TABLE 1.3

The 32 point groups

No.	Label		Elements
Triclinic			
1	1	C_1	E
2	$\bar{1}$	C_i	E, I
Monoclinic			
3	2	C_2	E, C_{2z}
4	m	C_s, C_{1h}	E, σ_z
5	$2/m$	C_{2h}	E, C_{2z}, I, σ_z
Orthorhombic			
6	222	D_2	$E, C_{2x}, C_{2y}, C_{2z}$
7	$mm2$	C_{2v}	$E, C_{2z}, \sigma_x, \sigma_y$
8	mmm	D_{2h}	$E, C_{2x}, C_{2y}, C_{2z}, I, \sigma_x, \sigma_y, \sigma_z$
Tetragonal			
9	4	C_4	$E, C_{4z}^+, C_{4z}^-, C_{2z}$
10	$\bar{4}$	S_4	$E, S_{4z}^-, S_{4z}^+, C_{2z}$
11	$4/m$	C_{4h}	$E, C_{4z}^+, C_{4z}^-, C_{2z}, I, S_{4z}^-, S_{4z}^+, \sigma_z$
12	422	D_4	$E, C_{4z}^+, C_{4z}^-, C_{2z}, C_{2x}, C_{2y}, C_{2a}, C_{2b}$
13	$4mm$	C_{4v}	$E, C_{4z}^+, C_{4z}^-, C_{2z}, \sigma_x, \sigma_y, \sigma_{da}, \sigma_{db}$
14	$\bar{4}2m$	D_{2d}	$E, S_{4z}^+, S_{4z}^-, C_{2z}, C_{2x}, C_{2y}, \sigma_{da}, \sigma_{db}$
15	$4/mmm$	D_{4h}	$E, C_{4z}^+, C_{4z}^-, C_{2z}, C_{2x}, C_{2y}, C_{2a}, C_{2b}$ $I, S_{4z}^-, S_{4z}^+, \sigma_z, \sigma_x, \sigma_y, \sigma_{da}, \sigma_{db}$
Trigonal			
16	3	C_3	E, C_3^+, C_3^-
17	$\bar{3}$	C_{3i}	$E, C_3^+, C_3^-, I, S_6^-, S_6^+$
18	32	D_3	$E, C_3^+, C_3^-, C'_{21}, C'_{22}, C'_{23}$
19	$3m$	C_{3v}	$E, C_3^+, C_3^-, \sigma_{d1}, \sigma_{d2}, \sigma_{d3}$
20	$\bar{3}m$	D_{3d}	$E, C_3^+, C_3^-, C'_{21}, C'_{22}, C'_{23}, I, S_6^-, S_6^+, \sigma_{d1}, \sigma_{d2}, \sigma_{d3}$
Hexagonal			
21	6	C_6	$E, C_6^+, C_6^-, C_3^+, C_3^-, C_2$
22	$\bar{6}$	C_{3h}	$E, S_3^-, S_3^+, C_3^+, C_3^-, \sigma_h$
23	$6/m$	C_{6h}	$E, C_6^+, C_6^-, C_3^+, C_3^-, C_2, I, S_3^-, S_3^+, S_6^-, S_6^+, \sigma_h$
24	622	D_6	$E, C_6^+, C_6^-, C_3^+, C_3^-, C_2, C'_{21}, C'_{22}, C'_{23}, C''_{21}, C''_{22}, C''_{23}$
25	$6mm$	C_{6v}	$E, C_6^+, C_6^-, C_3^+, C_3^-, C_2, \sigma_{d1}, \sigma_{d2}, \sigma_{d3}, \sigma_{v1}, \sigma_{v2}, \sigma_{v3}$
26	$\bar{6}2m$	D_{3h}	$E, S_3^-, S_3^+, C_3^+, C_3^-, \sigma_h, C'_{21}, C'_{22}, C'_{23}, \sigma_{v1}, \sigma_{v2}, \sigma_{v3}$
27	$6/mmm$	D_{6h}	$E, C_6^+, C_6^-, C_3^+, C_3^-, C_2, C'_{21}, C'_{22}, C'_{23}, C''_{21}, C''_{22}, C''_{23}$ $I, S_3^-, S_3^+, S_6^-, S_6^+, \sigma_h, \sigma_{d1}, \sigma_{d2}, \sigma_{d3}, \sigma_{v1}, \sigma_{v2}, \sigma_{v3}$
Cubic			
28	23	T	$E, C_{2m}, C_{3j}^+, C_{3j}^-$
29	$m3$	T_h	$E, C_{2m}, C_{3j}^+, C_{3j}^-, I, \sigma_m, S_{6j}^-, S_{6j}^+$
30	432	O	$E, C_{2m}, C_{3j}^+, C_{3j}^-, C_{2p}, C_{4m}^+, C_{4m}^-$
31	$\bar{4}3m$	T_d	$E, C_{2m}, C_{3j}^+, C_{3j}^-, \sigma_{dp}, S_{4m}^-, S_{4m}^+$
32	$m3m$	O_h	$E, C_{2m}, C_{3j}^+, C_{3j}^-, C_{2p}, C_{4m}^+, C_{4m}^-$ $I, \sigma_m, S_{6j}^-, S_{6j}^+, \sigma_{dp}, S_{4m}^-, S_{4m}^+$

Notes to Table 1.3

(i) The arbitrary numbers in column 1 are those of Koster, Dimmock, Wheeler, and Statz (1963).

(ii) The labels of the symmetry operations can be identified from Figs. 1.1–1.3; j = 1, 2, 3, and 4; $m = x, y$, and z; $p = a, b, c, d, e$, and f.

(iii) The principal axes have been set in the Oz direction but there are still possible alternative settings for some of the point groups, for example $\bar{4}2m$ (D_{2d}) may contain the elements, $E, S_{4z}^-, C_{2z}, S_{4z}^+, \sigma_x, \sigma_y, C_{2a}$, and C_{2b}; sometimes alternatives of this kind are important when one considers the space groups (see Chapter 3).

TABLE 1.2

Symmetry elements for the seven crystal systems

Triclinic	Monoclinic	Orthorhombic	Tetragonal	Trigonal	Hexagonal	Cubic
$\bar{1}$ (C_i)	$2/m$ (C_{2h})	mmm (D_{2h})	$4/mmm$ (D_{4h})	$\bar{3}m$ (D_{3d})	$6/mmm$ (D_{6h})	$m3m$ (O_h)
E, I	E, I C_{2z}, σ_z	E, I C_{2m}, σ_m	E, I $C_{4z}^{\pm}, S_{4z}^{\mp}$ C_{2m}, σ_m C_{2s}, σ_{ds}	E, I $C_3^{\pm}, S_6^{\mp}$ C'_{2i}, σ_{di}	E, I $C_6^{\pm}, S_3^{\mp}$ $C_3^{\pm}, S_6^{\mp}$ C_2, σ_h C'_{2i}, σ_{di} C''_{2i}, σ_{vi}	E, I C_{2m}, σ_m $C_{3j}^{\pm}, S_{6j}^{\mp}$ $C_{4m}^{\pm}, S_{4m}^{\mp}$ C_{2p}, σ_{dp}

Notes to Table 1.2

(i) There is an alternative setting for the trigonal system using C''_{2i} instead of C'_{2i} as a standard setting.

