Character Tables for the Crystal Point Groups

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Notes

The point groups are labelled by their *international* symbols (with the *Schoenflies* symbols in brackets).

The *classes* of group elements are indicated by one typical element followed in square brackets by the number of elements in that class. The symbol n stands for a rotation by $2\pi/n$, and n^r for $2\pi\, r/n$. The rotation axis is given by a suffix, e.g. x, y, and z; d means an axis at $\pi/4$ to Ox and Oy. The symbol m_z means a reflection in a plane perpendicular to the z-axis. $\bar{n}$ is an improper rotation by $2\pi/n$, i.e. a proper rotation by this angle followed by inversion through the origin. An inversion on its own is thus denoted by $\bar{1}$.

The *irreducible representations* are labelled according to two schemes, the first being the Γ_n notation of Bethe, following the convention of Koster, Dimmock, Wheeler and Statz in *Properties of the Thirty-Two Point Groups*, and the second is a systematic approach described as follows. A and B refer to one-dimensional representations, B being used if a rotation by $2\pi/n$ about the principal axis (chosen as the z-axis) has the character –1. E is used for a two-dimensional representation, and T for a three-dimensional one. A pair of complex conjugate one-dimensional representations are always bracketed together and regarded as a two-dimensional representation E because time-reversal symmetry makes them degenerate. If there are two representations in which the characters of m_z differ in sign, then they are distinguished by ′ and ″. Subscripts g and u (German: *gerade* and *ungerade*) indicate even and odd representations under inversion. In the event of both (′,″) and (g,u) labellings being applicable, (g,u) takes precedence over (′,″), which in turn precedes numerical subscripts, 1, 2, etc.

Some point groups are direct products, $\mathcal{G} \times \bar{1}$, where $\mathcal{G}$ contains only proper rotations R_1, R_2, etc, and $\bar{1}$ is the inversion group (E, $\bar{1}$). Their character tables may be constructed as follows. If D is an irreducible representation of $\mathcal{G}$, then the group $\mathcal{G} \times \bar{1}$ will contain two corresponding irreducible representations, D_g and D_u, with characters of opposite signs for the improper rotations, and the same sign for the proper rotations:

$\mathcal{G}$		R
Γ	D	$\chi(R)$

$\mathcal{G} \times \bar{1}$		R	$\bar{R}$
Γ^+	D_g	$\chi(R)$	$\chi(R)$
Γ^-	D_u	$\chi(R)$	$-\chi(R)$

On the right side of each character table are listed, in the row of the irreducible representation according to which they transform, the coordinate variables x, y, z, various products of these variables, and the infinitesimal rotations R_x, R_y and R_z (which transform as a pseudovector). For the direct product groups, x, y, z transform according to the appropriate *ungerade* representation, D_u (or Γ^-), and x^2, y^2, z^2, xy, yz, xz, R_x, R_y, R_z transform according to D_g (Γ^+).

Triclinic, monoclinic and orthorhombic point groups

1 (C_1)		E	
Γ_1	A	1	$x, y, z, x^2, y^2, z^2,$ $xy, yz, xz, R_x, R_y, R_z$

$\bar{1}$ (S_2/C_i)		E	$\bar{1}$	
Γ_1^+	A_g	1	1	$x^2, y^2, z^2, xy, yz, xz, R_x, R_y, R_z$
Γ_1^-	A_u	1	–1	x, y, z

2 (C_2)		E	2_z	
Γ_1	A	1	1	$z, x^2, y^2, z^2, xy, R_z$
Γ_2	B	1	–1	x, y, yz, xz, R_x, R_y

m (C_{1h}/C_s)		E	m_z	
Γ_1	A'	1	1	$x, y, x^2, y^2, z^2, xy, R_z$
Γ_2	A''	1	–1	z, yz, xz, R_x, R_y

222 (D_2/V)		E	2_x	2_y	2_z	
Γ_1	A	1	1	1	1	x^2, y^2, z^2
Γ_3	B_1	1	–1	–1	1	z, xy, R_z
Γ_2	B_2	1	–1	1	–1	y, xz, R_y
Γ_4	B_3	1	1	–1	–1	x, yz, R_x

$$mmm\ (D_{2h}/V_h) = 222 \times \bar{1}$$

$2mm$ (C_{2v})		E	2_z	m_y	m_x	
Γ_1	A_1	1	1	1	1	z, x^2, y^2, z^2
Γ_3	A_2	1	1	–1	–1	xy, R_z
Γ_2	B_1	1	–1	1	–1	x, xz, R_y
Γ_4	B_2	1	–1	–1	1	y, yz, R_x

