

Data Book

(revised Jan 2014)

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1 H hydrogen 1.008																	2 He helium 4.003
3 Li lithium 6.94	4 Be beryllium 9.012											5 B boron 10.81	6 C carbon 12.01	7 N nitrogen 14.01	8 O oxygen 16.00	9 F fluorine 19.00	10 Ne neon 20.18
11 Na sodium 22.99	12 Mg magnesium 24.31											13 Al aluminium 26.98	14 Si silicon 28.09	15 P phosphorus 30.97	16 S sulfur 32.06	17 Cl chlorine 35.45	18 Ar argon 39.95
19 K potassium 39.10	20 Ca calcium 40.08	21 Sc scandium 44.96	22 Ti titanium 47.87	23 V vanadium 50.94	24 Cr chromium 52.00	25 Mn manganese 54.94	26 Fe iron 55.85	27 Co cobalt 58.93	28 Ni nickel 58.69	29 Cu copper 63.55	30 Zn zinc 65.38(2)	31 Ga gallium 69.72	32 Ge germanium 72.63	33 As arsenic 74.92	34 Se selenium 78.96(3)	35 Br bromine 79.904	36 Kr krypton 83.80
37 Rb rubidium 85.47	38 Sr strontium 87.62	39 Y yttrium 88.91	40 Zr zirconium 91.22	41 Nb niobium 92.91	42 Mo molybdenum 95.96(2)	43 Tc technetium	44 Ru ruthenium 101.1	45 Rh rhodium 102.9	46 Pd palladium 106.4	47 Ag silver 107.9	48 Cd cadmium 112.4	49 In indium 114.8	50 Sn tin 118.7	51 Sb antimony 121.8	52 Te tellurium 127.6	53 I iodine 126.9	54 Xe xenon 131.3
55 Cs caesium 132.9	56 Ba barium 137.3	57-71 lanthanoids	72 Hf hafnium 178.5	73 Ta tantalum 180.9	74 W tungsten 183.8	75 Re rhenium 186.2	76 Os osmium 190.2	77 Ir iridium 192.2	78 Pt platinum 195.1	79 Au gold 197.0	80 Hg mercury 200.6	81 Tl thallium 204.37	82 Pb lead 207.2	83 Bi bismuth 209.0	84 Po polonium	85 At astatine	86 Rn radon
87 Fr francium	88 Ra radium	89-103 actinoids	104 Rf rutherfordium	105 Db dubnium	106 Sg seaborgium	107 Bh bohrium	108 Hs hassium	109 Mt meitnerium	110 Ds darmstadtium	111 Rg roentgenium	112 Cn copernicium		114 Fl flerovium		116 Lv livermorium		

Key:

atomic number
Symbol
name
standard atomic weight

57 La lanthanum 138.9	58 Ce cerium 140.1	59 Pr praseodymium 140.9	60 Nd neodymium 144.2	61 Pm promethium	62 Sm samarium 150.4	63 Eu europium 152.0	64 Gd gadolinium 157.3	65 Tb terbium 158.9	66 Dy dysprosium 162.5	67 Ho holmium 164.9	68 Er erbium 167.3	69 Tm thulium 168.9	70 Yb ytterbium 173.1	71 Lu lutetium 175.0
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89 Ac actinium	90 Th thorium 232.0	91 Pa protactinium 231.0	92 U uranium 238.0	93 Np neptunium	94 Pu plutonium	95 Am americium	96 Cm curium	97 Bk berkelium	98 Cf californium	99 Es einsteinium	100 Fm fermium	101 Md mendelevium	102 No nobelium	103 Lr lawrencium
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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 m s^{-1}
Planck's constant	h	6.6260693(11)	10^{-34} J s
	$\hbar = h/2\pi$	1.05457168(18)	10^{-34} J s
Avogadro's constant	N_A	6.0221415(10)	10^{23} mol^{-1}
Elementary charge	e	1.60217653(14)	10^{-19} C
Electron rest mass	m_e	0.91093826(16)	10^{-30} kg
Atomic mass unit	$m_u = 1 \text{ g mol}^{-1}/N_A$	1.66053886(28)	10^{-27} kg
Proton rest mass	m_p	1.67262171(29)	10^{-27} kg
Neutron rest mass	m_n	1.67492728(29)	10^{-27} kg
Faraday constant	$F = N_A e$	9.64853383(83)	10^4 C mol^{-1}
Boltzmann constant	k_B	1.3806505(24)	$10^{-23} \text{ J K}^{-1}$
Molar Gas constant	$R = N_A k_B$	8.314472(15)	$\text{J mol}^{-1} \text{ K}^{-1}$
Permeability of vacuum	μ_0	$4\pi \times 10^{-7}$	H m^{-1}
Permittivity of vacuum	$\epsilon_0 = 1/(\mu_0 c^2)$	8.8541878 ...	$10^{-12} \text{ F m}^{-1}$
	$4\pi\epsilon_0$	1.1126501 ...	$10^{-10} \text{ F m}^{-1}$
Bohr magneton	$\mu_B = e\hbar/2m_e$	9.27400949(80)	$10^{-24} \text{ J T}^{-1}$
Nuclear magneton	$\mu_N = e\hbar/2m_p$	5.05078343(43)	$10^{-27} \text{ J T}^{-1}$
Stefan-Boltzmann constant	$\sigma = 2\pi^5 k_B^4/15h^3 c^2$	5.670400(40)	$10^{-8} \text{ W m}^{-2} \text{ K}^{-4}$
Bohr radius	$a_0 = 4\pi\epsilon_0 \hbar^2/m_e e^2$	0.5291772108(18)	10^{-10} m
Hartree energy	$E_h = e^2/4\pi\epsilon_0 a_0$	4.35974417(75)	10^{-18} J
Fine structure constant	$\alpha = e^2/4\pi\epsilon_0 \hbar c$	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	kJ mol ⁻¹	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	219475	315773
1 eV	1.60218 · 10 ⁻¹⁹	96.485	8065.54	11604
1 kJ mol ⁻¹	1.66054 · 10 ⁻²¹	1	83.5935	120.27
1 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} m
Energy	cal	4.184 J
Pressure	atm = 760 Torr	101325 Pa
	Torr = mm Hg	133.3 Pa
	bar	10^5 Pa
Radioactivity	becquerel, Bq	1 s^{-1}
	curie, Ci	$3.7 \cdot 10^{10} \text{ Bq}$
Charge	esu	$3.33564 \cdot 10^{-10} \text{ C}$
Dipole moment	debye = 10^{-18} esu cm	$3.33564 \cdot 10^{-30} \text{ C m}$
	a.u. = $e a_0$	$8.478358 \cdot 10^{-30} \text{ C m}$
Temperature	°C	$0^\circ \text{C} = 273.15 \text{ K}$

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, $\text{J mol}^{-1} \text{ K}^{-1}$.

Greek Alphabet

A	α	alpha	H	η	eta	N	ν	nu	T	τ	tau
B	β	beta	Θ	θ, ϑ	theta	Ξ	ξ	xi	Υ	υ	upsilon
Γ	γ	gamma	I	ι	iota	O	o	omicron	Φ	ϕ, φ	phi
Δ	δ	delta	K	κ	kappa	Π	π	pi	X	χ	chi
E	ε	epsilon	Λ	λ	lambda	P	ρ	rho	Ψ	ψ	psi
Z	ζ	zeta	M	μ	mu	Σ	σ	sigma	Ω	ω	omega

Series

Geometrical progression

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

Power series

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

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

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

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

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

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 i th row and the j th column of \mathbf{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

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

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

$$\int_0^{\infty} r^n \exp(-ar) dr = \frac{n!}{a^{n+1}} \quad (n \geq 0; a > 0)$$