(ii) See Figs. 1.1, 1.2, and 1.3 for the positions of the following axes:
$m = x, y, z$; $s = a, b$; $i = 1, 2, 3$; $j = 1, 2, 3, 4$, and $p = a, b, c, d, e, f$.

group $6/mmm$ (D_{6h}) by $R_1, R_2, \ldots, R_{24}$; this scheme is very convenient when computers are being used. However, because the well-established notations, while far from perfect, do carry some meaning (which is not the case for an arbitrary labelling) we therefore use in this book the Schönflies notation for the actual symmetry operations of both point groups and space groups, elaborated so that each point-group

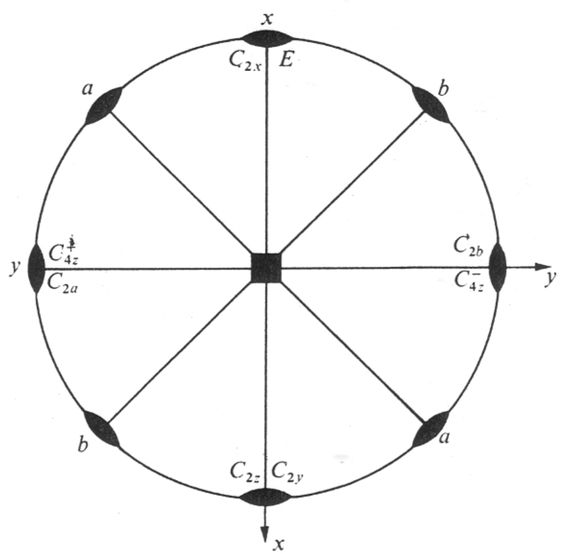
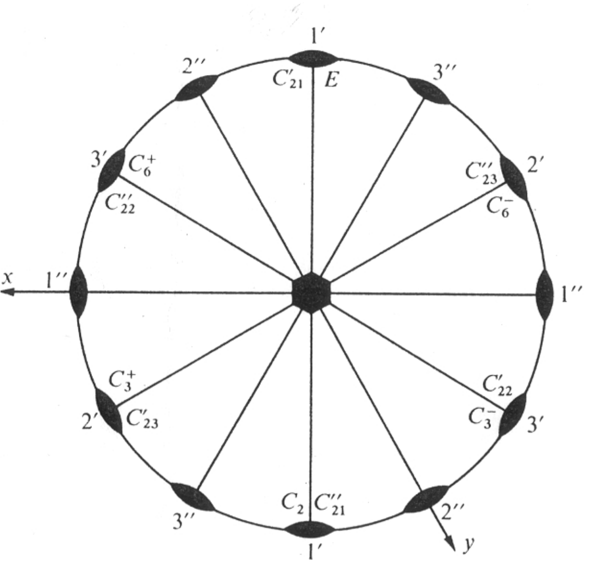


FIG. 1.1. Symmetry elements: triclinic, monoclinic, orthorhombic, and tetragonal systems. The point groups in these systems are subgroups of $m3m$ (O_h) and so the same notation is used. x, y, z form a right-handed set of axes. The labels of the symmetry operations are placed on the figure in the position to which the letter E is taken by that operation.



ments: trigonal and hexagonal systems. The z-axis is vertically upwards, out of the page. :try operations are placed on the figure in the position to which the letter E is taken by that operation.

:nd for their usefulness on a complete identification of the symmetry and so we shall give some attention to this matter. To identify the ts for point groups belonging to most crystal systems it is possible re such as a stereogram, and we do this for the triclinic, monoclinic, d tetragonal systems in Fig. 1.1 and for the trigonal and hexagonal 2. Two-sided paper models have been used by Schiff (1954) to help :rent non-cubic point groups. However, for the cubic system it is the symmetry elements from the figure of a cube; this is done in anti-clockwise rotation of the points of space through $2\pi/n$ radians oelled by r on the figure in question. C_{nr}^- is a clockwise rotation of e through $2\pi/n$ radians about the same axis. E is the identity and I ı Table 1.2 the operators that appear in a given system are listed for crystal systems; in each part of the table there are two columns, e right-hand column being the product of I with the corresponding :-hand column. The elements given in this table are those that appear :iate point group is in the standard setting with respect to the x, y,

so on). This is because S_n^+ denotes an anti-clockwise rotation by 2ı reflection in the plane perpendicular to the rotation and hence I $\sigma(C_{2n}^+)^{n+2} = (S_{2n}^+)^{n+2}$.

A final and very important point, which we have mentioned stressed and that is that when dealing with a point-group operato preted always as an *active* operator moving the points of space anc fixed; similarly, when dealing with a space-group operator written i: (see section 1.5) it too will be interpreted as active.

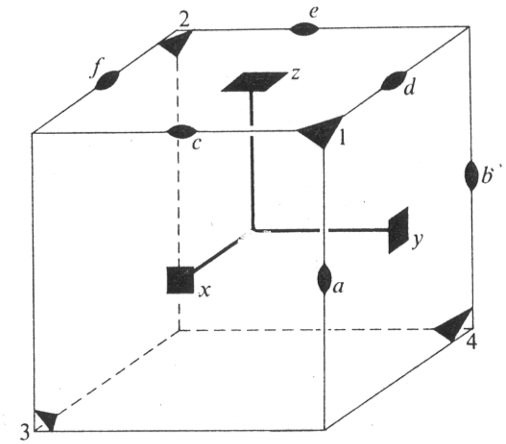


FIG. 1.3. Symmetry elements: cubic system (Altmann and Bradley 19

In Table 1.3 we identify the symmetry operations that are pres 32 crystallographic point groups. The point groups are arranged seven crystal systems and all the elements of each point group arı a point group has a principal axis this axis is set in the Oz directioı the *standard setting*, but of course many other settings are possib shown stereograms for the 32 crystallographic point groups; for de of stereographic projection see, for example, Phillips (1963). In system the point group that contains the largest number of symm called the *holosymmetric* point group of that system.

