UNIVERSITY OF CAMBRIDGE
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Chemistry Examination Data Book
(revised April 2026)

Contents

Periodic table of the elements

H 1 1.0080																	**He** 2 4.0026
Li 3 6.94	**Be** 4 9.0122						**symbol** atomic number abridged standard atomic weight					**B** 5 10.81	**C** 6 12.011	**N** 7 14.007	**O** 8 15.999	**F** 9 18.998	**Ne** 10 20.180
Na 11 22.990	**Mg** 12 24.305											**Al** 13 26.982	**Si** 14 28.085	**P** 15 30.974	**S** 16 32.06	**Cl** 17 35.45	**Ar** 18 39.95
K 19 39.098	**Ca** 20 40.078	**Sc** 21 44.956	**Ti** 22 47.867	**V** 23 50.942	**Cr** 24 51.996	**Mn** 25 54.938	**Fe** 26 55.845	**Co** 27 58.933	**Ni** 28 58.693	**Cu** 29 63.546	**Zn** 30 65.38	**Ga** 31 69.723	**Ge** 32 72.630	**As** 33 74.922	**Se** 34 78.971	**Br** 35 79.904	**Kr** 36 83.798
Rb 37 85.468	**Sr** 38 87.62	**Y** 39 88.906	**Zr** 40 91.224	**Nb** 41 92.906	**Mo** 42 95.95	**Tc** 43 [97]	**Ru** 44 101.07	**Rh** 45 102.91	**Pd** 46 106.42	**Ag** 47 107.87	**Cd** 48 112.41	**In** 49 114.82	**Sn** 50 118.71	**Sb** 51 121.76	**Te** 52 127.60	**I** 53 126.90	**Xe** 54 131.29
Cs 55 132.91	**Ba** 56 137.33	**La*** 57 138.91	**Hf** 72 178.49	**Ta** 73 180.95	**W** 74 183.84	**Re** 75 186.21	**Os** 76 190.23	**Ir** 77 192.22	**Pt** 78 195.08	**Au** 79 196.97	**Hg** 80 200.59	**Tl** 81 204.38	**Pb** 82 207.2	**Bi** 83 208.98	**Po** 84 [209]	**At** 85 [210]	**Rn** 86 [222]
Fr 87 [223]	**Ra** 88 [226]	**Ac†** 89 [227]	**Rf** 104 [267]	**Db** 105 [268]	**Sg** 106 [269]	**Bh** 107 [270]	**Hs** 108 [269]	**Mt** 109 [277]	**Ds** 110 [281]	**Rg** 111 [282]	**Cn** 112 [285]	**Nh** 113 [286]	**Fl** 114 [290]	**Mc** 115 [290]	**Lv** 116 [293]	**Ts** 117 [294]	**Og** 118 [294]

***Lanthanides**	**Ce** 58 140.12	**Pr** 59 140.91	**Nd** 60 144.24	**Pm** 61 [145]	**Sm** 62 150.36	**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** 70 173.05	**Lu** 71 174.97
†Actinides	**Th** 90 232.04	**Pa** 91 231.04	**U** 92 238.03	**Np** 93 [237]	**Pu** 94 [244]	**Am** 95 [243]	**Cm** 96 [247]	**Bk** 97 [247]	**Cf** 98 [251]	**Es** 99 [252]	**Fm** 100 [257]	**Md** 101 [258]	**No** 102 [259]	**Lr** 103 [262]

Data from IUPAC Periodic Table of the Elements 2022 Edition `https://iupac.org/wp-content/uploads/2022/05/IUPAC_Periodic_Table_150-04May22.jpg`

