

8. INTRODUCTION TO SPACE-GROUP SYMMETRY

Examples

In Fig. 8.3.3.1, the space group $P6_3/mcm$ is a minimal supergroup of $P6c2$, ..., $P3c1$; $P6c2$ is a minimal supergroup of $P6$, $P3c1$ and $P312$; etc.

If \mathcal{G} is a maximal t subgroup of \mathcal{R} then \mathcal{R} is a minimal t supergroup of \mathcal{G} . If \mathcal{G} is a maximal k subgroup of \mathcal{R} then \mathcal{R} is a minimal k supergroup of \mathcal{G} . Finally, if \mathcal{G} is a maximal isomorphic subgroup of \mathcal{R} , then \mathcal{R} is a minimal isomorphic supergroup of \mathcal{G} . Data on minimal t and minimal non-isomorphic k supergroups are listed in the space-group tables; cf. Section 2.2.15. Data on minimal isomorphic supergroups are not listed because they can be derived easily from the corresponding subgroup relations.

The complete data on maximal subgroups of plane and space groups are listed in Volume A1 of *International Tables for Crystallography* (2004). For each space group, all maximal subgroups of index [2], [3] and [4] are listed individually. The infinitely many maximal isomorphic subgroups are listed as members of a few (infinite) series. The main parameter in these series is the index p , p^2 or p^3 , where p runs through the infinite number of primes.

8.3.4. Sequence of space-group types

The sequence of space-group entries in the space-group tables follows that introduced by Schoenflies (1891) and is thus established historically. Within each geometric crystal class, Schoenflies has numbered the space-group types in an obscure way. As early as 1919, Niggli (1919) considered this Schoenflies sequence to be unsatisfactory and suggested that another sequence might be more appropriate. Fedorov (1891) used a different sequence in order to distinguish between symmorphic, hemi-symmorphic and asymmorphic space groups.

The basis of the Schoenflies symbols and thus of the Schoenflies listing is the geometric crystal class. For the present *Tables*, a sequence might have been preferred in which, in addition, space-group types belonging to the same arithmetic crystal class were grouped together. It was decided, however, that the long-established sequence in the earlier editions of *International Tables* should not be changed.

In Table 8.3.4.1, those geometric crystal classes are listed in which the Schoenflies sequence separates space groups belonging to the same arithmetic crystal class. The space groups are rearranged in such a way that space groups of the same arithmetic crystal class are grouped together. The arithmetic crystal classes are separated by broken lines, the geometric crystal classes by full lines. In all cases not listed in Table 8.3.4.1, the Schoenflies sequence, as used in these *Tables*, does not break up arithmetic crystal classes. Nevertheless, some rearrangement would be desirable in other arithmetic crystal classes too. For example, the symmorphic space group should always be the first entry of each arithmetic crystal class.

8.3.5. Space-group generators

In group theory, a *set of generators of a group* is a set of group elements such that each group element may be obtained as an ordered product of the generators. For space groups of one, two and three dimensions, generators may always be chosen and ordered in such a way that each symmetry operation W can be written as the product of powers of h generators G_j ($j = 1, 2, \dots, h$). Thus,

$$W = G_h^{k_h} * G_{h-1}^{k_{h-1}} * \dots * G_3^{k_3} * G_2^{k_2} * G_1,$$

where the powers k_j are positive or negative integers (including zero).

Description of a group by means of generators has the advantage of compactness. For instance, the 48 symmetry operations in point

Table 8.3.4.1. Listing of space-group types according to their geometric and arithmetic crystal classes

No.	Hermann–Mauguin symbol	Schoenflies symbol	Geometric crystal class
10	$P2/m$	C_{2h}^1	$2/m$
11	$P2_1/m$	C_{2h}^2	
13	$P2/c$	C_{2h}^4	
14	$P2_1/c$	C_{2h}^5	
12	$C2/m$	C_{2h}^3	
15	$C2/c$	C_{2h}^6	
149	$P312$	D_3^1	32
151	$P3_112$	D_3^2	
153	$P3_212$	D_3^3	
150	$P321$	D_3^4	
152	$P3_121$	D_3^5	
154	$P3_221$	D_3^6	
155	$R32$	D_3^7	
156	$P3m1$	C_{3v}^1	$3m$
158	$P3c1$	C_{3v}^3	
157	$P31m$	C_{3v}^2	
159	$P31c$	C_{3v}^4	
160	$R3m$	C_{3v}^5	
161	$R3c$	C_{3v}^6	
195	$P23$	T^1	23
198	$P2_13$	T^4	
196	$F23$	T^2	
197	$I23$	T^3	
199	$I2_13$	T^5	
200	$Pm\bar{3}$	T_h^1	$m\bar{3}$
201	$Pn\bar{3}$	T_h^2	
205	$Pa\bar{3}$	T_h^6	
202	$Fm\bar{3}$	T_h^3	
203	$Fd\bar{3}$	T_h^4	
204	$Im\bar{3}$	T_h^5	
206	$Ia\bar{3}$	T_h^7	
207	$P432$	O^1	432
208	$P4_232$	O^2	
213	$P4_132$	O^7	
212	$P4_332$	O^6	
209	$F432$	O^3	
210	$F4_132$	O^4	
211	$I432$	O^5	
214	$I4_132$	O^8	
215	$P\bar{4}3m$	T_d^1	$\bar{4}3m$
218	$P\bar{4}3n$	T_d^4	
216	$F\bar{4}3m$	T_d^2	
219	$F\bar{4}3c$	T_d^5	
217	$I\bar{4}3m$	T_d^3	
220	$I\bar{4}3d$	T_d^6	