The multiplication of point-group operations

TABLE 1.5

The group multiplication table for the point group 432 (O)

E	C_{2x}	C_{2y}	C_{2z}	C_{4x}^{-}	C_{4y}^{-}	C_{4z}^{-}	C_{4x}^{+}	C_{4y}^{+}	C_{4z}^{+}	C_{31}^{-}	C_{32}^{-}	C_{33}^{-}	C_{34}^{-}	C_{31}^{+}	C_{32}^{+}	C_{33}^{+}	C_{34}^{+}	C_{2a}	C_{2b}	C_{2c}	C_{2d}	C_{2e}	C_{2f}
C_{2x}	E	C_{2z}	C_{2y}	C_{4x}^{+}	C_{2e}	C_{2a}	C_{4x}^{-}	C_{2c}	C_{2b}	C_{32}^{-}	C_{31}^{-}	C_{34}^{-}	C_{33}^{-}	C_{34}^{+}	C_{33}^{+}	C_{32}^{+}	C_{31}^{+}	C_{4z}^{-}	C_{4z}^{+}	C_{4y}^{+}	C_{2f}	C_{4y}^{-}	C_{2d}
C_{2y}	C_{2z}	E	C_{2x}	C_{2d}	C_{4y}^{+}	C_{2b}	C_{2f}	C_{4y}^{-}	C_{2a}	C_{33}^{-}	C_{34}^{-}	C_{31}^{-}	C_{32}^{-}	C_{32}^{+}	C_{31}^{+}	C_{34}^{+}	C_{33}^{+}	C_{4z}^{+}	C_{4z}^{-}	C_{2e}	C_{4x}^{-}	C_{2c}	C_{4x}^{+}
C_{2z}	C_{2y}	C_{2x}	E	C_{2f}	C_{2c}	C_{4z}^{+}	C_{2d}	C_{2e}	C_{4z}^{-}	C_{34}^{-}	C_{33}^{-}	C_{32}^{-}	C_{31}^{-}	C_{33}^{+}	C_{34}^{+}	C_{31}^{+}	C_{32}^{+}	C_{2b}	C_{2a}	C_{4y}^{-}	C_{4x}^{+}	C_{4y}^{+}	C_{4x}^{-}
C_{4x}^{-}	C_{4x}^{+}	C_{2f}	C_{2d}	C_{2x}	C_{32}^{+}	C_{31}^{-}	E	C_{34}^{+}	C_{33}^{-}	C_{2a}	C_{4z}^{-}	C_{2b}	C_{4z}^{+}	C_{4y}^{+}	C_{2e}	C_{4y}^{-}	C_{2c}	C_{32}^{-}	C_{34}^{-}	C_{31}^{+}	C_{2y}	C_{33}^{+}	C_{2z}
C_{4y}^{-}	C_{2c}	C_{4y}^{+}	C_{2e}	C_{31}^{-}	C_{2y}	C_{33}^{+}	C_{34}^{-}	E	C_{32}^{+}	C_{2d}	C_{4x}^{+}	C_{4x}^{-}	C_{2f}	C_{4z}^{+}	C_{2a}	C_{2b}	C_{4z}^{-}	C_{31}^{+}	C_{34}^{+}	C_{2z}	C_{33}^{-}	C_{2x}	C_{32}^{-}
C_{4z}^{-}	C_{2b}	C_{2a}	C_{4z}^{+}	C_{34}^{+}	C_{31}^{-}	C_{2z}	C_{33}^{+}	C_{32}^{-}	E	C_{2c}	C_{2e}	C_{4y}^{+}	C_{4y}^{-}	C_{4x}^{+}	C_{4x}^{-}	C_{2d}	C_{2f}	C_{2x}	C_{2y}	C_{34}^{-}	C_{31}^{+}	C_{33}^{-}	C_{32}^{+}
C_{4x}^{+}	C_{4x}^{-}	C_{2d}	C_{2f}	E	C_{33}^{+}	C_{32}^{-}	C_{2x}	C_{31}^{+}	C_{34}^{-}	C_{4z}^{-}	C_{2a}	C_{4z}^{+}	C_{2b}	C_{2c}	C_{4y}^{-}	C_{2e}	C_{4y}^{+}	C_{31}^{-}	C_{33}^{-}	C_{34}^{+}	C_{2z}	C_{32}^{+}	C_{2y}
C_{4y}^{+}	C_{2e}	C_{4y}^{-}	C_{2c}	C_{33}^{-}	E	C_{34}^{+}	C_{32}^{-}	C_{2y}	C_{31}^{+}	C_{4x}^{-}	C_{2f}	C_{2d}	C_{4x}^{+}	C_{2a}	C_{4z}^{+}	C_{4z}^{-}	C_{2b}	C_{32}^{+}	C_{33}^{+}	C_{2x}	C_{31}^{-}	C_{2z}	C_{34}^{-}
C_{4z}^{+}	C_{2a}	C_{2b}	C_{4z}^{-}	C_{32}^{+}	C_{34}^{-}	E	C_{31}^{+}	C_{33}^{-}	C_{2z}	C_{4y}^{-}	C_{4y}^{+}	C_{2e}	C_{2c}	C_{2d}	C_{2f}	C_{4x}^{+}	C_{4x}^{-}	C_{2y}	C_{2x}	C_{31}^{-}	C_{33}^{+}	C_{32}^{-}	C_{34}^{+}
C_{31}^{-}	C_{34}^{-}	C_{32}^{-}	C_{33}^{-}	C_{2c}	C_{2a}	C_{2d}	C_{4y}^{-}	C_{4z}^{-}	C_{4x}^{-}	C_{31}^{+}	C_{33}^{+}	C_{34}^{+}	C_{32}^{+}	E	C_{2x}	C_{2y}	C_{2z}	C_{4x}^{+}	C_{2f}	C_{4z}^{+}	C_{4y}^{+}	C_{2b}	C_{2e}
C_{32}^{-}	C_{33}^{-}	C_{31}^{-}	C_{34}^{-}	C_{4y}^{+}	C_{4z}^{-}	C_{2f}	C_{2e}	C_{2a}	C_{4x}^{+}	C_{34}^{+}	C_{32}^{+}	C_{31}^{+}	C_{33}^{+}	C_{2x}	E	C_{2z}	C_{2y}	C_{4x}^{-}	C_{2d}	C_{2b}	C_{2c}	C_{4z}^{+}	C_{4y}^{-}
