

1.2. REPRESENTATIONS OF CRYSTALLOGRAPHIC GROUPS

Table 1.2.6.1. Finite point groups in three dimensions

Isomorphism class	First class with determinants > 0	Second class with $-E$	Third class without $-E$	Order
$C_n$	$n$		$\bar{n}$ ( $n$ even, $> 2$ ) $m$ ( $n = 2$ )	$n$
$D_n$	$n22$ ( $n$ even) $n2$ ( $n$ odd, $> 1$ )		$mmm$ ( $n$ even) $\bar{n}2m$ ( $n$ even) $nm$ ( $n$ odd)	$2n$
$C_n \times C_2$		$\bar{n}$ ( $n$ odd) $n/m$ ( $n$ even)		$2n$
$D_n \times C_2$		$n/mmm$ ( $n$ even, $\geq 4$ ) $mmm$ ( $n = 2$ ) $\bar{n}m$ ( $n$ odd, $> 0$ )		$4n$
$T$	23			12
$O$	432		$\bar{4}3m$	24
$I$	532			60
$T \times C_2$		$m\bar{3}$		24
$O \times C_2$		$m\bar{3}m$		48
$I \times C_2$		$\bar{5}3m$		120

Table 1.2.6.5. The character tables for the 32 three-dimensional crystallographic point groups. The groups are grouped by isomorphism class (there are 18 isomorphism classes).

For each isomorphism class, the character table is given, including the symbol for the isomorphism class, the number  $n$  of elements per conjugacy class and the order of the elements in each such class. The conjugation classes are specified by representative elements expressed in terms of the generators  $\alpha, \beta, \dots$ . The irreps are denoted by  $\Gamma_i$ , where  $i$  takes as many values as there are conjugation classes. In each isomorphism class for each point group, given by its international symbol and its Schoenflies symbol, identification is made between the generators of the abstract group ( $\alpha, \beta$ ) and the generating orthogonal transformations. Notation:  $C_{nx}$  is a rotation of  $2\pi/n$  along the  $x$  axis,  $\sigma_x$  is a reflection from a plane perpendicular to the  $x$  axis,  $S_{nz}$  is a rotation over  $2\pi/n$  along the  $z$  axis multiplied by  $-E$  and  $\sigma_v$  is a reflection from a plane through the unique axis.

The notation for the irreducible representations can be given as  $\Gamma_i$ , but other systems have been used as well. Indicated below are the relations between  $\Gamma_i$  and a system that uses a characterization according to the dimension of the representation and (for

groups of the second kind) the sign of the representative of  $-E$ . This nomenclature is often used by spectroscopists.

- $A, A_1, A_2, A', A''$  one-dimensional
- $B, B_1, B_2, B_3$  one-dimensional
- $E$  two-dimensional
- $T, T_1, T_2$  three-dimensional
- $A_g, B_g$  etc. gerade
- $A_u, B_u$  etc. ungerade

The other notation for which the relation with the present notation is indicated is that of Kopský, and is used in the accompanying software.

The three functions  $x, y$  and  $z$  transform according to the vector representation of the point group, which is generally reducible. The reduction into irreducible components of this three-dimensional vector representation is indicated.

The six bilinear functions  $x^2, xy, xz, y^2, yz, z^2$  transform according to the symmetrized product of the vector representation. The basis functions of the irreducible components are indicated. Because the basis functions are real, one should consider the physically irreducible representations.

Table 1.2.6.6. The point groups of the second class containing  $-E$  are obtained from those of the first class by taking the direct product with the group generated by  $\bar{1}$ . From the point groups, one obtains nonmagnetic point groups by the direct product with the group generated by the time reversal  $1'$ . The relation between the characters of a point group and its direct products with

Table 1.2.6.2. Crystallographic point groups in three dimensions

Isomorphism class	First class	Second class with $-E$	Third class without $-E$	Order
$C_1$	1			1
$C_2$	2	$\bar{1}$	$m$	2
$C_3$	3			3
$C_4$	4		4	4
$D_2$	222	$2/m$	$2mm$	4
$C_6$	6	$\bar{3}$	$\bar{6}$	6
$D_3$	32		$3m$	6
$C_4 \times C_2$		$4/m$		8
$D_4$	422		$4mm, \bar{4}2m$	8
$D_2 \times C_2$		$mmm$		8
$D_6$	622	$\bar{3}m$	$6mm, \bar{6}2m$	12
$T$	23			12
$C_6 \times C_2$		$6/m$		12
$D_4 \times C_2$		$4/mmm$		16
$O$	432		$\bar{4}3m$	24
$D_6 \times C_2$		$6/mmm$		24
$T \times C_2$		$m\bar{3}$		24
$O \times C_2$		$m\bar{3}m$		48

Table 1.2.6.3. Irreducible representations for cyclic groups  $C_n$

$\omega = \exp(2\pi i/n)$ , s.c.m. = smallest common multiple.

$n_i$	$\epsilon$	$\alpha$	$\alpha^2$	$\alpha^3$	...	$\alpha^{n-1}$
Order	1	$n$	s.c.m.( $n, 2$ )	s.c.m.( $n, 3$ )	...	$n$
$\Gamma_1$	1	1	1	1	...	1
$\Gamma_2$	1	$\omega$	$\omega^2$	$\omega^3$	...	$\omega^{-1}$
$\vdots$	1	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
$\Gamma_n$	1	$\omega^{-1}$	$\omega^{-2}$	$\omega^{-3}$	...	$\omega$

Table 1.2.6.4. Irreducible representations for dihedral groups  $D_n$

(a)  $n$  odd.  $m = 1, \dots, (n-1)/2$ ;  $j = 1, \dots, (n-1)/2$ , s.c.m. = smallest common multiple.

$n_i$	$\epsilon$	$\alpha^j$	...	$\beta$
Order	1	s.c.m.( $n, j$ )	...	$n$
$\Gamma_1$	1	1	...	1
$\Gamma_2$	1	1	...	-1
$\Gamma_{2+m}$	2	$2\cos(2\pi mj/n)$	...	0

(b)  $n$  even.  $m = 1, \dots, (n/2 - 1)$ ;  $j = 1, \dots, (n/2 - 1)$ , s.c.m. = smallest common multiple.

$n_i$	$\epsilon$	$\alpha^{n/2}$	$\alpha^j$	...	$\beta$	$\alpha\beta$
Order	1	2	s.c.m.( $n, j$ )	...	$n/2$	$n/2$
$\Gamma_1$	1	1	1	...	1	1
$\Gamma_2$	1	1	1	...	-1	-1
$\Gamma_3$	1	$(-1)^{n/2}$	$(-1)^j$	...	1	-1
$\Gamma_4$	1	$(-1)^{n/2}$	$(-1)^j$	...	-1	1
$\Gamma_{4+m}$	2	$(-1)^{m/2}$	$2\cos(2\pi mj/n)$	...	0	0