UNIVERSITY OF CAMBRIDGE

Department of Chemistry

Data Book
(revised October 2005)

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H 1 1.008																	**He** 2 4.003
Li 3 6.94	**Be** 4 9.01						**symbol** atomic number mean atomic mass					**B** 5 10.81	**C** 6 12.01	**N** 7 14.01	**O** 8 16.00	**F** 9 19.00	**Ne** 10 20.18
Na 11 22.99	**Mg** 12 24.31											**Al** 13 26.98	**Si** 14 28.09	**P** 15 30.97	**S** 16 32.06	**Cl** 17 35.45	**Ar** 18 39.95
K 19 39.102	**Ca** 20 40.08	**Sc** 21 44.96	**Ti** 22 47.90	**V** 23 50.94	**Cr** 24 52.00	**Mn** 25 54.94	**Fe** 26 55.85	**Co** 27 58.93	**Ni** 28 58.71	**Cu** 29 63.55	**Zn** 30 65.37	**Ga** 31 69.72	**Ge** 32 72.59	**As** 33 74.92	**Se** 34 78.96	**Br** 35 79.904	**Kr** 36 83.80
Rb 37 85.47	**Sr** 38 87.62	**Y** 39 88.91	**Zr** 40 91.22	**Nb** 41 92.91	**Mo** 42 95.94	**Tc** 43	**Ru** 44 101.07	**Rh** 45 102.91	**Pd** 46 106.4	**Ag** 47 107.87	**Cd** 48 112.40	**In** 49 114.82	**Sn** 50 118.69	**Sb** 51 121.75	**Te** 52 127.60	**I** 53 126.90	**Xe** 54 131.30
Cs 55 132.91	**Ba** 56 137.34	**La*** 57 138.91	**Hf** 72 178.49	**Ta** 73 180.95	**W** 74 183.85	**Re** 75 186.2	**Os** 76 190.2	**Ir** 77 192.2	**Pt** 78 195.09	**Au** 79 196.97	**Hg** 80 200.59	**Tl** 81 204.37	**Pb** 82 207.2	**Bi** 83 208.98	**Po** 84	**At** 85	**Rn** 86
Fr 87	**Ra** 88	**Ac+** 89															

***Lanthanides**	**Ce** 58 140.12	**Pr** 59 140.91	**Nd** 60 144.24	**Pm** 61	**Sm** 62 150.4	**Eu** 63 151.96	**Gd** 64 157.25	**Tb** 65 158.93	**Dy** 66 162.50	**Ho** 67 164.93	**Er** 68 167.26	**Tm** 69 168.93	**Yb** 70 173.04	**Lu** 71 174.97
+Actinides	**Th** 90 232.01	**Pa** 91	**U** 92 238.03	**Np** 93	**Pu** 94	**Am** 95	**Cm** 96	**Bk** 97	**Cf** 98	**Es** 99	**Fm** 100	**Md** 101	**No** 102	**Lr** 103

Constants

Name	Symbol and definition	Value (uncertainty)	Unit
	π	3.141592653589...	
	e	2.718281828459...	
	$\ln 10 = 1/\log_{10} e$	2.302585092994...	
Speed of light	c	2.99792458	$10^{8}\,\mathrm{m\,s^{-1}}$
Planck's constant	h	6.6260693(11)	$10^{-34}\,\mathrm{J\,s}$
	$\hbar = h/2\pi$	1.05457168(18)	$10^{-34}\,\mathrm{J\,s}$
Avogadro's constant	N_A	6.0221415(10)	$10^{23}\,\mathrm{mol^{-1}}$
Elementary charge	e	1.60217653(14)	$10^{-19}\,\mathrm{C}$
Electron rest mass	m_e	0.91093826(16)	$10^{-30}\,\mathrm{kg}$
Atomic mass unit	$m_u = 1\,\mathrm{g\,mol^{-1}}/N_A$	1.66053886(28)	$10^{-27}\,\mathrm{kg}$
Proton rest mass	m_p	1.67262171(29)	$10^{-27}\,\mathrm{kg}$
Neutron rest mass	m_n	1.67492728(29)	$10^{-27}\,\mathrm{kg}$
Faraday constant	$F = N_A e$	9.64853383(83)	$10^{4}\,\mathrm{C\,mol^{-1}}$
Boltzmann constant	k_B	1.3806505(24)	$10^{-23}\,\mathrm{J\,K^{-1}}$
Molar Gas constant	$R = N_A k_B$	8.314472(15)	$\mathrm{J\,mol^{-1}\,K^{-1}}$
Permeability of vacuum	μ_0	$4\pi \times 10^{-7}$	$\mathrm{H\,m^{-1}}$
Permittivity of vacuum	$\varepsilon_0 = 1/(\mu_0 c^2)$	8.8541878...	$10^{-12}\,\mathrm{F\,m^{-1}}$
	$4\pi\varepsilon_0$	1.1126501...	$10^{-10}\,\mathrm{F\,m^{-1}}$
Bohr magneton	$\mu_B = e\hbar/2m_e$	9.27400949(80)	$10^{-24}\,\mathrm{J\,T^{-1}}$
Nuclear magneton	$\mu_N = e\hbar/2m_p$	5.05078343(43)	$10^{-27}\,\mathrm{J\,T^{-1}}$
Stefan-Boltzmann constant	$\sigma = 2\pi^5 k_B^4/15h^3c^2$	5.670400(40)	$10^{-8}\,\mathrm{W\,m^{-2}\,K^{-4}}$
Bohr radius	$a_0 = 4\pi\varepsilon_0\hbar^2/m_e e^2$	0.5291772108(18)	$10^{-10}\,\mathrm{m}$
Hartree energy	$E_h = e^2/4\pi\varepsilon_0 a_0$	4.35974417(75)	$10^{-18}\,\mathrm{J}$
Fine structure constant	$\alpha = e^2/4\pi\varepsilon_0\hbar c$	7.297352568(24)	10^{-3}
	α^{-1}	137.035986	

CODATA recommended values, December 2002
http://physics.nist.gov/constants
The estimated standard uncertainty, in parentheses after the value, applies to the least significant digits of the value.

Energy Conversion Factors

	J	$\mathrm{kJ\,mol^{-1}}$	$\mathrm{cm^{-1}}$	K
1 J	1	$6.0221\,.\,10^{20}$	$5.0341\,.\,10^{22}$	$7.2429\,.\,10^{22}$
1 hartree	$4.35974\,.\,10^{-18}$	2625.5	219 475	315 773
1 eV	$1.60218\,.\,10^{-19}$	96.485	8065.54	11 604
1 $\mathrm{kJ\,mol^{-1}}$	$1.66054\,.\,10^{-21}$	1	83.5935	120.27
1 $\mathrm{cm^{-1}}$	$1.98645\,.\,10^{-23}$	$11.963\,.\,10^{-3}$	1	1.4388
1 K	$1.38065\,.\,10^{-23}$	$8.3145\,.\,10^{-3}$	0.69504	1
1 Hz	$6.62607\,.\,10^{-34}$	$3.9903\,.\,10^{-13}$	$3.3356\,.\,10^{-11}$	$4.7992\,.\,10^{-11}$

Note: the energy of a photon with reciprocal wavelength (wavenumber) $1/\lambda$ and frequency ν is $hc/\lambda = h\nu$. The energy corresponding to a temperature T is $k_B T$.