C_{33}^{-}	C_{32}^{-}	C_{34}^{-}	C_{31}^{-}	C_{2e}	C_{4z}^{+}	C_{4x}^{-}	C_{4y}^{+}	C_{2b}	C_{2d}	C_{32}^{+}	C_{34}^{+}	C_{33}^{+}	C_{31}^{+}	C_{2y}	C_{2z}	E	C_{2x}	C_{2f}	C_{4x}^{+}	C_{2a}	C_{4y}^{-}	C_{4z}^{-}	C_{2c}
C_{34}^{-}	C_{31}^{-}	C_{33}^{-}	C_{32}^{-}	C_{4y}^{-}	C_{2b}	C_{4x}^{+}	C_{2c}	C_{4z}^{+}	C_{2f}	C_{33}^{+}	C_{31}^{+}	C_{32}^{+}	C_{34}^{+}	C_{2z}	C_{2y}	C_{2x}	E	C_{2d}	C_{4x}^{-}	C_{4z}^{-}	C_{2e}	C_{2a}	C_{4y}^{+}
C_{31}^{+}	C_{32}^{+}	C_{33}^{+}	C_{34}^{+}	C_{4z}^{+}	C_{4x}^{+}	C_{4y}^{+}	C_{2a}	C_{2d}	C_{2c}	E	C_{2y}	C_{2z}	C_{2x}	C_{31}^{-}	C_{34}^{-}	C_{32}^{-}	C_{33}^{-}	C_{4y}^{-}	C_{2e}	C_{4x}^{-}	C_{4z}^{-}	C_{2f}	C_{2b}
C_{32}^{+}	C_{31}^{+}	C_{34}^{+}	C_{33}^{+}	C_{2a}	C_{2f}	C_{4y}^{-}	C_{4z}^{+}	C_{4x}^{-}	C_{2e}	C_{2y}	E	C_{2x}	C_{2z}	C_{33}^{-}	C_{32}^{-}	C_{34}^{-}	C_{31}^{-}	C_{4y}^{+}	C_{2c}	C_{2d}	C_{2b}	C_{4x}^{+}	C_{4z}^{-}
C_{33}^{+}	C_{34}^{+}	C_{31}^{+}	C_{32}^{+}	C_{4z}^{-}	C_{2d}	C_{2e}	C_{2b}	C_{4x}^{+}	C_{4y}^{-}	C_{2z}	C_{2x}	E	C_{2y}	C_{34}^{-}	C_{31}^{-}	C_{33}^{-}	C_{32}^{-}	C_{2c}	C_{4y}^{+}	C_{2f}	C_{4z}^{+}	C_{4x}^{-}	C_{2a}
C_{34}^{+}	C_{33}^{+}	C_{32}^{+}	C_{31}^{+}	C_{2b}	C_{4x}^{-}	C_{2c}	C_{4z}^{-}	C_{2f}	C_{4y}^{+}	C_{2x}	C_{2z}	C_{2y}	E	C_{32}^{-}	C_{33}^{-}	C_{31}^{-}	C_{34}^{-}	C_{2e}	C_{4y}^{-}	C_{4x}^{+}	C_{2a}	C_{2d}	C_{4z}^{+}
C_{2a}	C_{4z}^{+}	C_{4z}^{-}	C_{2b}	C_{31}^{+}	C_{32}^{-}	C_{2y}	C_{32}^{+}	C_{31}^{-}	C_{2x}	C_{4y}^{+}	C_{4y}^{-}	C_{2c}	C_{2e}	C_{4x}^{-}	C_{4x}^{+}	C_{2f}	C_{2d}	E	C_{2z}	C_{33}^{-}	C_{34}^{+}	C_{34}^{-}	C_{33}^{+}
C_{2b}	C_{4z}^{-}	C_{4z}^{+}	C_{2a}	C_{33}^{+}	C_{33}^{-}	C_{2x}	C_{34}^{+}	C_{34}^{-}	C_{2y}	C_{2e}	C_{2c}	C_{4y}^{-}	C_{4y}^{+}	C_{2f}	C_{2d}	C_{4x}^{-}	C_{4x}^{+}	C_{2z}	E	C_{32}^{-}	C_{32}^{+}	C_{31}^{-}	C_{31}^{+}
C_{2c}	C_{4y}^{-}	C_{2e}	C_{4y}^{+}	C_{34}^{-}	C_{2x}	C_{31}^{+}	C_{31}^{-}	C_{2z}	C_{34}^{+}	C_{4x}^{+}	C_{2d}	C_{2f}	C_{4x}^{-}	C_{4z}^{-}	C_{2b}	C_{2a}	C_{4z}^{+}	C_{33}^{+}	C_{32}^{+}	E	C_{32}^{-}	C_{2y}	C_{33}^{-}
C_{2d}	C_{2f}	C_{4x}^{+}	C_{4x}^{-}	C_{2z}	C_{31}^{+}	C_{33}^{-}	C_{2y}	C_{33}^{+}	C_{31}^{-}	C_{4z}^{+}	C_{2b}	C_{4z}^{-}	C_{2a}	C_{4y}^{-}	C_{2c}	C_{4y}^{+}	C_{2e}	C_{34}^{-}	C_{32}^{-}	C_{32}^{+}	E	C_{34}^{+}	C_{2x}
C_{2e}	C_{4y}^{+}	C_{2c}	C_{4y}^{-}	C_{32}^{-}	C_{2z}	C_{32}^{+}	C_{33}^{-}	C_{2x}	C_{33}^{+}	C_{2f}	C_{4x}^{-}	C_{4x}^{+}	C_{2d}	C_{2b}	C_{4z}^{-}	C_{4z}^{+}	C_{2a}	C_{34}^{+}	C_{31}^{+}	C_{2y}	C_{34}^{-}	E	C_{31}^{-}
C_{2f}	C_{2d}	C_{4x}^{-}	C_{4x}^{+}	C_{2y}	C_{34}^{+}	C_{34}^{-}	C_{2z}	C_{32}^{+}	C_{32}^{-}	C_{2b}	C_{4z}^{+}	C_{2a}	C_{4z}^{-}	C_{2e}	C_{4y}^{+}	C_{2c}	C_{4y}^{-}	C_{33}^{-}	C_{31}^{-}	C_{33}^{+}	C_{2x}	C_{31}^{+}	E