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

so that

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

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

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

Integration by parts

$$\int_a^b u \frac{dv}{dx} dx = [uv]_a^b - \int_a^b \frac{du}{dx} v dx$$

Trigonometrical formulae

$$\sin(A \pm B) = \sin A \cos B \pm \cos A \sin B$$

$$\cos(A \pm B) = \cos A \cos B \mp \sin A \sin B$$

$$\cos A \cos B = \frac{1}{2} (\cos(A+B) + \cos(A-B))$$

$$\sin A \sin B = \frac{1}{2} (\cos(A-B) - \cos(A+B))$$

$$\sin A \cos B = \frac{1}{2} (\sin(A+B) + \sin(A-B))$$

$$\sin A + \sin B = 2 \sin \frac{A+B}{2} \cos \frac{A-B}{2}$$

$$\sin A - \sin B = 2 \cos \frac{A+B}{2} \sin \frac{A-B}{2}$$

$$\cos A + \cos B = 2 \cos \frac{A+B}{2} \cos \frac{A-B}{2}$$

$$\cos A - \cos B = -2 \sin \frac{A+B}{2} \sin \frac{A-B}{2}$$

Cosine formula

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

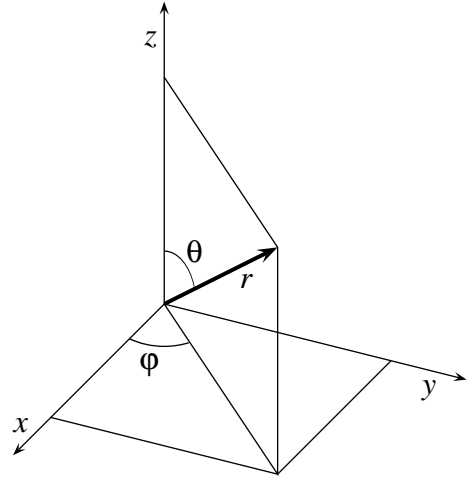
Spherical Polar Coordinates

Relationship with Cartesian coordinates

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

Integration

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



Laplacian

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

Spherical Harmonics

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

where

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

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

$$C_{00} = 1,$$

$$C_{10} = \cos \theta = z/r,$$

$$C_{1,\pm 1} = \mp \sqrt{\frac{1}{2}} \sin \theta e^{\pm i\varphi} = \mp \sqrt{\frac{1}{2}} (x \pm iy)/r,$$

$$C_{20} = \frac{1}{2} (3 \cos^2 \theta - 1) = \frac{1}{2} (3z^2 - r^2)/r^2,$$

$$C_{2,\pm 1} = \mp \sqrt{\frac{3}{2}} \cos \theta \sin \theta e^{\pm i\varphi} = \mp \sqrt{\frac{3}{2}} (zx \pm izy)/r^2,$$

$$C_{2,\pm 2} = \sqrt{\frac{3}{8}} \sin^2 \theta e^{\pm 2i\varphi} = \sqrt{\frac{3}{8}} (x^2 - y^2 \pm 2ixy)/r^2.$$

Ladder Operators

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

Character tables for some important symmetry groups

C_i	E	i	
A_g	1	1	$R_x; R_y; R_z \quad x^2; y^2; z^2; xy; xz; yz$
A_u	1	-1	$x; y; z$

C_s	E	σ_h	
A'	1	1	$x; y \quad R_z \quad x^2; y^2; z^2; xy$
A''	1	-1	$z \quad R_x; R_y \quad xz; yz$

C_2	E	C_2^z	
A	1	1	$z \quad R_z \quad x^2; y^2; z^2; xy$
B	1	-1	$x; y \quad R_x; R_y \quad xz; yz$

C_{2v}	E	C_2^z	σ^{xz}	σ^{yz}	
A_1	1	1	1	1	$z \quad x^2; y^2; z^2$
A_2	1	1	-1	-1	$R_z \quad xy$
B_1	1	-1	1	-1	$x \quad R_y \quad xz$
B_2	1	-1	-1	1	$y \quad R_x \quad yz$

C_{2h}	E	C_2^z	i	σ^{xy}	
A_g	1	1	1	1	$R_z \quad x^2; y^2; z^2; xy$
B_g	1	-1	1	-1	$R_x; R_y \quad xz; yz$
A_u	1	1	-1	-1	z
B_u	1	-1	-1	1	$x; y$

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	$z \quad R_z \quad xy$
B_2	1	-1	1	-1	$y \quad R_y \quad xz$
B_3	1	-1	-1	1	$x \quad R_x \quad yz$

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	$z \quad xy$
E	2	0	-2	0	0	$(x, y) \quad (R_x, R_y) \quad (xz, yz)$

2

\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

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	$x + iy$	$R_x + iR_y$	$xz + iyz; x^2 - 2ixy - y^2$	

C_{3v}	E	$2C_3$	$3C_2$			
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	$2C_3$	$3C_2$			
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)

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 C_{4v} coincide with the xz and yz planes.

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 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 $\eta_+ \eta_- = 1$.