Other conversion factors

Length	Å	$10^{-10}\,\mathrm{m}$
Energy	cal	4.184 J
Pressure	atm = 760 Torr	101 325 Pa
	Torr = mm Hg	133.3 Pa
	bar	$10^{5}\,\mathrm{Pa}$
Radioactivity	becquerel, Bq	$1\,\mathrm{s^{-1}}$
	curie, Ci	$3.7\,.\,10^{10}\,\mathrm{Bq}$
Charge	esu	$3.33564\,.\,10^{-10}\,\mathrm{C}$
Dipole moment	debye $= 10^{-18}$ esu cm	$3.33564\,.\,10^{-30}\,\mathrm{C\,m}$
	a.u. $= ea_0$	$8.478358\,.\,10^{-30}\,\mathrm{C\,m}$
Temperature	°C	0 °C = 273.15 K

The 'entropy unit' (e.u.) used for entropies of activation is usually the c.g.s. unit cal/mol/°C. However some authors use the same symbol for the SI unit, $\mathrm{J\,mol^{-1}\,K^{-1}}$.

Greek Alphabet

Α	α	alpha	Η	η	eta	Ν	ν	nu	Τ	τ	tau
Β	β	beta	Θ	θ, ϑ	theta	Ξ	ξ	xi	ϒ	υ	upsilon
Γ	γ	gamma	Ι	ι	iota	Ο	*o*	omicron	Φ	ϕ, φ	phi
Δ	δ	delta	Κ	κ	kappa	Π	π	pi	Χ	χ	chi
Ε	ε	epsilon	Λ	λ	lambda	Ρ	ρ	rho	Ψ	ψ	psi
Ζ	ζ	zeta	Μ	μ	mu	Σ	σ	sigma	Ω	ω	omega

Series

Geometrical progression

$$S_n = a + az + az^2 + \cdots + az^{n-1} = a\frac{1-z^n}{1-z}. \qquad S_\infty = \frac{a}{1-z} \quad \text{when } |z| < 1.$$

Power series

$$\exp z = 1 + z + \frac{z^2}{2!} + \frac{z^3}{3!} + \cdots + \frac{z^n}{n!} + \cdots$$

$$\cos z = \frac{e^{iz} + e^{-iz}}{2} = 1 - \frac{z^2}{2!} + \frac{z^4}{4!} - \frac{z^6}{6!} + \cdots$$

$$\sin z = \frac{e^{iz} - e^{-iz}}{2i} = z - \frac{z^3}{3!} + \frac{z^5}{5!} - \frac{z^7}{7!} + \cdots$$

$$(1+z)^p = 1 + pz + \frac{p(p-1)}{2!}z^2 + \frac{p(p-1)(p-2)}{3!}z^3 + \cdots, \qquad |z| < 1$$

$$\ln(1+z) = z - \frac{z^2}{2} + \frac{z^3}{3} - \cdots - \frac{(-z)^n}{n} - \cdots, \qquad |z| < 1$$

Stirling's formula

$$\ln n! \approx n \ln n - n \quad \text{for large } n$$

Determinants

$$\begin{vmatrix} a & b \\ c & d \end{vmatrix} = ad - bc$$

In general,

$$\det(\mathbf{A}) = \sum_j A_{ij} C_{ji} \quad (i \text{ fixed at any value}),$$

where the cofactor C_{ji} is $(-1)^{i+j}$ times the determinant of the matrix obtained by deleting the ith row and the jth column of **A**. For example,

$$\begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} = a_{11} \begin{vmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{vmatrix} - a_{12} \begin{vmatrix} a_{21} & a_{23} \\ a_{31} & a_{33} \end{vmatrix} + a_{13} \begin{vmatrix} a_{21} & a_{22} \\ a_{31} & a_{32} \end{vmatrix}$$

$$= a_{11}a_{22}a_{33} - a_{11}a_{23}a_{32} + a_{12}a_{23}a_{31} - a_{12}a_{21}a_{33} + a_{13}a_{21}a_{32} - a_{13}a_{22}a_{31}.$$

Integrals

$$\int_{-\infty}^{\infty} \exp\left(-ax^2\right) dx = \sqrt{\pi/a}, \qquad (a > 0)$$

$$\int_{-\infty}^{\infty} x^{2n} \exp\left(-ax^2\right) dx = 1 \times 3 \times 5 \times \ldots \times (2n-1) \frac{\sqrt{\pi/a}}{(2a)^n} \qquad (n \geq 1;\ a > 0)$$

$$\int_{0}^{\infty} r^n \exp(-ar)\, dr = \frac{n!}{a^{n+1}} \qquad (n \geq 0;\ a > 0)$$

$$\int_0^{\pi/2} \sin^m\theta \cos^n\theta\, d\theta = \frac{m-1}{m+n} \int_0^{\pi/2} \sin^{m-2}\theta \cos^n\theta\, d\theta$$
$$= \frac{n-1}{m+n} \int_0^{\pi/2} \sin^m\theta \cos^{n-2}\theta\, d\theta,$$

so that

$$\int_0^{\pi/2} \sin^m\theta \cos^n\theta\, d\theta = \frac{(m-1)(m-3)\ldots(n-1)(n-3)\ldots}{(m+n)(m+n-2)(m+n-4)\ldots} \times C,$$

where $C = \pi/2$ if m and n are both *even*, and $C = 1$ otherwise. E.g.:

$$\int_0^{\pi/2} \sin\theta \cos^3\theta\, d\theta = \frac{2}{4.2} = \frac{1}{4}; \qquad \int_0^{\pi/2} \sin^2\theta \cos^2\theta\, d\theta = \frac{1.1}{4.2}\frac{\pi}{2} = \frac{\pi}{16}.$$

Integration by parts

$$\int_a^b u \frac{\mathrm{d}v}{\mathrm{d}x}\, \mathrm{d}x = [uv]_a^b - \int_a^b \frac{\mathrm{d}u}{\mathrm{d}x} v\, \mathrm{d}x$$