TABLE 1.6

The group multiplication table for the point group 622 (D_6)

E	C_6^+	C_3^+	C_2	C_3^-	C_6^-	C'_{21}	C'_{22}	C'_{23}	C''_{21}	C''_{22}	C''_{23}
C_6^+	C_3^+	C_2	C_3^-	C_6^-	E	C''_{22}	C''_{23}	C''_{21}	C'_{22}	C'_{23}	C'_{21}
C_3^+	C_2	C_3^-	C_6^-	E	C_6^+	C'_{23}	C'_{21}	C'_{22}	C''_{23}	C''_{21}	C''_{22}
C_2	C_3^-	C_6^-	E	C_6^+	C_3^+	C''_{21}	C''_{22}	C''_{23}	C'_{21}	C'_{22}	C'_{23}
C_3^-	C_6^-	E	C_6^+	C_3^+	C_2	C'_{22}	C'_{23}	C'_{21}	C''_{22}	C''_{23}	C''_{21}
C_6^-	E	C_6^+	C_3^+	C_2	C_3^-	C''_{23}	C''_{21}	C''_{22}	C'_{23}	C'_{21}	C'_{22}
C'_{21}	C''_{23}	C'_{22}	C''_{21}	C'_{23}	C''_{22}	E	C_3^+	C_3^-	C_2	C_6^-	C_6^+
C'_{22}	C''_{21}	C'_{23}	C''_{22}	C'_{21}	C''_{23}	C_3^-	E	C_3^+	C_6^+	C_2	C_6^-
C'_{23}	C''_{22}	C'_{21}	C''_{23}	C'_{22}	C''_{21}	C_3^+	C_3^-	E	C_6^-	C_6^+	C_2
C''_{21}	C'_{23}	C''_{22}	C'_{21}	C''_{23}	C'_{22}	C_2	C_6^-	C_6^+	E	C_3^+	C_3^-
C''_{22}	C'_{21}	C''_{23}	C'_{22}	C''_{21}	C'_{23}	C_6^+	C_2	C_6^-	C_3^-	E	C_3^+
C''_{23}	C'_{22}	C''_{21}	C'_{23}	C''_{22}	C'_{21}	C_6^-	C_6^+	C_2	C_3^+	C_3^-	E

exactly similar array of atoms or molecules to the array that he would see if he were to view the crystal from any other of these lattice points. Strictly speaking, in order to obtain complete similarity of the environment of each lattice point it is necessary that a mathematical lattice be of infinite extent. A real crystal clearly cannot contain such an infinite lattice but, remembering the actual sizes of atoms, it will be a close approximation to an infinite lattice. We may illustrate the idea of a lattice with a 2-dimensional example; if the set of points in Fig. 1.6, which are arranged at the

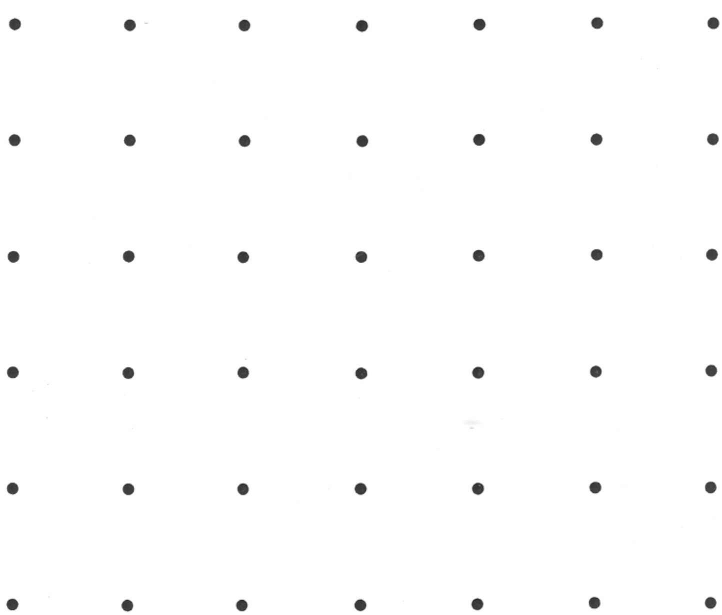


FIG. 1.6. The square 2-dimensional Bravais lattice, *p*.

β is equal to $\frac{1}{2}\pi$ (see Table 2.1), and so we can calculate
hose l values for which $d^l(\frac{1}{2}\pi)$ is known. In fact, surface
epresentations of the cubic groups have been evaluated
. But to have base functions up to $l = 12$ is sufficient for
present time.

eness, we quote two other theorems concerning the

$$W^i_{ts} W^j_{pq} = \delta^{ij}\,\delta_{sp} W^i_{tq}. \tag{2.2.6}$$

$$W^{i\dagger}_{ts} = W^i_{st} \tag{2.2.7}$$

adjoint operator in the space V.

ems are given, for example, by Altmann (1962).

groups

a point group **G** with elements R, S, ..., and a matrix
.... For the generating functions we take the spherical
iire to evaluate $W^i_{ts} Y^m_l(\theta, \phi)$. Using eqn. (2.2.2) we obtain

$$\ldots^m(\theta, \phi) = \frac{d_i}{|\mathbf{G}|} \sum_{R \in \mathbf{G}} \mathbf{D}^i(R)^*_{ts} R Y^m_l(\theta, \phi). \tag{2.3.1}$$

we need an expression for $RY^m_l(\theta, \phi)$. Now R is either a
ct of the inversion, I, with a proper rotation, that is, an
a proper rotation then we find its Euler angles (α, β, γ)
$RY^m_l(\theta, \phi)$ directly by means of eqn. (2.1.3). On the other
xpress $R = IQ$ and use the Euler angles (α, β, γ) for the
ng $QY^m_l(\theta, \phi)$ by means of eqn. (2.1.3); to complete the
use eqn. (2.1.12) for the transforms of $IY^n_l(\theta, \phi)$. This
$(-1)^l$ if R is an improper rotation.
1) becomes

$$\ldots \sum_{R \in \mathbf{G}} P_R \mathbf{D}^i(R)^*_{ts} \exp(-im\alpha) \sum_n C_{nm} \exp(-in\gamma) \times d^l(\beta)_{nm} Y^n_l(\theta, \phi), \tag{2.3.2}$$

Before tabulating the results for all the point groups we deal with one further theoretical problem. This is that the surface harmonics generated by means of eqn. (2.3.2) for a given row of a given rep, that is for fixed i and t, are not necessarily orthogonal. For practical purposes it is desirable that any two bases for the same representation should consist of mutually orthogonal functions. All the expansions given in the tables that follow have been orthogonalized with the help of Theorems 2.2.2 and 2.2.3.

2.4. Symmetry-adapted functions for the crystallographic point groups

In Table 2.2 we give the character tables of the (single-valued) reps of the 32 crystallographic point groups. The reps are labelled in the notation of Mulliken (1933) which we shall follow in this book, but the Γ labels, given for example by Koster, Dimmock, Wheeler, and Statz (1963), are also included for reference. In Table 2.3 we give the matrices that we use for the degenerate point-group reps. The method of section 2.3 can be applied to the determination of the surface harmonics for the cyclic, dihedral, and cubic point groups and these functions are given in Tables 2.4–2.6, respectively (Altmann 1957, Altmann and Bradley 1963*b*, Altmann and Cracknell 1965). We give a few examples of the interpretation of these tables of surface harmonics.