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	$(x^2 - y^2, 2xy)$

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	$(x^2 - y^2, 2xy)$

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	$(x^2 - y^2, 2xy)$
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	z
A_2''	1	1	1	-1	-1	-1	-1	1	(R_x, R_y)
E_1''	2	η_-	$-\eta_+$	0	-2	$-\eta_-$	η_+	0	(xz, yz)
E_2''	2	$-\eta_+$	η_-	0	-2	η_+	$-\eta_-$	0	(xz, yz)

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
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)
E_2	2	-1	-1	2	0	0	(R_x, R_y)
							(xz, yz)
							$(x^2 - y^2, 2xy)$

\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
B_1	1	-1	1	-1	1	-1	R_z
B_2	1	-1	1	-1	-1	1	
E_1	2	1	-1	-2	0	0	(x, y)
E_2	2	-1	-1	2	0	0	(R_x, R_y)
							(xz, yz)
							$(x^2 - y^2, 2xy)$

\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)
E_{2g}	2	-1	-1	2	0	0	2	-1	-1	2	0	0	(xz, yz)
													$(x^2 - y^2, 2xy)$
A_{1u}	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1	z
A_{2u}	1	1	1	1	-1	-1	-1	-1	-1	-1	1	1	
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

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	$z^2 + \omega^2 x^2 + \omega y^2$		
	1	ω^2	ω	1	$z^2 + \omega x^2 + \omega^2 y^2$		
T_2	3	0	0	-1	(x, y, z)	(R_x, R_y, R_z)	(yz, xz, xy)

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	$((2z^2 - x^2 - y^2), \sqrt{3}(x^2 - y^2))$	
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	$((2z^2 - x^2 - y^2), \sqrt{3}(x^2 - y^2))$	
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	$((2z^2 - x^2 - y^2), \sqrt{3}(x^2 - y^2))$	
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	$(\sqrt{\frac{1}{12}}(2z^2 - x^2 - y^2), \frac{1}{2}(x^2 - y^2), xz, xy, yz)$	
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	$2C^z(\alpha)$	\dots	$\infty\sigma_v$		
$\Sigma^+ (A_1)$	1	1	\dots	1	z	$x^2 + y^2; z^2$
$\Sigma^- (A_2)$	1	1	\dots	-1	R_z	
$\Pi (E_1)$	2	$2\cos\alpha$	\dots	0	(x, y)	(xz, yz)
$\Delta (E_2)$	2	$2\cos 2\alpha$	\dots	0		$(x^2 - y^2, 2xy)$
$\Phi (E_3)$	2	$2\cos 3\alpha$	\dots	0		
\dots	\dots	\dots	\dots	\dots		

$\mathcal{D}_{\infty h}$	E	$2C^z(\alpha)$	\dots	$\infty\sigma_v$	i	$2S^z(\alpha)$	\dots	∞C_2	
$\Sigma_g^+ (A_{1g})$	1	1	\dots	1	1	1	\dots	1	$x^2 + y^2; z^2$
$\Sigma_g^- (A_{2g})$	1	1	\dots	-1	1	1	\dots	-1	R_z
$\Pi_g (E_{1g})$	2	$2\cos\alpha$	\dots	0	2	$-2\cos\alpha$	\dots	0	(R_x, R_y)
$\Delta_g (E_{2g})$	2	$2\cos 2\alpha$	\dots	0	2	$2\cos 2\alpha$	\dots	0	(xz, yz)
$\Phi_g (E_{3g})$	2	$2\cos 3\alpha$	\dots	0	2	$-2\cos 3\alpha$	\dots	0	$(x^2 - y^2, 2xy)$
\dots	\dots	\dots	\dots	\dots	\dots	\dots	\dots	\dots	
$\Sigma_u^+ (A_{1u})$	1	1	\dots	1	-1	-1	\dots	-1	z
$\Sigma_u^- (A_{2u})$	1	1	\dots	-1	-1	-1	\dots	1	
$\Pi_u (E_{1u})$	2	$2\cos\alpha$	\dots	0	-2	$2\cos\alpha$	\dots	0	(x, y)
$\Delta_u (E_{2u})$	2	$2\cos 2\alpha$	\dots	0	-2	$-2\cos 2\alpha$	\dots	0	
$\Phi_u (E_{3u})$	2	$2\cos 3\alpha$	\dots	0	-2	$2\cos 3\alpha$	\dots	0	
\dots	\dots	\dots	\dots	\dots	\dots	\dots	\dots	\dots	

Selected tables for descent in symmetry

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

\mathcal{D}_{3h}	C_{3v}	C_{2v}	C_s	C_s
		$(\sigma_h \rightarrow \sigma^{yz})$	(E, σ_h)	(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	$A_2 \oplus B_1$	$2A''$	$A' \oplus A''$