Trigonometrical formulae

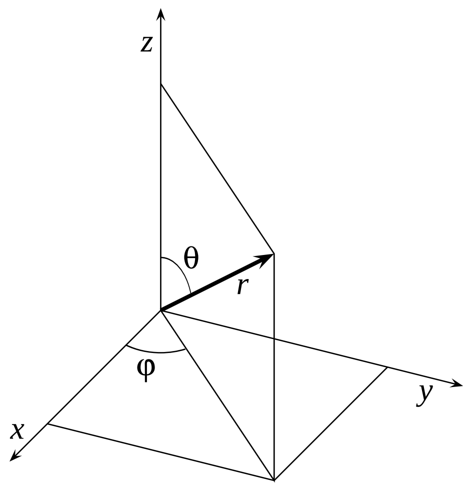
$$\sin(A \pm B) = \sin A \cos B \pm \cos A \sin B$$
$$\cos(A \pm B) = \cos A \cos B \mp \sin A \sin B$$
$$\cos A \cos B = \tfrac{1}{2}\left(\cos(A+B) + \cos(A-B)\right)$$
$$\sin A \sin B = \tfrac{1}{2}\left(\cos(A-B) - \cos(A+B)\right)$$
$$\sin A \cos B = \tfrac{1}{2}\left(\sin(A+B) + \sin(A-B)\right)$$
$$\sin A + \sin B = 2 \sin\frac{A+B}{2} \cos\frac{A-B}{2}$$
$$\sin A - \sin B = 2 \cos\frac{A+B}{2} \sin\frac{A-B}{2}$$
$$\cos A + \cos B = 2 \cos\frac{A+B}{2} \cos\frac{A-B}{2}$$
$$\cos A - \cos B = -2 \sin\frac{A+B}{2} \sin\frac{A-B}{2}$$

Cosine formula

$$a^2 = b^2 + c^2 - 2bc\cos A$$

Spherical Polar Coordinates

Relationship with Cartesian coordinates



$$x = r\sin\theta\cos\varphi \qquad r = \sqrt{x^2+y^2+z^2}$$
$$y = r\sin\theta\sin\varphi \qquad \theta = \arccos(z/r)$$
$$z = r\cos\theta \qquad \varphi = \arctan(y/x)$$

Integration

$$\int \ldots dV = \int_{r=0}^{\infty}\int_{\theta=0}^{\pi}\int_{\varphi=0}^{2\pi} \ldots r^2\sin\theta\, dr\, d\theta\, d\varphi$$

Laplacian

$$\nabla^2\psi = \frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}$$
$$= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\varphi^2}$$

Spherical Harmonics

$$Y_{lm}(\theta,\varphi) = \sqrt{\frac{2l+1}{4\pi}}C_{lm}(\theta,\varphi),$$

where

$$C_{lm}(\theta,\varphi) = \left[\frac{(l-|m|)!}{(l+|m|)!}\right]^{\frac{1}{2}} P_l^{|m|}(\cos\theta)e^{im\varphi} \times \begin{cases}(-1)^m & \text{for } m>0,\\ 1 & \text{for } m\le 0.\end{cases}$$

Here P_l^m is an associated Legendre polynomial. In particular,

$$C_{00} = 1,$$
$$C_{10} = \cos\theta = z/r,$$
$$C_{1,\pm1} = \mp\sqrt{\tfrac{1}{2}}\sin\theta e^{\pm i\varphi} = \mp\sqrt{\tfrac{1}{2}}(x\pm iy)/r,$$
$$C_{20} = \tfrac{1}{2}(3\cos^2\theta - 1) = \tfrac{1}{2}(3z^2 - r^2)/r^2,$$
$$C_{2,\pm1} = \mp\sqrt{\tfrac{3}{2}}\cos\theta\sin\theta e^{\pm i\varphi} = \mp\sqrt{\tfrac{3}{2}}(zx \pm izy)/r^2,$$
$$C_{2,\pm2} = \sqrt{\tfrac{3}{8}}\sin^2\theta e^{\pm 2i\varphi} = \sqrt{\tfrac{3}{8}}(x^2 - y^2 \pm 2ixy)/r^2.$$

Ladder Operators

$$\hat{J}_\pm \equiv \hat{J}_x \pm i\hat{J}_y; \qquad \hat{J}_\pm|J,M\rangle = \sqrt{J(J+1)-M(M\pm1)}\,|J,M\pm1\rangle$$

Character tables for some important symmetry groups

$\mathcal{C}_i$	E	i			
A_g	1	1		$R_x;R_y;R_z$	$x^2;y^2;z^2;xy;xz;yz$
A_u	1	−1	$x;y;z$		

$\mathcal{C}_s$	E	σ_h			
A'	1	1	$x;y$	R_z	$x^2;y^2;z^2;xy$
A''	1	−1	z	$R_x;R_y$	$xz;yz$

$\mathcal{C}_2$	E	C_2^z			
A	1	1	z	R_z	$x^2;y^2;z^2;xy$
B	1	−1	$x;y$	$R_x;R_y$	$xz;yz$

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$\mathcal{C}_{2v}$	E	C_2^z	σ^{xz}	σ^{yz}			
A_1	1	1	1	1	z		$x^2;y^2;z^2$
A_2	1	1	−1	−1		R_z	xy
B_1	1	−1	1	−1	x	R_y	xz
B_2	1	−1	−1	1	y	R_x	yz

$\mathcal{C}_{2h}$	E	C_2^z	i	σ^{xy}		
A_g	1	1	1	1	R_z	$x^2;y^2;z^2;xy$
B_g	1	−1	1	−1	$R_x;R_y$	$xz;yz$
A_u	1	1	−1	−1	z	
B_u	1	−1	−1	1	$x;y$	

$\mathcal{D}_2$	E	C_2^z	C_2^y	C_2^x			
A	1	1	1	1			$x^2;y^2;z^2$
B_1	1	1	−1	−1	z	R_z	xy
B_2	1	−1	1	−1	y	R_y	xz
B_3	1	−1	−1	1	x	R_x	yz

$\mathcal{D}_{2d}$	E	$2S_4$	C_2^z	$2C_2'$	$2\sigma_d$			
A_1	1	1	1	1	1			$x^2+y^2;z^2$
A_2	1	1	1	−1	−1		R_z	
B_1	1	−1	1	1	−1			x^2-y^2
B_2	1	−1	1	−1	1	z		xy
E	2	0	−2	0	0	(x,y)	(R_x,R_y)	(xz,yz)

$\mathcal{D}_{2h}$	E	C_2^z	C_2^y	C_2^x	i	σ^{xy}	σ^{xz}	σ^{yz}		
A_g	1	1	1	1	1	1	1	1		$x^2;y^2;z^2$
B_{1g}	1	1	−1	−1	1	1	−1	−1	R_z	xy
B_{2g}	1	−1	1	−1	1	−1	1	−1	R_y	xz
B_{3g}	1	−1	−1	1	1	−1	−1	1	R_x	yz
A_u	1	1	1	1	−1	−1	−1	−1		
B_{1u}	1	1	−1	−1	−1	−1	1	1	z	
B_{2u}	1	−1	1	−1	−1	1	−1	1	y	
B_{3u}	1	−1	−1	1	−1	1	1	−1	x	