TABLE 2.2

Character tables for the crystallographic point groups
$(\omega = \exp(2\pi i/3))$

$1(C_1)$		E
A	Γ_1	1

$\bar{1}(C_i)$		$2(C_2)$		$m(C_{1h})$		E E E	I C_{2z} σ_z
A_g	Γ_1^+	A	Γ_1	A'	Γ_1	1	1
A_u	Γ_1^-	B	Γ_2	A''	Γ_2	1	-1

$2/m = 2 \otimes \bar{1}\ (C_{2h} = C_2 \otimes C_i)$

$mm2$ (C_{2v})				E	C_{2z}	σ_y	σ_x
		222 (D_2)		E	C_{2z}	C_{2y}	C_{2x}
A_1	Γ_1	A	Γ_1	1	1	1	1
B_2	Γ_4	B_3	Γ_4	1	−1	−1	1
A_2	Γ_3	B_1	Γ_3	1	1	−1	−1
B_1	Γ_2	B_2	Γ_2	1	−1	1	−1

$mmm = 222 \otimes \bar{1}$ ($D_{2h} = D_2 \otimes C_i$)

4 (C_4)				E	C_{2z}	C_{4z}^+	C_{4z}^-
		$\bar{4}$ (S_4)		E	C_{2z}	S_{4z}^-	S_{4z}^+
A	Γ_1	A	Γ_1	1	1	1	1
B	Γ_2	B	Γ_2	1	1	−1	−1
^1E	Γ_4	^1E	Γ_4	1	−1	−i	i
^2E	Γ_3	^2E	Γ_3	1	−1	i	−i

$4/m = 4 \otimes \bar{1}$ ($C_{4h} = C_4 \otimes C_i$)

3 (C_3)		E	C_3^+	C_3^-
A	Γ_1	1	1	1
^1E	Γ_3	1	ω^*	ω
^2E	Γ_2	1	ω	ω^*

$\bar{3} = 3 \otimes \bar{1}$ ($C_{3i} = C_3 \otimes C_i$)

32 (D_3)				E	$C_3^\pm$	C'_{2i}
		$3m$ (C_{3v})		E	$C_3^\pm$	σ_{di}
A_1	Γ_1	A_1	Γ_1	1	1	1
A_2	Γ_2	A_2	Γ_2	1	1	−1
E	Γ_3	E	Γ_3	2	−1	0

$\bar{3}m = 32 \otimes \bar{1}$ ($D_{3d} = D_3 \otimes C_i$)

6 (C_6)				E	C_6^+	C_3^+	C_2	C_3^-	C_6^-
		$\bar{6}$ (C_{3h})		E	S_3^-	C_3^+	σ_h	C_3^-	S_3^+
A	Γ_1	A'	Γ_1	1	1	1	1	1	1
B	Γ_4	A''	Γ_4	1	−1	1	−1	1	−1
$^1E_1$	Γ_6	$^1E'$	Γ_3	1	ω	ω^*	1	ω	ω^*
$^2E_1$	Γ_5	$^2E'$	Γ_2	1	ω^*	ω	1	ω^*	ω
$^1E_2$	Γ_3	$^1E''$	Γ_6	1	$-\omega$	ω^*	−1	ω	$-\omega^*$
$^2E_2$	Γ_2	$^2E''$	Γ_5	1	$-\omega^*$	ω	−1	ω^*	$-\omega$

$6/m = 6 \otimes \bar{1}$ ($C_{6h} = C_6 \otimes C_i$)

422 (D_4)						E	C_{2z}	$C_{4z}^\pm$	C_{2x}, C_{2y}	C_{2a}, C_{2b}
		$4mm$ (C_{4v})				E	C_{2z}	$C_{4z}^\pm$	σ_x, σ_y	σ_{da}, σ_{db}
				$\bar{4}2m$ (D_{2d})		E	C_{2z}	$S_{4z}^\pm$	C_{2x}, C_{2y}	σ_{da}, σ_{db}
A_1	Γ_1	A_1	Γ_1	A_1	Γ_1	1	1	1	1	1
A_2	Γ_2	A_2	Γ_2	A_2	Γ_2	1	1	1	−1	−1
B_1	Γ_3	B_1	Γ_3	B_1	Γ_3	1	1	−1	1	−1
B_2	Γ_4	B_2	Γ_4	B_2	Γ_4	1	1	−1	−1	1
E	Γ_5	E	Γ_5	E	Γ_5	2	−2	0	0	0

$4/mmm = 422 \otimes \bar{1}$ ($D_{4h} = D_4 \otimes C_i$)

622 (D_6)						E	C_2	$C_3^\pm$	$C_6^\pm$	C'_{2i}	C''_{2i}
		$6mm$ (C_{6v})				E	C_2	$C_3^\pm$	$C_6^\pm$	σ_{di}	σ_{vi}
				$\bar{6}2m$ (D_{3h})		E	σ_h	$C_3^\pm$	$S_3^\pm$	C'_{2i}	σ_{vi}
A_1	Γ_1	A_1	Γ_1	A'_1	Γ_1	1	1	1	1	1	1
A_2	Γ_2	A_2	Γ_2	A'_2	Γ_2	1	1	1	1	−1	−1
B_1	Γ_3	B_2	Γ_3	A''_1	Γ_3	1	−1	1	−1	1	−1
B_2	Γ_4	B_1	Γ_4	A''_2	Γ_4	1	−1	1	−1	−1	1
E_2	Γ_6	E_2	Γ_6	E'	Γ_6	2	2	−1	−1	0	0
E_1	Γ_5	E_1	Γ_5	E''	Γ_5	2	−2	−1	1	0	0

$6/mmm = 622 \otimes \bar{1}$ ($D_{6h} = D_6 \otimes C_i$)

23 (T)		E	C_{2m}	C_{3j}^+	C_{3j}^-
A	Γ_1	1	1	1	1
^1E	Γ_2	1	1	ω	ω^*
^2E	Γ_3	1	1	ω^*	ω
T	Γ_4	3	−1	0	0

$m3 = 23 \otimes \bar{1}$ ($T_h = T \otimes C_i$)

432 (O)				E	$C_{3j}^\pm$	C_{2m}	C_{2p}	$C_{4m}^\pm$
		$\bar{4}3m$ (T_d)		E	$C_{3j}^\pm$	C_{2m}	σ_{dp}	$S_{4m}^\pm$
A_1	Γ_1	A_1	Γ_1	1	1	1	1	1
A_2	Γ_2	A_2	Γ_2	1	1	1	−1	−1
E	Γ_3	E	Γ_3	2	−1	2	0	0
T_2	Γ_5	T_2	Γ_5	3	0	−1	1	−1
T_1	Γ_4	T_1	Γ_4	3	0	−1	−1	1

$m3m = 432 \otimes \bar{1}$ ($O_h = O \otimes C_i$)

'es to Table 2.2

(i) The names of the point groups are given in both the international and Schönflies notations. Sometimes two hree point groups have identical characters; such groups are tabulated together.