$2/m$ (C_{2h})		E	2_z	m_z	$\bar{1}$	
Γ_1^+	A_g	1	1	1	1	x^2, y^2, z^2, xy, R_z
Γ_2^+	B_g	1	–1	–1	1	yz, xz, R_x, R_y
Γ_1^-	A_u	1	1	–1	–1	z
Γ_2^-	B_u	1	–1	1	–1	x, y

Tetragonal point groups

4 (C_4)		E	2_z	4_z	$(4_z)^3$	
Γ_1	A	1	1	1	1	z, x^2+y^2, z^2, R_z
Γ_2	B	1	1	–1	–1	$x^2–y^2$, xy
Γ_3	E {	1	–1	i	$–i$	(x, y), (xz, yz), (R_x, R_y)
Γ_4		1	–1	$–i$	i	

$4/m$ (C_{4h}) $= 4 \times \bar{1}$

$\bar{4}$ (S_4)		E	2_z	$\bar{4}_z$	$(\bar{4}_z)^3$	
Γ_1	A	1	1	1	1	x^2+y^2, z^2, R_z
Γ_2	B	1	1	–1	–1	z, $x^2–y^2$, xy
Γ_3	E {	1	–1	i	$–i$	(x, y), (xz, yz), (R_x, R_y)
Γ_4		1	–1	$–i$	i	

422 (D_4)		E	2_z	4_z [2]	2_x [2]	2_d [2]	
Γ_1	A_1	1	1	1	1	1	x^2+y^2, z^2
Γ_2	A_2	1	1	1	–1	–1	z, R_z
Γ_3	B_1	1	1	–1	1	–1	x^2-y^2
Γ_4	B_2	1	1	–1	–1	1	xy
Γ_5	E	2	–2	0	0	0	(x, y), (xz, yz), (R_x, R_y)

$4/mmm$ (D_{4h}) = $422 \times \bar{1}$

$4mm$ (C_{4v})		E	2_z	4_z [2]	m_x [2]	m_d [2]	
Γ_1	A_1	1	1	1	1	1	z, x^2+y^2, z^2
Γ_2	A_2	1	1	1	–1	–1	R_z
Γ_3	B_1	1	1	–1	1	–1	x^2-y^2
Γ_4	B_2	1	1	–1	–1	1	xy
Γ_5	E	2	–2	0	0	0	(x, y), (xz, yz), (R_x, R_y)

$\bar{4}2m$ (D_{2d}/V_d)		E	2_z	$\bar{4}_z$ [2]	2_x [2]	m_d [2]	
Γ_1	A_1	1	1	1	1	1	x^2+y^2, z^2
Γ_2	A_2	1	1	1	–1	–1	R_z
Γ_3	B_1	1	1	–1	1	–1	x^2-y^2
Γ_4	B_2	1	1	–1	–1	1	z, xy
Γ_5	E	2	–2	0	0	0	(x, y), (xz, yz), (R_x, R_y)

Trigonal and hexagonal point groups

$3\ (C_3)$		E	3_z	$(3_z)^2$	$\omega = e^{2\pi i/3}$
Γ_1	A	1	1	1	$z,\ x^2+y^2,\ z^2,\ R_z$
Γ_2	E {	1	ω	ω^2	$(x, y),\ (x^2-y^2, xy),\ (yz, xz),\ (R_x, R_y)$
Γ_3		1	ω^2	ω	

$\bar{3}\ (S_6/C_{3i}) \quad = \quad 3 \times \bar{1}$

$32\ (D_3)$		E	3_z [2]	2_y [3]	
Γ_1	A_1	1	1	1	$x^2+y^2,\ z^2$
Γ_2	A_2	1	1	–1	$z,\ R_z$
Γ_3	E	2	–1	0	$(x, y),\ (x^2-y^2, xy),\ (yz, xz),\ (R_x, R_y)$

$\bar{3}\,m\ (D_{3d}) \quad = \quad 32 \times \bar{1}$

$3m\ (C_{3v})$		E	3_z [2]	m_x [3]	
Γ_1	A_1	1	1	1	$z,\ x^2+y^2,\ z^2$
Γ_2	A_2	1	1	–1	R_z
Γ_3	E	2	–1	0	$(x, y),\ (x^2-y^2, xy),\ (yz, xz),\ (R_x, R_y)$

$6\ (C_6)$		E	6_z	3_z	2_z	$(3_z)^2$	$(6_z)^5$	$\omega = e^{2\pi i/3}$
Γ_1	A	1	1	1	1	1	1	z, x^2+y^2, z^2, R_z
Γ_4	B	1	–1	1	–1	1	–1	
Γ_5	E_1 {	1	$-\omega^2$	ω	–1	ω^2	$-\omega$	(x, y), (xz, yz), (R_x, R_y)
Γ_6		1	$-\omega$	ω^2	–1	ω	$-\omega^2$	
Γ_3	E_2 {	1	ω	ω^2	1	ω	ω^2	x^2-y^2, xy
Γ_2		1	ω^2	ω	1	ω^2	ω	