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$\mathcal{C}_3$	E	C_3	C_3^2	$\omega = \exp(2\pi i/3)$		
A	1	1	1	z	R_z	$x^2+y^2;\ z^2$
E {	1	ω	ω^2	$x-iy$	$R_x - iR_y$	$xz-iyz;\ x^2+2ixy-y^2$
	1	ω^2	ω	$x+iy$	$R_x + iR_y$	$xz+iyz;\ x^2-2ixy-y^2$

$\mathcal{C}_{3v}$	E	$2C_3^z$	$3\sigma_v$			
A_1	1	1	1	z		$x^2+y^2;z^2$
A_2	1	1	−1		R_z	
E	2	−1	0	(x,y)	(R_x,R_y)	$(xz,yz);\ (x^2-y^2,2xy)$

$\mathcal{D}_3$	E	$2C_3^z$	$3C_2$			
A_1	1	1	1			$x^2+y^2;z^2$
A_2	1	1	−1	z	R_z	
E	2	−1	0	(x,y)	(R_x,R_y)	$(xz,yz);\ (x^2-y^2,2xy)$

$\mathcal{D}_{3d}$	E	$2C_3$	$3C_2$	i	$2S_6$	$3\sigma_d$			
A_{1g}	1	1	1	1	1	1			$x^2+y^2;z^2$
A_{2g}	1	1	−1	1	1	−1		R_z	
E_g	2	−1	0	2	−1	0		(R_x,R_y)	$(xz,yz);\ (x^2-y^2,2xy)$
A_{1u}	1	1	1	−1	−1	−1			
A_{2u}	1	1	−1	−1	−1	1	z		
E_u	2	−1	0	−2	1	0	(x,y)		

$\mathcal{D}_{3h}$	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$			
A_1'	1	1	1	1	1	1			$x^2+y^2;z^2$
A_2'	1	1	−1	1	1	−1		R_z	
E'	2	−1	0	2	−1	0	(x,y)		$(x^2-y^2,2xy)$
A_1''	1	1	1	−1	−1	−1			
A_2''	1	1	−1	−1	−1	1	z		
E''	2	−1	0	−2	1	0		(R_x,R_y)	(xz,yz)

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$\mathcal{C}_{4v}$	E	$2C_4$	C_4^2	$2\sigma_v$	$2\sigma_d$			
A_1	1	1	1	1	1	z		$x^2+y^2; z^2$
A_2	1	1	1	-1	-1		R_z	
B_1	1	-1	1	1	-1			x^2-y^2
B_2	1	-1	1	-1	1			xy
E	2	0	-2	0	0	(x,y)	(R_x,R_y)	(xz,yz)

Note: The σ_v planes in $\mathcal{C}_{4v}$ coincide with the xz and yz planes.

$\mathcal{D}_{4h}$	E	$2C_4$	C_4^2	$2C_2$	$2C_2'$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$		
A_{1g}	1	1	1	1	1	1	1	1	1	1		$x^2+y^2; z^2$
A_{2g}	1	1	1	-1	-1	1	1	1	-1	-1	R_z	
B_{1g}	1	-1	1	1	-1	1	-1	1	1	-1		x^2-y^2
B_{2g}	1	-1	1	-1	1	1	-1	1	-1	1		xy
E_g	2	0	-2	0	0	2	0	-2	0	0	(R_x,R_y)	(xz,yz)
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1		
A_{2u}	1	1	1	-1	-1	-1	-1	-1	1	1	z	
B_{1u}	1	-1	1	1	-1	-1	1	-1	-1	1		
B_{2u}	1	-1	1	-1	1	-1	1	-1	1	-1		
E_u	2	0	-2	0	0	-2	0	2	0	0	(x,y)	

Note: The C_2 axes in $\mathcal{D}_{4h}$ coincide with the x and y axes, and the σ_v planes with the xz and yz planes.

Note that the quantities $\eta_\pm \equiv \frac{1}{2}(\sqrt{5}\pm 1)$ satisfy $\eta_\pm{}^2 = 1 \pm \eta_\pm$ and $\eta_+\eta_- = 1$.

5

$\mathcal{C}_{5v}$	E	$2C_5$	$2C_5^2$	$5\sigma_v$	$\eta_\pm = \frac{1}{2}(\sqrt{5}\pm 1)$		
A_1	1	1	1	1	z		$x^2+y^2; z^2$
A_2	1	1	1	-1		R_z	
E_1	2	η_-	$-\eta_+$	0	(x,y)	(R_x,R_y)	(xz,yz)
E_2	2	$-\eta_+$	η_-	0			$\left(x^2-y^2, 2xy\right)$

$\mathcal{D}_5$	E	$2C_5$	$2C_5^2$	$5C_2$	$\eta_\pm = \frac{1}{2}(\sqrt{5}\pm 1)$		
A_1	1	1	1	1			$x^2+y^2; z^2$
A_2	1	1	1	-1	z	R_z	
E_1	2	η_-	$-\eta_+$	0	(x,y)	(R_x,R_y)	(xz,yz)
E_2	2	$-\eta_+$	η_-	0			$\left(x^2-y^2, 2xy\right)$

$\mathcal{D}_{5d}$	E	$2C_5$	$2C_5^2$	$5C_2$	i	$2S_{10}^3$	$2S_{10}$	$5\sigma_d$	$\eta_\pm = \frac{1}{2}(\sqrt{5}\pm 1)$		
A_{1g}	1	1	1	1	1	1	1	1			$x^2+y^2; z^2$
A_{2g}	1	1	1	-1	1	1	1	-1		R_z	
E_{1g}	2	η_-	$-\eta_+$	0	2	η_-	$-\eta_+$	0		(R_x,R_y)	(xz,yz)
E_{2g}	2	$-\eta_+$	η_-	0	2	$-\eta_+$	η_-	0			$\left(x^2-y^2, 2xy\right)$
A_{1u}	1	1	1	1	-1	-1	-1	-1			
A_{2u}	1	1	1	-1	-1	-1	-1	1	z		
E_{1u}	2	η_-	$-\eta_+$	0	-2	$-\eta_-$	η_+	0	(x,y)		
E_{2u}	2	$-\eta_+$	η_-	0	-2	η_+	$-\eta_-$	0			