(ii) For each point group the names of the representations appear in the column headed by the name of the point up. The standard Mulliken notation for the representations is used (Margenau and Murphy 1956, Mulliken 1933). : Γ notation of Koster, Dimmock, Wheeler, and Statz (1963) is also included for reference, though we shall not ually use it in this book.

iii) For each point group the names of the operators appear in the row begun by the name of that group. They to be identified with respect to axes *Oxyz* by means of Figs. 1.1–1.4 and Tables 1.2–1.6. Note that we have en the first setting of the *International tables for X-ray crystallography* (Henry and Lonsdale 1965) for the point ups of the monoclinic system; the *z*-axis (being the polar axis) is more appropriate than the *y*-axis in the study ıarmonic functions.

iv) We have not given the character tables of those groups that are direct products of some other point group ı $\bar{1}$ (C_i); the character tables of these direct product groups can be constructed as follows. If a group **G**′ is given ı direct product of the form $\mathbf{G} \otimes \bar{1}$ then the reps of **G**′ fall into pairs; each pair M_g and M_u arise out of a single M of **G** and the characters of M_g and M_u obey the following rules. If $R' = R\bar{I}$ then for all $R \in \mathbf{G}$ the character R in M_g and M_u is equal to the character of R in M; the character of R' in M_g is equal to the character of ı M, but the character of R' in M_u is minus the character of R in M. In the Γ notation of Koster, Dimmock, eeler, and Statz (1963), if $\Gamma \equiv M$ in **G**, then $\Gamma^+ \equiv M_g$ and $\Gamma^- \equiv M_u$ in **G**′.

v) By using Theorem 1.3.9 one can easily show that all the point-group reps are of the first kind, except reps with ıplex characters and these are of the third kind.

vi) The Kronecker products of the various reps of each point group and the compatibilities between the reps of ɔint group and those of its subgroups are given in the tables of Koster, Dimmock, Wheeler, and Statz (1963).

TABLE 2.3

Matrices for the degenerate representations of the crystallographic point groups

Tetragonal groups

Key: ε $\begin{bmatrix}1 & 0\\0 & 1\end{bmatrix}$ λ $\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}$ κ $\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}$ ρ $\begin{bmatrix}0 & -1\\1 & 0\end{bmatrix}$

Group / Rep	422 (D_4) E	4*mm* (C_{4v}) E	$\bar{4}2m$ (D_{2d}) E	Group / Rep	422 (D_4) E	4*mm* (C_{4v}) E	$\bar{4}2m$ (D_{2d}) E
E	ε	ε	ε	C_{2b}	−κ	.	.
C_{2z}	−ε	−ε	−ε	σ_y	.	λ	.
C_{4z}^+	ρ	ρ	.	σ_x	.	−λ	.
C_{4z}^-	−ρ	−ρ	.	σ_{db}	.	κ	κ
C_{2x}	λ	.	λ	σ_{da}	.	−κ	−κ
C_{2y}	−λ	.	−λ	S_{4z}^+	.	.	ρ
C_{2a}	κ	.	.	S_{4z}^-	.	.	−ρ

Trigonal and hexagonal groups

Key: ε $\begin{bmatrix}1 & 0\\0 & 1\end{bmatrix}$ α $\begin{bmatrix}-\frac{1}{2} & -\frac{1}{2}\sqrt{3}\\ \frac{1}{2}\sqrt{3} & -\frac{1}{2}\end{bmatrix}$ β $\begin{bmatrix}-\frac{1}{2} & \frac{1}{2}\sqrt{3}\\ -\frac{1}{2}\sqrt{3} & -\frac{1}{2}\end{bmatrix}$ λ $\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}$ μ $\begin{bmatrix}-\frac{1}{2} & -\frac{1}{2}\sqrt{3}\\ -\frac{1}{2}\sqrt{3} & \frac{1}{2}\end{bmatrix}$ ν $\begin{bmatrix}-\frac{1}{2} & \frac{1}{2}\sqrt{3}\\ \frac{1}{2}\sqrt{3} & \frac{1}{2}\end{bmatrix}$

Group / Rep	32 (D_3) E	3*m* (C_{3v}) E	622 (D_6) E_1	622 (D_6) E_2	6*mm* (C_{6v}) E_1	6*mm* (C_{6v}) E_2	$\bar{6}2m$ (D_{3h}) E_1	$\bar{6}2m$ (D_{3h}) E_2
E	ε	ε	ε	ε	ε	ε	ε	ε
C_6^+	.	.	−β	α	−β	α	.	.
C_6^-	.	.	−α	β	−α	β	.	.
C_3^+	α	α	α	β	α	β	α	α
C_3^-	β	β	β	α	β	α	β	β
C_2	.	.	−ε	ε	−ε	ε	.	.
C'_{21}	λ	.	λ	λ	.	.	λ	−λ
C'_{22}	μ	.	μ	ν	.	.	μ	−μ
C'_{23}	ν	.	ν	μ	.	.	ν	−ν
C''_{21}	.	.	−λ	λ	.	.	.	.
C''_{22}	.	.	−μ	ν	.	.	.	.
C''_{23}	.	.	−ν	μ	.	.	.	.
σ_{v1}	.	.	.	.	λ	λ	λ	λ
σ_{v2}	.	.	.	.	μ	ν	μ	μ
σ_{v3}	.	.	.	.	ν	μ	ν	ν
σ_{d1}	.	λ	.	.	−λ	λ	.	.
σ_{d2}	.	μ	.	.	−μ	ν	.	.
σ_{d3}	.	ν	.	.	−ν	μ	.	.
σ_h	.	.	.	.	.	.	ε	−ε
S_3^+	.	.	.	.	.	.	α	−α
S_3^-	.	.	.	.	.	.	β	−β

The doubly-degenerate representations, E, of the cubic groups

432 (O), $\bar{4}3m$ (T_d):	E, C_{2x}, C_{2y}, C_{2z}	ε
432 (O), $\bar{4}3m$ (T_d):	C_{31}^+, C_{32}^+, C_{33}^+, C_{34}^+	α
432 (O), $\bar{4}3m$ (T_d);	C_{31}^-, C_{32}^-, C_{33}^-, C_{34}^-	β
432 (O):	C_{2a}, C_{4z}^+, C_{4z}^-, C_{2b}	λ
$\bar{4}3m$ (T_d):	σ_{da}, S_{4z}^-, S_{4z}^+, σ_{db}	λ
432 (O):	C_{4x}^-, C_{4x}^+, C_{2f}, C_{2d}	μ
$\bar{4}3m$ (T_d):	S_{4x}^+, S_{4x}^-, σ_{df}, σ_{dd}	μ
432 (O):	C_{4y}^+, C_{4y}^-, C_{2c}, C_{2e}	ν
$\bar{4}3m$ (T_d):	S_{4y}^-, S_{4y}^+, σ_{dc}, σ_{de}	ν

See key to trigonal and hexagonal groups, above, for the identification of the matrices.