Constants

Name	Symbol and definition	Value (Uncertainty)
	π	$3.14159265358979\ldots$
	e	$2.718281828459\ldots$
	$\ln 10 = 1/\log_{10} \mathrm{e}$	$2.302585092994\ldots$
Speed of light	c	$2.99792458 \times 10^{8}\,\mathrm{m\,s^{-1}}$
Planck constant	h	$6.62607015 \times 10^{-34}\,\mathrm{J\,s}$
Reduced Planck constant	$\hbar = h/2\pi$	$1.054571817\cdots \times 10^{-34}\,\mathrm{J\,s}$
Avogadro constant	N_{A}	$6.02214076 \times 10^{23}\,\mathrm{mol^{-1}}$
Elementary charge	e	$1.602176634 \times 10^{-19}\,\mathrm{C}$
Electron mass	m_{e}	$9.1093837139(28) \times 10^{-31}\,\mathrm{kg}$
Atomic mass unit	u	$1.66053906892(52) \times 10^{-27}\,\mathrm{kg}$
Proton mass	m_{p}	$1.67262192595(52) \times 10^{-27}\,\mathrm{kg}$
Neutron mass	m_{n}	$1.67492750056(85) \times 10^{-27}\,\mathrm{kg}$
Faraday constant	$F = N_{\mathrm{A}} e$	$9.648533212\cdots \times 10^{4}\,\mathrm{C\,mol^{-1}}$
Boltzmann constant	k_{B}	$1.380649 \times 10^{-23}\,\mathrm{J\,K^{-1}}$
Molar gas constant	$R = N_{\mathrm{A}} k_{\mathrm{B}}$	$8.314462618\,\mathrm{J\,mol^{-1}\,K^{-1}}$
Vacuum magnetic permeability	μ_0	$1.25663706127(20) \times 10^{-6}\,\mathrm{N\,A^{-2}}$
Vacuum electric permittivity	$\varepsilon_0 = 1/(\mu_0 c^2)$	$8.8541878188(14) \times 10^{-12}\,\mathrm{F\,m^{-1}}$
Bohr magneton	$\mu_{\mathrm{B}} = e\hbar/2m_{\mathrm{e}}$	$9.2740100657(29) \times 10^{-24}\,\mathrm{J\,T^{-1}}$
Nuclear magneton	$\mu_{\mathrm{N}} = e\hbar/2m_{\mathrm{p}}$	$5.0507837393(16) \times 10^{-27}\,\mathrm{J\,T^{-1}}$
Stefan–Boltzmann constant	$\sigma = 2\pi^5 k^4/15h^3c^2$	$5.670374419\cdots \times 10^{-8}\,\mathrm{W\,m^{-2}\,K^{-4}}$
Bohr radius	$a_0 = 4\pi\varepsilon_0\hbar^2/m_{\mathrm{e}}e^2$	$5.29177210544(82) \times 10^{-11}\,\mathrm{m}$
Hartree energy	$E_{\mathrm{h}} = e^2/4\pi\varepsilon_0 a_0$	$4.3597447222060(48) \times 10^{-18}\,\mathrm{J}$
Fine-structure constant	$\alpha = e^2/4\pi\varepsilon_0\hbar c$	$7.2973525643(11) \times 10^{-3}$
	α^{-1}	$137.035999177(21)$
Rydberg constant	$R_\infty = m_{\mathrm{e}}e^4/8\varepsilon_0^2 h^3 c$	$1.0973731568157(12) \times 10^{7}\,\mathrm{m^{-1}}$
Rydberg energy	$hcR_\infty = m_{\mathrm{e}}e^4/8\varepsilon_0^2 h^2$	$2.1798723611030(24) \times 10^{-18}\,\mathrm{J}$
Newtonian constant of gravitation	G	$6.67430(15) \times 10^{-11}\,\mathrm{m^3\,kg^{-1}\,s^{-2}}$
Electron g factor	g_{e^-}	$-2.00231930436092(36)$

SI prefixes

Name	Symbol	Factor	Name	Symbol	Factor
deca	da	10^{1}	deci	d	10^{-1}
hecto	h	10^{2}	centi	c	10^{-2}
kilo	k	10^{3}	milli	m	10^{-3}
mega	M	10^{6}	micro	µ	10^{-6}
giga	G	10^{9}	nano	n	10^{-9}
tera	T	10^{12}	pico	p	10^{-12}
peta	P	10^{15}	femto	f	10^{-15}
exa	E	10^{18}	atto	a	10^{-18}
zetta	Z	10^{21}	zepto	z	10^{-21}
yotta	Y	10^{24}	yocto	y	10^{-24}