$\mathcal{D}_{5h}$	E	$2C_5$	$2C_5^2$	$5C_2$	σ_h	$2S_5$	$2S_5^3$	$5\sigma_v$	$\eta_\pm = \frac{1}{2}(\sqrt{5}\pm 1)$		
A_1'	1	1	1	1	1	1	1	1			$x^2+y^2;z^2$
A_2'	1	1	1	−1	1	1	1	−1		R_z	
E_1'	2	η_-	$-\eta_+$	0	2	η_-	$-\eta_+$	0	(x,y)		
E_2'	2	$-\eta_+$	η_-	0	2	$-\eta_+$	η_-	0			$(x^2-y^2,2xy)$
A_1''	1	1	1	1	−1	−1	−1	−1			
A_2''	1	1	1	−1	−1	−1	−1	1	z		
E_1''	2	η_-	$-\eta_+$	0	−2	$-\eta_-$	η_+	0		(R_x,R_y)	(xz,yz)
E_2''	2	$-\eta_+$	η_-	0	−2	η_+	$-\eta_-$	0			

$\mathcal{C}_{6v}$	E	$2C_6$	$2C_6^2$	C_6^3	$3\sigma_v$	$3\sigma_d$			
A_1	1	1	1	1	1	1	z		$x^2+y^2;z^2$
A_2	1	1	1	1	−1	−1		R_z	
B_1	1	−1	1	−1	1	−1			
B_2	1	−1	1	−1	−1	1			
E_1	2	1	−1	−2	0	0	(x,y)	(R_x,R_y)	(xz,yz)
E_2	2	−1	−1	2	0	0			$(x^2-y^2,2xy)$

$\mathcal{D}_6$	E	$2C_6$	$2C_6^2$	C_6^3	$3C_2$	$3C_2'$			
A_1	1	1	1	1	1	1			$x^2+y^2;z^2$
A_2	1	1	1	1	−1	−1	z	R_z	
B_1	1	−1	1	−1	1	−1			
B_2	1	−1	1	−1	−1	1			
E_1	2	1	−1	−2	0	0	(x,y)	(R_x,R_y)	(xz,yz)
E_2	2	−1	−1	2	0	0			$(x^2-y^2,2xy)$

$\mathcal{D}_{6h}$	E	$2C_6$	$2C_6^2$	C_6^3	$3C_2$	$3C_2'$	i	$2S_3$	$2S_6$	σ_h	$3\sigma_d$	$3\sigma_v$		
A_{1g}	1	1	1	1	1	1	1	1	1	1	1	1		$x^2+y^2;z^2$
A_{2g}	1	1	1	1	−1	−1	1	1	1	1	−1	−1	R_z	
B_{1g}	1	−1	1	−1	1	−1	1	−1	1	−1	1	−1		
B_{2g}	1	−1	1	−1	−1	1	1	−1	1	−1	−1	1		
E_{1g}	2	1	−1	−2	0	0	2	1	−1	−2	0	0	(R_x,R_y)	(xz,yz)
E_{2g}	2	−1	−1	2	0	0	2	−1	−1	2	0	0		$(x^2-y^2,2xy)$
A_{1u}	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1		
A_{2u}	1	1	1	1	−1	−1	−1	−1	−1	−1	1	1	z	
B_{1u}	1	−1	1	−1	1	−1	−1	1	−1	1	−1	1		
B_{2u}	1	−1	1	−1	−1	1	−1	1	−1	1	1	−1		
E_{1u}	2	1	−1	−2	0	0	−2	−1	1	2	0	0	(x,y)	
E_{2u}	2	−1	−1	2	0	0	−2	1	1	−2	0	0		

Cubic

$\mathcal{T}$	E	$4C_3$	$4C_3^2$	$3C_2$		$\omega = \exp(2\pi i/3)$
A_1	1	1	1	1		$x^2+y^2+z^2$
E	1	ω	ω^2	1		$z^2+\omega^2x^2+\omega y^2$
	1	ω^2	ω	1		$z^2+\omega x^2+\omega^2y^2$
T_2	3	0	0	-1	(x,y,z) (R_x,R_y,R_z)	(yz,xz,xy)

$\mathcal{T}_d$	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$		
A_1	1	1	1	1	1		$x^2+y^2+z^2$
A_2	1	1	1	-1	-1		
E	2	-1	2	0	0		$\left((2z^2-x^2-y^2), \sqrt{3}(x^2-y^2)\right)$
T_1	3	0	-1	1	-1	(R_x,R_y,R_z)	
T_2	3	0	-1	-1	1	(x,y,z)	(yz,xz,xy)

O	E	$8C_3$	$3C_4^2$	$6C_4$	$6C_2$		
A_1	1	1	1	1	1		$x^2+y^2+z^2$
A_2	1	1	1	-1	-1		
E	2	-1	2	0	0		$\left((2z^2-x^2-y^2), \sqrt{3}(x^2-y^2)\right)$
T_1	3	0	-1	1	-1	(x,y,z) (R_x,R_y,R_z)	
T_2	3	0	-1	-1	1		(xz,xy,yz)

O_h	E	$8C_3$	$3C_4^2$	$6C_4$	$6C_2$	i	$8S_6$	$3\sigma_h$	$6S_4$	$6\sigma_d$		
A_{1g}	1	1	1	1	1	1	1	1	1	1		$x^2+y^2+z^2$
A_{2g}	1	1	1	-1	-1	1	1	1	-1	-1		
E_g	2	-1	2	0	0	2	-1	2	0	0		$\left((2z^2-x^2-y^2), \sqrt{3}(x^2-y^2)\right)$
T_{1g}	3	0	-1	1	-1	3	0	-1	1	-1	(R_x,R_y,R_z)	
T_{2g}	3	0	-1	-1	1	3	0	-1	-1	1		(xz,xy,yz)
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1		
A_{2u}	1	1	1	-1	-1	-1	-1	-1	1	1		
E_u	2	-1	2	0	0	-2	1	-2	0	0		
T_{1u}	3	0	-1	1	-1	-3	0	1	-1	1	(x,y,z)	
T_{2u}	3	0	-1	-1	1	-3	0	1	1	-1		

Icosahedral

I_h	E	$12C_5$	$12C_5^2$	$20C_3$	$15C_2$	i	$12S_{10}^3$	$12S_{10}$	$20S_6$	15σ		$\eta_\pm = \frac{1}{2}(\sqrt{5}\pm 1)$
A_g	1	1	1	1	1	1	1	1	1	1		$x^2+y^2+z^2$
T_{1g}	3	η_+	$-\eta_-$	0	-1	3	η_+	$-\eta_-$	0	-1	(R_x,R_y,R_z)	
T_{2g}	3	$-\eta_-$	η_+	0	-1	3	$-\eta_-$	η_+	0	-1		
G_g	4	-1	-1	1	0	4	-1	-1	1	0		
H_g	5	0	0	-1	1	5	0	0	-1	1		$\left(\sqrt{\frac{1}{12}}(2z^2-x^2-y^2), \frac{1}{2}(x^2-y^2), xz, xy, yz\right)$
A_u	1	1	1	1	1	-1	-1	-1	-1	-1		
T_{1u}	3	η_+	$-\eta_-$	0	-1	-3	$-\eta_+$	η_-	0	1	(x,y,z)	
T_{2u}	3	$-\eta_-$	η_+	0	-1	-3	η_-	$-\eta_+$	0	1		
G_u	4	-1	-1	1	0	-4	1	1	-1	0		
H_u	5	0	0	-1	1	-5	0	0	1	-1		