$\mathcal{D}_{\infty h}$	C_{2v}
$(x, y, z) \rightarrow$	(x, z, y)
Σ_g^+	A_1
Σ_g^-	B_1
Π_g	$A_2 \oplus B_2$
Δ_g	$A_1 \oplus B_1$
\dots	\dots
Σ_u^+	B_2
Σ_u^-	A_2
Π_u	$A_1 \oplus B_1$
Δ_u	$A_2 \oplus B_2$
\dots	\dots

$O(3)$	O_h	\mathcal{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	$A_{1g} \oplus E_g \oplus T_{1g} \oplus T_{2g}$	$A_1 \oplus E \oplus T_1 \oplus T_2$
\dots	\dots	\dots
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	$A_{1u} \oplus E_u \oplus T_{1u} \oplus T_{2u}$	$A_2 \oplus E \oplus T_2 \oplus T_1$
\dots	\dots	\dots

Reduction of a representation

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

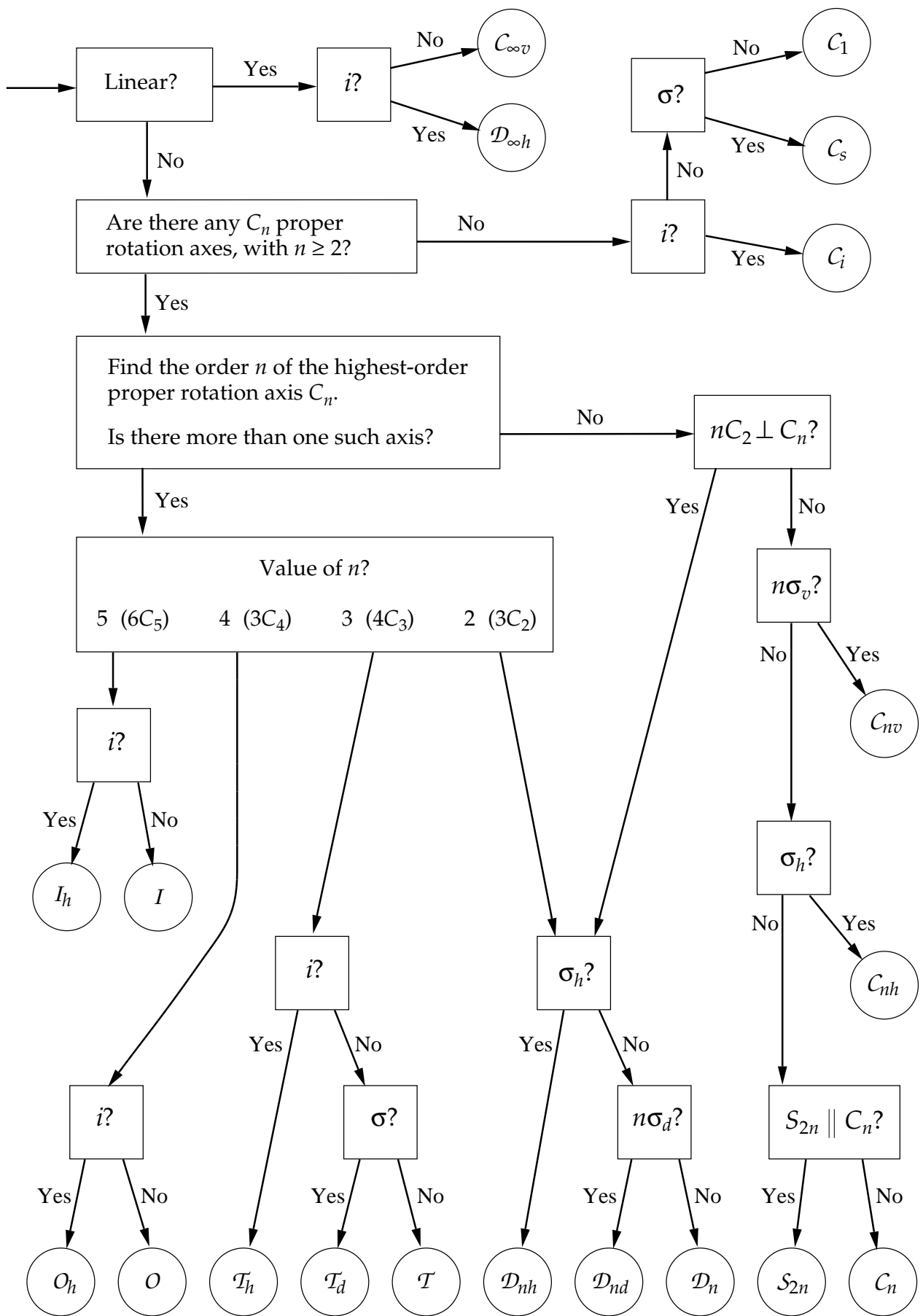
Examples

For $E \otimes E$ in 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 .