Other conversion factors

Length	Å	$10^{-10}\,\mathrm{m}$
Energy	cal	$4.184\,\mathrm{J}$
Pressure	$1\,\mathrm{atm} = 760\,\mathrm{Torr}$	$101\,325\,\mathrm{Pa}$
	$1\,\mathrm{Torr} = 1\,\mathrm{mmHg}$	$133.3224\,\mathrm{Pa}$
	$1\,\mathrm{bar}$	$10^{5}\,\mathrm{Pa}$
Radioactivity	becquerel, Bq	$1\,\mathrm{s^{-1}}$
	curie, Ci	$3.7 \times 10^{10}\,\mathrm{Bq}$
Charge	esu	$3.33564 \times 10^{-10}\,\mathrm{C}$
Dipole moment	debye	$10^{-18}\,\mathrm{esu\,cm}$
	debye	$3.33564 \times 10^{-30}\,\mathrm{C\,m}$
	$\mathrm{a.u.} = ea_0$	$8.4783536198(13) \times 10^{-30}\,\mathrm{C\,m}$
Temperature	°C	$t/°\mathrm{C} = T/\mathrm{K} - 273.15$
Parts per million	ppm	1×10^{-6}
Parts per billion	ppb	1×10^{-9}

CODATA recommended values, 2022 `https://physics.nist.gov/cuu/Constants/index.html`
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}	7.2430×10^{22}
1 E_h	4.35974×10^{-18}	2625.5	219 475	315 775
1 eV	1.60218×10^{-19}	96.485	8065.54	11 605
1 $\mathrm{kJ\,mol^{-1}}$	1.66054×10^{-21}	1	83.5935	120.27
1 $\mathrm{cm^{-1}}$	1.98645×10^{-23}	0.011963	1	1.4388
1 K	1.38065×10^{-23}	8.3145×10^{-3}	0.69503	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 $k_\mathrm{B}T$.

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, ϵ	epsilon	Λ	λ	lambda	P	ρ	rho	Ψ	ψ	psi
Z	ζ	zeta	M	μ	mu	Σ	σ, ς	sigma	Ω	ω	omega

Series

Arithmetic progression

$$S_n = a + (a + d) + (a + 2d) + \cdots + (a + [n-1]\,d) = \frac{n\,(2a + [n-1]\,d)}{2}.$$

Geometric 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

$$f(x) = f(a) + f'(a)\,(x-a) + \frac{f''(a)}{2!}\,(x-a)^2 + \frac{f'''(a)}{3!}\,(x-a)^3 + \cdots$$

$$\mathrm{e}^z = 1 + z + \frac{z^2}{2!} + \frac{z^3}{3!} + \cdots$$

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

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

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

$$\sinh z = \frac{\mathrm{e}^{z} - \mathrm{e}^{-z}}{2} = z + \frac{z^3}{3!} + \frac{z^5}{5!} + \frac{z^7}{7!} + \cdots$$

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

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

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,

$$\det(\mathbf{A}) = \sum_j A_{ij} M_{ij} \left(-1\right)^{i+j} \quad (i \text{ fixed at any value}),$$

where M_{ij} is the determinant of the matrix obtained by deleting the ith row and the jth column of $\mathbf{A}$. For example,

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

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

Multinomial examples

Binomial theorem

$$(x+y)^n = \sum_{k=0}^{n} \binom{n}{k} x^{n-k} y^k,$$

where the binomial coefficents are given by

$$\binom{n}{k} = \frac{n!}{k!\,(n-k)!}.$$

Trinomial theorem

$$(x_1 + x_2 + x_3)^n = \sum_{k=0}^{n} \sum_{l=0}^{n-k} \frac{n!}{k!l!(n-k-l)!} x_1^k x_2^l x_3^{n-k-l}$$