$C_{\infty v}$		E	$2C^z(\alpha)$	$\cdots$	$\infty\sigma_v$			
Σ^+	(A_1)	1	1	$\cdots$	1	z		$x^2+y^2; z^2$
Σ^-	(A_2)	1	1	$\cdots$	-1		R_z	
Π	(E_1)	2	$2\cos\alpha$	$\cdots$	0	(x,y)	(R_x,R_y)	(xz,yz)
Δ	(E_2)	2	$2\cos 2\alpha$	$\cdots$	0			$(x^2-y^2, 2xy)$
Φ	(E_3)	2	$2\cos 3\alpha$	$\cdots$	0			
$\cdots$		$\cdots$	$\cdots$	$\cdots$	$\cdots$			

$D_{\infty h}$		E	$2C^z(\alpha)$	$\cdots$	$\infty\sigma_v$	i	$2S^z(\alpha)$	$\cdots$	∞C_2		
Σ_g^+	(A_{1g})	1	1	$\cdots$	1	1	1	$\cdots$	1		$x^2+y^2; z^2$
Σ_g^-	(A_{2g})	1	1	$\cdots$	-1	1	1	$\cdots$	-1	R_z	
Π_g	(E_{1g})	2	$2\cos\alpha$	$\cdots$	0	2	$-2\cos\alpha$	$\cdots$	0	(R_x,R_y)	(xz,yz)
Δ_g	(E_{2g})	2	$2\cos 2\alpha$	$\cdots$	0	2	$2\cos 2\alpha$	$\cdots$	0		$(x^2-y^2, 2xy)$
Φ_g	(E_{3g})	2	$2\cos 3\alpha$	$\cdots$	0	2	$-2\cos 3\alpha$	$\cdots$	0		
$\cdots$		$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$		
Σ_u^+	(A_{1u})	1	1	$\cdots$	1	-1	-1	$\cdots$	-1	z	
Σ_u^-	(A_{2u})	1	1	$\cdots$	-1	-1	-1	$\cdots$	1		
Π_u	(E_{1u})	2	$2\cos\alpha$	$\cdots$	0	-2	$2\cos\alpha$	$\cdots$	0	(x,y)	
Δ_u	(E_{2u})	2	$2\cos 2\alpha$	$\cdots$	0	-2	$-2\cos 2\alpha$	$\cdots$	0		
Φ_u	(E_{3u})	2	$2\cos 3\alpha$	$\cdots$	0	-2	$2\cos 3\alpha$	$\cdots$	0		
$\cdots$		$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$		

Selected tables for descent in symmetry

C_{2v}	C_2	C_s (E,σ^{xz})	C_s (E,σ^{yz})
A_1	A	A'	A'
A_2	A	A''	A''
B_1	B	A'	A''
B_2	B	A''	A'

D_{3h}	C_{3v}	C_{2v} $(\sigma_h \to \sigma^{yz})$	C_s (E,σ_h)	C_s (E,σ_v)
A_1'	A_1	A_1	A'	A'
A_2'	A_2	B_2	A'	A''
E'	E	$A_1 \oplus B_2$	$2A'$	$A' \oplus A''$
A_1''	A_2	A_2	A''	A''
A_2''	A_1	B_1	A''	A'
E''	E	$A_2 \oplus B_1$	$2A''$	$A' \oplus A''$

$D_{\infty h}$ (x,y,z) $\to$	C_{2v} (x,z,y)
Σ_g^+	A_1
Σ_g^-	B_1
Π_g	$A_2 \oplus B_2$
Δ_g	$A_1 \oplus B_1$
$\cdots$	$\cdots$
Σ_u^+	B_2
Σ_u^-	A_2
Π_u	$A_1 \oplus B_1$
Δ_u	$A_2 \oplus B_2$
$\cdots$	$\cdots$

$O(3)$	O_h	T_d
S_g	A_{1g}	A_1
P_g	T_{1g}	T_1
D_g	$E_g \oplus T_{2g}$	$E \oplus T_2$
F_g	$A_{2g} \oplus T_{1g} \oplus T_{2g}$	$A_2 \oplus T_1 \oplus T_2$
G_g	$A_{1g} \oplus E_g \oplus T_{1g} \oplus T_{2g}$	$A_1 \oplus E \oplus T_1 \oplus T_2$
$\cdots$	$\cdots$	$\cdots$
S_u	A_{1u}	A_2
P_u	T_{1u}	T_2
D_u	$E_u \oplus T_{2u}$	$E \oplus T_1$
F_u	$A_{2u} \oplus T_{1u} \oplus T_{2u}$	$A_1 \oplus T_2 \oplus T_1$
G_u	$A_{1u} \oplus E_u \oplus T_{1u} \oplus T_{2u}$	$A_2 \oplus E \oplus T_2 \oplus T_1$
$\cdots$	$\cdots$	$\cdots$

Reduction of a representation

If $\Gamma = a_1\Gamma^{(1)} \oplus a_2\Gamma^{(2)} \oplus \cdots \oplus a_n\Gamma^{(n)}$, then

$$a_k = \frac{1}{h}\sum_R \chi^{(k)}(R)^* \chi(R),$$

where $\chi(R)$ is the character of the operation R in the representation Γ, $\chi^{(k)}(R)$ is the character of the operation R in the representation $\Gamma^{(k)}$, and h is the number of elements in the group.

Projection operators

The projection operator for representation $\Gamma^{(k)}$ is

$$\mathcal{P}^{(k)} = \frac{n_k}{h}\sum_R \chi^{(k)}(R)^* R.$$

The projected function $\mathcal{P}^{(k)} f$ obtained by applying $\mathcal{P}^{(k)}$ to any function f is either zero or a component of a basis for representation $\Gamma^{(k)}$.

Direct Products

Generally,

$$\chi^{\Gamma\otimes\Gamma'}(R) = \chi^{\Gamma}(R)\chi^{\Gamma'}(R),$$

and if the resulting representation is reducible it can be reduced in the usual way. Alternatively the following rules can be applied.

Treat g/u and $'/''$ symmetry separately. For groups with an inversion centre,

$$g\otimes g = u\otimes u = g \quad \text{and} \quad g\otimes u = u.$$

For groups with a horizontal plane σ_h but no inversion centre, single and double primes, $'$ and $''$, are used to denote symmetry and antisymmetry with respect to σ_h. Then

$$'\otimes' = ''\otimes'' = ' \quad \text{and} \quad '\otimes'' = ''.$$

Direct products involving nondegenerate representations are easily worked out from the character table. The product of any A or B with any E is an E, and the product of any A or B with any T is a T.