The threefold degenerate representations of the cubic groups

Given a representation of 432 (O) or $\bar{4}3m$ (T_d), the representatives for the operations of these groups that do not belong to 23 (T), which are listed under the headings 432 (O) and $\bar{4}3m$ (T_d) in the first part of the table, are obtained as follows: take the corresponding matrix from the first part of the table and post-multiply it with the matrix that appears under the representation chosen at the bottom of the table.

23 (T), 432 (O) $\bar{4}3m$ (T_d)	432 (O)	$\bar{4}3m$ (T_d)	
E	C_{2a}	σ_{da}	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$
C_{2x}	C_{4z}^-	S_{4z}^+	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$
C_{2y}	C_{4z}^+	S_{4z}^-	$\begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$
C_{2z}	C_{2b}	σ_{db}	$\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$
C_{31}^-	C_{4x}^+	S_{4x}^-	$\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$
C_{32}^-	C_{4x}^-	S_{4x}^+	$\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ -1 & 0 & 0 \end{bmatrix}$
C_{33}^-	C_{2f}	σ_{df}	$\begin{bmatrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ -1 & 0 & 0 \end{bmatrix}$
C_{34}^-	C_{2d}	σ_{dd}	$\begin{bmatrix} 0 & -1 & 0 \\ 0 & 0 & -1 \\ 1 & 0 & 0 \end{bmatrix}$
C_{31}^+	C_{4y}^-	S_{4y}^+	$\begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$
C_{32}^+	C_{4y}^+	S_{4y}^-	$\begin{bmatrix} 0 & 0 & -1 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \end{bmatrix}$
C_{33}^+	C_{2c}	σ_{dc}	$\begin{bmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$
C_{34}^+	C_{2e}	σ_{de}	$\begin{bmatrix} 0 & 0 & 1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{bmatrix}$

432 (O)	$\bar{4}3m$ (T_d)	T_1	T_2
C_{2a}	σ_{da}	$\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$	$\begin{bmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$

Note to Table 2.3

See Note (iv) to Table 2.2 concerning direct product groups. The note applies here with 'm substituted for 'character' wherever the word 'character' appears.

TABLE 2.4

Surface harmonics for the cyclic groups

$\bar{1}$ (C_i)	l
A_g	0
A_u	1

2 (C_2)	m mod 2
A	0
B	1

m (C_{1h})	l	m mod 2
A'	0	0
	1	1
A''	2	1
	1	0

3 (C_3)	m mod 3
A	0
^1E	1
^2E	2

$\bar{6}$ (C_{3h})	l
A'	0
	3
A''	1
	4
$^1E'$	1
	2
$^2E'$	1
	2
$^1E''$	2
	3
$^2E''$	2
	3

4 (C_4)	m mod 4
A	0
B	2
^1E	1
^2E	3

$\bar{4}$ (S_4)	l
A	0
	3
B	1
	2
^1E	1
	2
^2E	1
	2

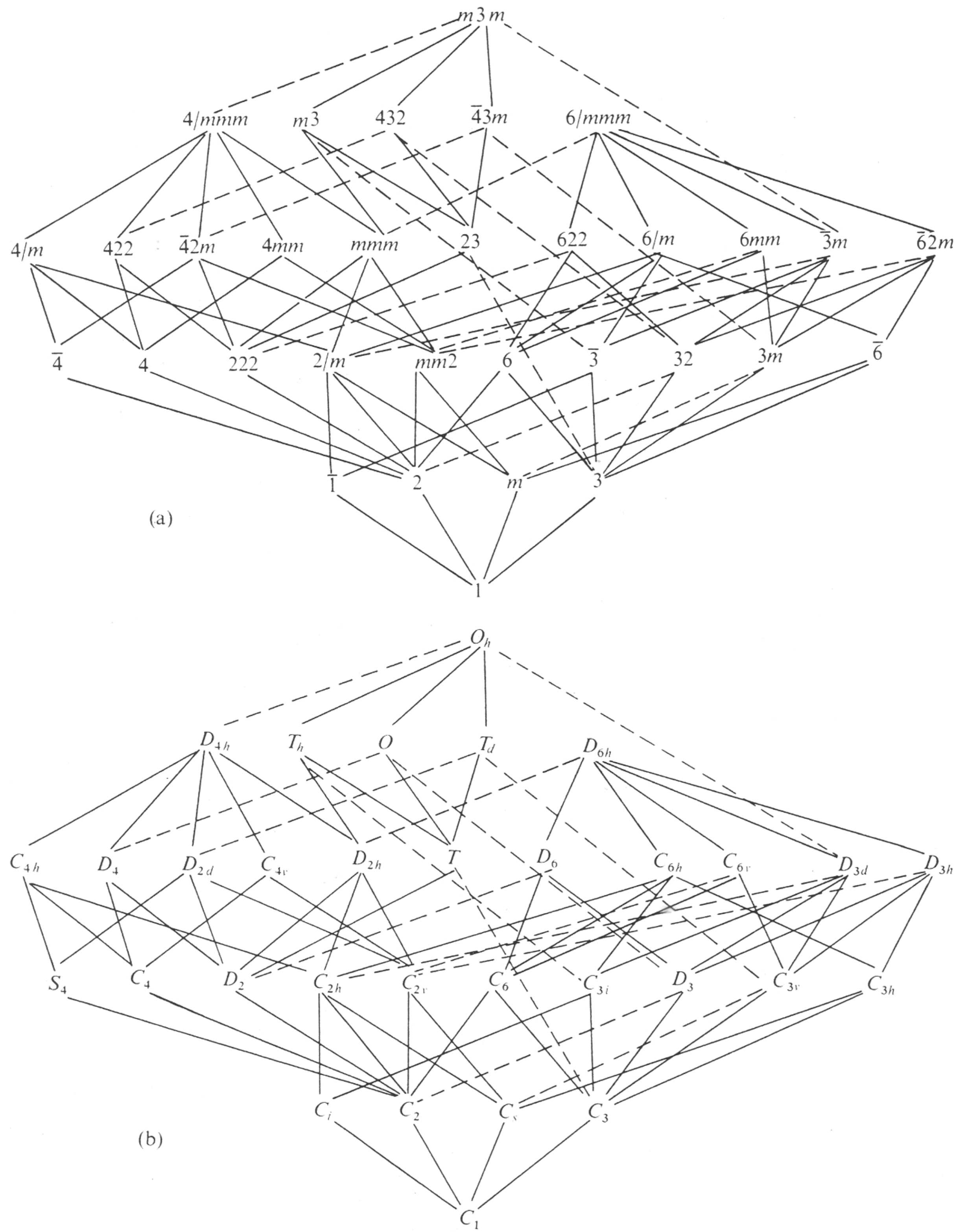


FIG. 4.1. The genealogical relations between the point groups. A continuous line indicates that a subgroup is invariant. (a) international notation. (b) Schönflies notation.