Double factorial

The double factorial of n is the product of all positive integers up to n that have the same parity.

$$n!! = \begin{cases} 1 \times 3 \times 5 \times \ldots \times n & \text{odd}\, n \\ 2 \times 4 \times 6 \times \ldots \times n & \text{even}\, n \end{cases}.$$

Integrals

$$\int_{-\infty}^{\infty} \mathrm{e}^{-ax^2}\,\mathrm{d}x = \sqrt{\pi/a}, \qquad (a>0)$$

$$\int_{-\infty}^{\infty} x^{2n}\mathrm{e}^{-ax^2}\,\mathrm{d}x = (2n-1)!!\frac{\sqrt{\pi/a}}{(2a)^n} \qquad (n\geq 1;\ a>0)$$

$$\int_{0}^{\infty} x^{2n-1}\mathrm{e}^{-ax^2}\,\mathrm{d}x = \frac{(n-1)!}{2a^n} \qquad (n\geq 1;\ a>0)$$

$$\int_{0}^{\infty} x^{n}\mathrm{e}^{-ax}\,\mathrm{d}x = \frac{n!}{a^{n+1}} \qquad (n\geq 0;\ a>0)$$

$$\int_{0}^{\pi/2} \sin^m\theta\cos^n\theta\,\mathrm{d}\theta = \frac{(m-1)!!(n-1)!!}{(m+n)!!}\times C,$$

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

$$\int_{0}^{\pi/2} \sin\theta\cos^3\theta\,\mathrm{d}\theta = \frac{2}{4\times 2} = \frac{1}{4}; \qquad \int_{0}^{\pi/2} \sin^2\theta\cos^2\theta\,\mathrm{d}\theta = \frac{1\times 1}{4\times 2}\frac{\pi}{2} = \frac{\pi}{16}.$$

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

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

$$2\cos A\cos B = \cos(A+B)+\cos(A-B)$$
$$2\sin A\sin B = \cos(A-B)-\cos(A+B)$$
$$2\sin A\cos B = \sin(A+B)+\sin(A-B)$$

$$\sin 2A + \sin 2B = 2\sin(A+B)\cos(A-B)$$
$$\sin 2A - \sin 2B = 2\cos(A+B)\sin(A-B)$$
$$\cos 2A + \cos 2B = 2\cos(A+B)\cos(A-B)$$
$$\cos 2A - \cos 2B = -2\sin(A+B)\sin(A-B)$$

$$\operatorname{arsinh} A = \ln\left(A+\sqrt{A^2+1}\right)$$
$$\operatorname{arcosh} A = \ln\left(A\pm\sqrt{A^2-1}\right)$$
$$\operatorname{artanh} A = \tfrac{1}{2}\ln\frac{1+A}{1-A}$$

Cosine formula

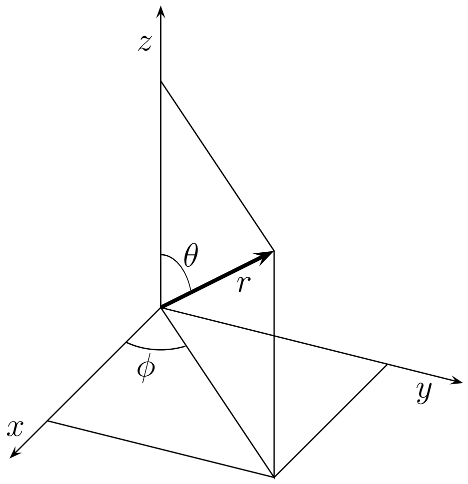
$$a^2 = b^2 + c^2 - 2bc\cos A$$

Spherical polar coordinates

Relationship with Cartesian coordinates

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

These definitions do not take into account the quadrant of the position vector.