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:

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

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

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

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

Space group $P2_12_12_1$

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:

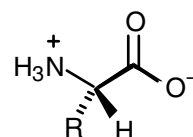
None

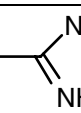

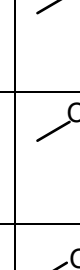
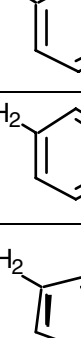
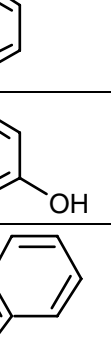
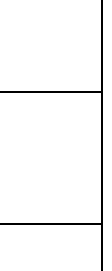
*Parameters for selected magnetic nuclei**

isotope	natural abundance (%)	spin, I
^1H	100	$\frac{1}{2}$
^2H	1.5×10^{-2}	1
^3H	0	$\frac{1}{2}$
^6Li	7	1
^7Li	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.

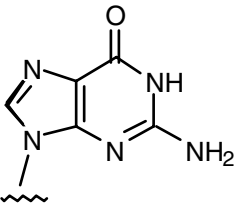
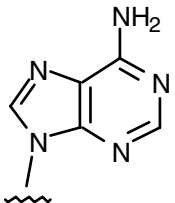
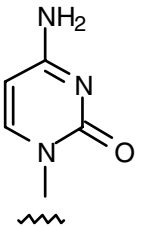
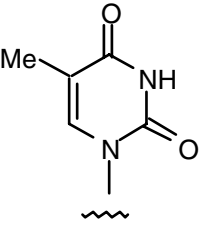
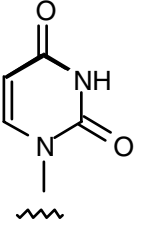
Amino acids



Name	Three-letter code	Single-letter code	Side chain, R =
Serine	Ser	S	—CH ₂ OH
Threonine	Thr	T	—CH(CH ₃)OH
Cysteine	Cys	C	—CH ₂ SH
Methionine	Met	M	—CH ₂ CH ₂ SMe
Aspartic acid	Asp	D	—CH ₂ COO ⁻
Asparagine	Asn	N	—CH ₂ CONH ₂
Glutamic acid	Glu	E	—CH ₂ CH ₂ COO ⁻
Glutamine	Gln	Q	—CH ₂ CH ₂ CONH ₂
Lysine	Lys	K	—CH ₂ CH ₂ CH ₂ CH ₂ NH ₃ ⁺
Arginine	Arg	R	—CH ₂ CH ₂ CH ₂ NH— 
Glycine	Gly	G	—H
Alanine	Ala	A	—Me
Leucine	Leu	L	—CH ₂ CHMe ₂
Isoleucine	Ile	I	—CH(Me)CH ₂ Me
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	 <p>The structure of Guanine is a purine base consisting of a fused bicyclic ring system (a six-membered ring fused to a five-membered ring). It features a carbonyl group (=O) at the 6-position, an amino group (-NH₂) at the 2-position, and a wavy line at the 9-position representing the attachment point to the sugar-phosphate backbone.</p>
Adenine	A	 <p>The structure of Adenine is a purine base consisting of a fused bicyclic ring system. It features an amino group (-NH₂) at the 6-position and a wavy line at the 9-position representing the attachment point to the sugar-phosphate backbone.</p>
Cytosine	C	 <p>The structure of Cytosine is a pyrimidine base consisting of a single six-membered ring. It features an amino group (-NH₂) at the 4-position, a carbonyl group (=O) at the 2-position, and a wavy line at the 1-position representing the attachment point to the sugar-phosphate backbone.</p>
Thymine	T	 <p>The structure of Thymine is a pyrimidine base consisting of a single six-membered ring. It features a methyl group (-Me) at the 5-position, carbonyl groups (=O) at the 2 and 4 positions, and a wavy line at the 1-position representing the attachment point to the sugar-phosphate backbone.</p>
Uracil	U	 <p>The structure of Uracil is a pyrimidine base consisting of a single six-membered ring. It features carbonyl groups (=O) at the 2 and 4 positions and a wavy line at the 1-position representing the attachment point to the sugar-phosphate backbone.</p>