In the cubic groups $\mathcal{T}_d$, O and O_h,

$$E\otimes E = A_1\oplus A_2\oplus E,$$

$$E\otimes T_1 = E\otimes T_2 = T_1\oplus T_2,$$

$$T_1\otimes T_1 = T_2\otimes T_2 = A_1\oplus E\oplus T_1\oplus T_2,$$

$$T_1\otimes T_2 = A_2\oplus E\oplus T_1\oplus T_2.$$

For products of E_i with E_j in the axial groups the rules are complicated. If there is only one E representation, apart from g/u or $'/''$ labels, it should be considered as E_1. We need the order n of the principal axis, which is usually obvious — e.g. $n=5$ for $\mathcal{D}_{5h}$ — *but* for $\mathcal{D}_{md}$ with *m even*, $n=2m$ (because $\mathcal{D}_{md}$ has an S_{2m} axis when m is even).

(a) For $E_i\otimes E_i$:

(i) If E_{2i} exists, then

$$E_i\otimes E_i = A_1\oplus A_2\oplus E_{2i}.$$

(ii) Otherwise, if $4i=n$ then

$$E_i\otimes E_i = A_1\oplus A_2\oplus B_1\oplus B_2$$

(iii) Otherwise

$$E_i\otimes E_i = A_1\oplus A_2\oplus E_{|2i-n|}.$$

(b) For $E_i\otimes E_j$ with $i\neq j$:

(i) If E_{i+j} exists, then

$$E_i\otimes E_j = E_{|i-j|}\oplus E_{i+j}.$$

(ii) If $2(i+j)=n$, then

$$E_i\otimes E_j = E_{|i-j|}\oplus B_1\oplus B_2$$

(iii) Otherwise

$$E_i\otimes E_j = E_{|i-j|}\oplus E_{|i+j-n|}.$$

If there is only one A representation, apart from g/u or $'/''$ labels, read A_1 and A_2 above as A; similarly for B.

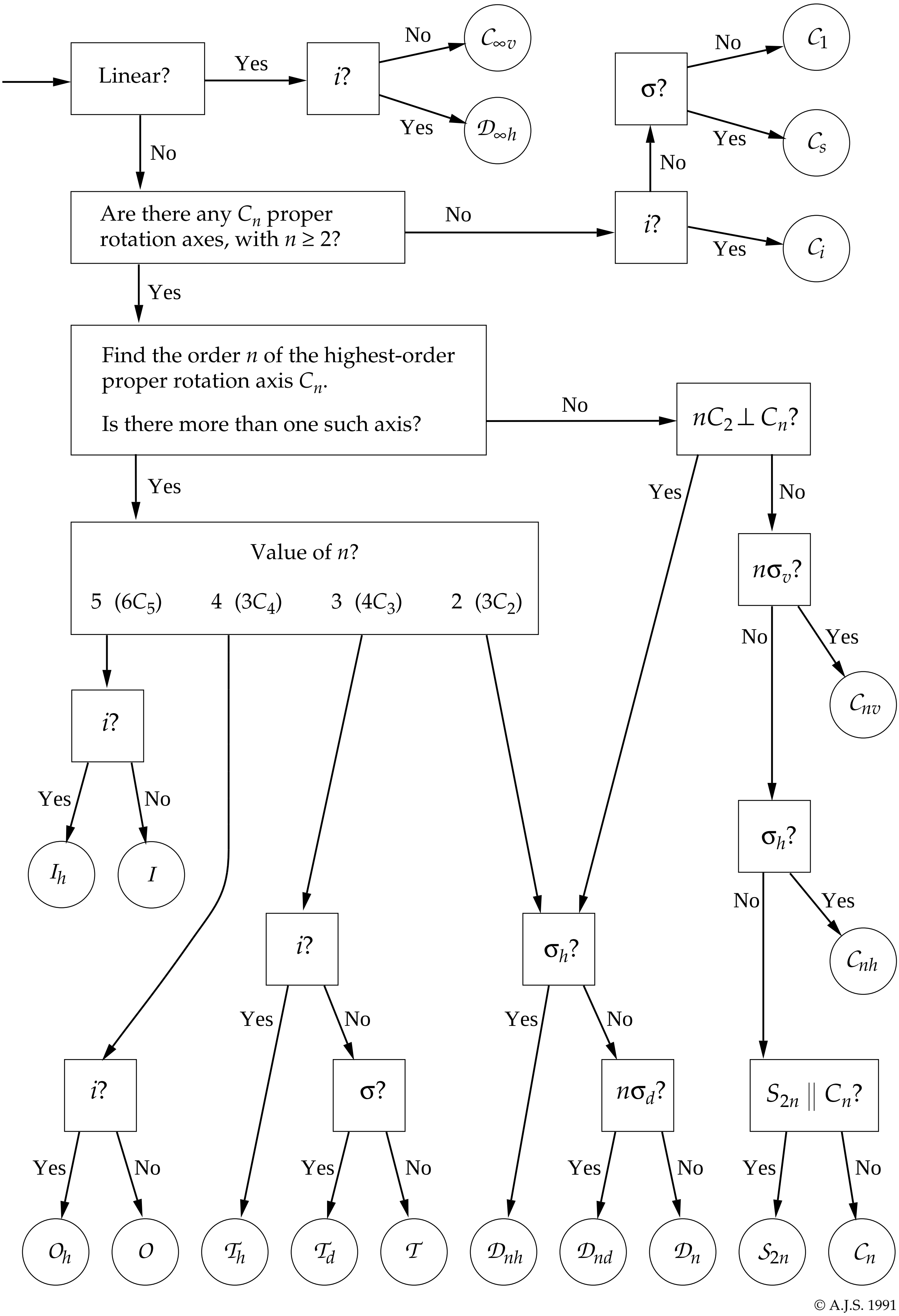
Examples

For $E\otimes E$ in $\mathcal{C}_{4v}$: there is only one E representation, so treat it as E_1. Rule a(i) doesn't apply, because E_2 doesn't exist, but a(ii) applies, so $E\otimes E = A_1\oplus A_2\oplus B_1\oplus B_2$.

For $E_{1g}\otimes E_{2u}$ in $\mathcal{D}_{5d}$, note first that $g\otimes u = u$. Then we need $E_1\otimes E_2$, for which rule b(iii) applies, with $n=5$, so the result is $E_{1g}\otimes E_{2u} = E_{1u}\oplus E_{2u}$.

Antisymmetrized Squares

The antisymmetric component of $E\otimes E$ or $E_i\otimes E_i$ is always A_2. In the cubic groups, the antisymmetric part of $T_1\otimes T_1$ and $T_2\otimes T_2$ is T_1.