$6/m\ (C_{6h}) = 6 \times \bar{1}$

$\bar{6}\ (C_{3h})$		E	3_z	$(3_z)^2$	m_z	$\bar{6}_z$	$(\bar{6}_z)^5$	$\omega = e^{2\pi i/3}$
Γ_1	A'	1	1	1	1	1	1	x^2+y^2, z^2, R_z
Γ_4	A''	1	1	1	–1	–1	–1	z
Γ_2	E' {	1	ω	ω^2	1	ω	ω^2	
Γ_3		1	ω^2	ω	1	ω^2	ω	(x, y), (x^2-y^2, xy)
Γ_5	E'' {	1	ω	ω^2	–1	$-\omega$	$-\omega^2$	
Γ_6		1	ω^2	ω	–1	$-\omega^2$	$-\omega$	(xz, yz), (R_x, R_y)

$622\ (D_6)$		E	2_z	3_z [2]	6_z [2]	2_y [3]	2_x [3]	
Γ_1	A_1	1	1	1	1	1	1	x^2+y^2, z^2
Γ_2	A_2	1	1	1	1	–1	–1	z, R_z
Γ_3	B_1	1	–1	1	–1	1	–1	
Γ_4	B_2	1	–1	1	–1	–1	1	
Γ_5	E_1	2	–2	–1	1	0	0	(x, y), (xz, yz), (R_x, R_y)
Γ_6	E_2	2	2	–1	–1	0	0	(x^2-y^2, xy)

$6/mmm\ (D_{6h}) = 622 \times \bar{1}$

$6mm$ (C_{6v})		E	2_z	3_z [2]	6_z [2]	m_y [3]	m_x [3]	
Γ_1	A_1	1	1	1	1	1	1	z, x^2+y^2, z^2
Γ_2	A_2	1	1	1	1	–1	–1	R_z
Γ_3	B_1	1	–1	1	–1	–1	1	
Γ_4	B_2	1	–1	1	–1	1	–1	
Γ_5	E_1	2	–2	–1	1	0	0	(x, y), (xz, yz), (R_x, R_y)
Γ_6	E_2	2	2	–1	–1	0	0	(x^2-y^2, xy)

$\bar{6}\,m2$ (D_{3h})		E	m_z	3_z [2]	$\bar{6}_z$ [2]	2_y [3]	m_x [3]	
Γ_1	A'_1	1	1	1	1	1	1	x^2+y^2, z^2
Γ_2	A'_2	1	1	1	1	–1	–1	R_z
Γ_3	A''_1	1	–1	1	–1	1	–1	
Γ_4	A''_2	1	–1	1	–1	–1	1	z
Γ_6	E'	2	2	–1	–1	0	0	(x, y), (x^2-y^2, xy)
Γ_5	E''	2	–2	–1	1	0	0	(xz, yz), (R_x, R_y)

Cubic point groups

23 (T)		E	2_z [3]	3 [4]	$(3)^2$ [4]	$\omega = e^{2\pi i/3}$
Γ_1	A	1	1	1	1	$x^2+y^2+z^2 = r^2$
Γ_2	E {	1	1	ω	ω^2	$(x^2-y^2, 3z^2-r^2)$
Γ_3		1	1	ω^2	ω	
Γ_4	T	3	–1	0	0	$(x, y, z), (xy, yz, xz), (R_x, R_y, R_z)$

$m3$ (T_h) = $23 \times \bar{1}$

432 (O)		E	3 [8]	2_z [3]	2_d [6]	4_z [6]	
Γ_1	A_1	1	1	1	1	1	$x^2+y^2+z^2 = r^2$
Γ_2	A_2	1	1	1	–1	–1	
Γ_3	E	2	–1	2	0	0	$(x^2-y^2, 3z^2-r^2)$
Γ_4	T_1	3	0	–1	–1	1	$(x, y, z), (R_x, R_y, R_z)$
Γ_5	T_2	3	0	–1	1	–1	(xy, xz, yz)

$m3m$ (O_h) = $432 \times \bar{1}$

$\bar{4}3m$ (T_d)		E	3 [8]	2_z [3]	m_d [6]	$\bar{4}_z$ [6]	
Γ_1	A_1	1	1	1	1	1	$x^2+y^2+z^2 = r^2$
Γ_2	A_2	1	1	1	–1	–1	
Γ_3	E	2	–1	2	0	0	$(x^2-y^2, 3z^2-r^2)$
Γ_4	T_1	3	0	–1	–1	1	(R_x, R_y, R_z)
Γ_5	T_2	3	0	–1	1	–1	$(x, y, z), (xy, xz, yz)$