Linear?
Yes
No
i?
No
Yes
$\mathcal{C}_{\infty v}$
$\mathcal{D}_{\infty h}$
σ?
No
Yes
$\mathcal{C}_1$
$\mathcal{C}_s$
Are there any C_n proper rotation axes, with $n \geq 2$?
No
i?
Yes
$\mathcal{C}_i$
Yes
Find the order n of the highest-order proper rotation axis C_n.
Is there more than one such axis?
No
$nC_2 \perp C_n$?
Yes
No
$n\sigma_v$?
$\mathcal{C}_{nv}$
Value of n?
5 ($6C_5$)
4 ($3C_4$)
3 ($4C_3$)
2 ($3C_2$)
i?
$\mathcal{I}_h$
$\mathcal{I}$
σ_h?
$\mathcal{C}_{nh}$
σ?
$n\sigma_d$?
$S_{2n} \parallel C_n$?
$\mathcal{O}_h$
$\mathcal{O}$
$\mathcal{T}_h$
$\mathcal{T}_d$
$\mathcal{T}$
$\mathcal{D}_{nh}$
$\mathcal{D}_{nd}$
$\mathcal{D}_n$
$\mathcal{S}_{2n}$
$\mathcal{C}_n$
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Space Groups

General Equivalent Positions (GEPs) and Special Equivalent Positions (SEPs)

Space group P2_1

GEPs:

2 @ $(x_n, y_n, z_n),\ (-x_n, \frac{1}{2}+y_n, -z_n)$

SEPs:

None

Space group P2_1**/c**

GEPs:

4 @ $(x_n, y_n, z_n),\ (-x_n, \frac{1}{2}+y_n, \frac{1}{2}-z_n),\ (x_n, \frac{1}{2}-y_n, \frac{1}{2}+z_n),\ (-x_n, -y_n, -z_n)$

SEPs:

4 pairs:

2 @ $(0,0,0)$ and $(0,\frac{1}{2},\frac{1}{2})$

2 @ $(0,0,\frac{1}{2})$ and $(0,\frac{1}{2},0)$

2 @ $(\frac{1}{2},0,0)$ and $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$

2 @ $(\frac{1}{2},\frac{1}{2},0)$ and $(\frac{1}{2},0,\frac{1}{2})$

Space group P$2_12_12_1$

GEPs:

4 @ $(x_n, y_n, z_n),\ (-x_n, \frac{1}{2}+y_n, \frac{1}{2}-z_n),\ (\frac{1}{2}+x_n, \frac{1}{2}-y_n, -z_n),\ (\frac{1}{2}-x_n, -y_n, \frac{1}{2}+z_n)$

SEPs:

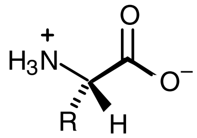
None

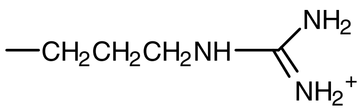
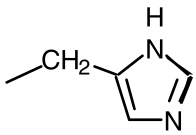
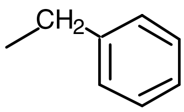
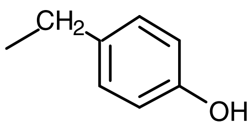
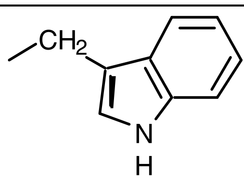
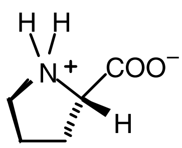
*Parameters for selected magnetic nuclei**

isotope	natural abundance (%)	spin, I
^{1}H	100	$\frac{1}{2}$
^{2}H	1.5×10^{-2}	1
^{3}H	0	$\frac{1}{2}$
^{6}Li	7	1
^{7}Li	93	$\frac{3}{2}$
^{10}B	20	3
^{11}B	80	$\frac{3}{2}$
^{13}C	1	$\frac{1}{2}$
^{14}N	100	1
^{15}N	0.4	$\frac{1}{2}$
^{17}O	3.7×10^{-2}	$\frac{5}{2}$
^{19}F	100	$\frac{1}{2}$
^{23}Na	100	$\frac{3}{2}$
^{27}Al	100	$\frac{5}{2}$
^{29}Si	5	$\frac{1}{2}$
^{31}P	100	$\frac{1}{2}$
^{51}V	100	$\frac{7}{2}$
^{57}Fe	2	$\frac{1}{2}$
^{77}Se	8	$\frac{1}{2}$
^{103}Rh	100	$\frac{1}{2}$
^{107}Ag	52	$\frac{1}{2}$
^{109}Ag	48	$\frac{1}{2}$
^{113}Cd	12	$\frac{1}{2}$
^{119}Sn	9	$\frac{1}{2}$
^{129}Xe	26	$\frac{1}{2}$
^{195}Pt	34	$\frac{1}{2}$
^{203}Tl	30	$\frac{1}{2}$
^{205}Tl	70	$\frac{1}{2}$
^{207}Pb	23	$\frac{1}{2}$

*The list is not exhaustive.

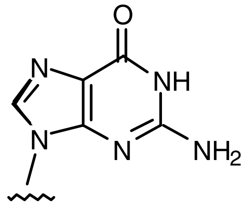
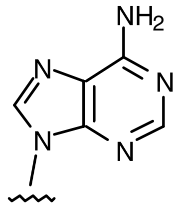
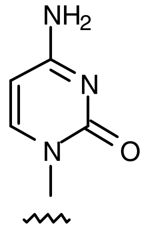
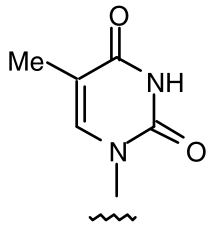
Amino acids



Name	Three-letter code	Single-letter code	Side chain, R =
Serine	Ser	S	$—CH_2OH$
Threonine	Thr	T	$—CH(CH_3)OH$
Cysteine	Cys	C	$—CH_2SH$
Methionine	Met	M	$—CH_2CH_2SMe$
Aspartic acid	Asp	D	$—CH_2COO^-$
Asparagine	Asn	N	$—CH_2CONH_2$
Glutamic acid	Glu	E	$—CH_2CH_2COO^-$
Glutamine	Gln	Q	$—CH_2CH_2CONH_2$
Lysine	Lys	K	$—CH_2CH_2CH_2CH_2NH_3^+$
Arginine	Arg	R	
Glycine	Gly	G	—H
Alanine	Ala	A	—Me
Leucine	Leu	L	$—CH_2CHMe_2$
Isoleucine	Ile	I	$—CH(Me)CH_2Me$
Valine	Val	V	$—CHMe_2$
Histidine	His	H	
Phenylalanine	Phe	F	
Tyrosine	Tyr	Y	
Tryptophan	Trp	W	
Proline*	Pro	P	

*For proline the complete structure of the amino acid is shown.

Nucleotide bases

Name	Abbreviation	Structure
Guanine	G	
Adenine	A	
Cytosine	C	
Thymine	T	
Uracil	U