Integration

$$\int \ldots \,\mathrm{d}V = \int_{r=0}^{\infty}\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi} \ldots\, r^2\sin\theta\,\mathrm{d}r\,\mathrm{d}\theta\,\mathrm{d}\phi$$

Selected spherical harmonics, Y_{J,M_J}

$$Y_{0,0}(\theta,\phi) = \frac{1}{2}\sqrt{\frac{1}{\pi}}$$
$$Y_{1,0}(\theta,\phi) = \frac{1}{2}\sqrt{\frac{3}{\pi}}\cos\theta = \frac{1}{2}\sqrt{\frac{3}{\pi}}\frac{z}{r}$$
$$Y_{1,\pm1}(\theta,\phi) = \mp\frac{1}{2}\sqrt{\frac{3}{2\pi}}\mathrm{e}^{\pm\mathrm{i}\phi}\sin\theta = \mp\frac{1}{2}\sqrt{\frac{3}{2\pi}}\frac{x\pm\mathrm{i}y}{r}$$
$$Y_{2,0}(\theta,\phi) = \frac{1}{4}\sqrt{\frac{5}{\pi}}\left(3\cos^2\theta-1\right) = \frac{1}{4}\sqrt{\frac{5}{\pi}}\frac{(3z^2-r^2)}{r^2}$$
$$Y_{2,\pm1}(\theta,\phi) = \mp\frac{1}{2}\sqrt{\frac{15}{2\pi}}\mathrm{e}^{\pm\mathrm{i}\phi}\sin\theta\cos\theta = \mp\frac{1}{2}\sqrt{\frac{15}{2\pi}}\frac{(x\pm\mathrm{i}y)\,z}{r^2}$$
$$Y_{2,\pm2}(\theta,\phi) = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\mathrm{e}^{\pm2\mathrm{i}\phi}\sin^2\theta = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\frac{(x\pm\mathrm{i}y)^2}{r^2}$$

Angular momentum ladder operators

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

Differentiation

Euler's cyclic chain rule

$$\left(\frac{\partial x}{\partial y}\right)_z\left(\frac{\partial y}{\partial z}\right)_x\left(\frac{\partial z}{\partial x}\right)_y = -1$$

l'Hôpital's rule

$$\lim_{x\to a}\frac{f(x)}{g(x)} = \lim_{x\to a}\frac{f'(x)}{g'(x)} \qquad \text{if } \lim_{x\to a} f(x) = \lim_{x\to a} g(x) \in \{0,\, \pm\infty\}$$

Gradient

$$\begin{aligned}\boldsymbol{\nabla} f &= \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}\right) \cdot (\hat{\boldsymbol{x}}, \hat{\boldsymbol{y}}, \hat{\boldsymbol{z}}) \\ &= \left(\frac{\partial f}{\partial r}, \frac{1}{r}\frac{\partial f}{\partial \theta}, \frac{1}{r\sin\theta}\frac{\partial f}{\partial \phi}\right) \cdot \left(\hat{\boldsymbol{r}}, \hat{\boldsymbol{\theta}}, \hat{\boldsymbol{\phi}}\right)\end{aligned}$$

Divergence

$$\begin{aligned}\boldsymbol{\nabla} \cdot \boldsymbol{A} &= \frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \frac{\partial A_z}{\partial z} \\ &= \frac{1}{r^2}\frac{\partial}{\partial r} r^2 A_r + \frac{1}{r\sin\theta}\frac{\partial}{\partial \theta} A_\theta \sin\theta + \frac{1}{r\sin\theta}\frac{\partial A_\phi}{\partial \phi}\end{aligned}$$

Curl

$$\begin{aligned}\boldsymbol{\nabla} \times \boldsymbol{A} &= \left(\frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z}, \frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x}, \frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right) \cdot (\hat{\boldsymbol{x}}, \hat{\boldsymbol{y}}, \hat{\boldsymbol{z}}) \\ &= \left(\frac{1}{r\sin\theta}\left(\frac{\partial}{\partial \theta} A_\phi \sin\theta - \frac{\partial A_\theta}{\partial \phi}\right), \frac{1}{r}\left(\frac{1}{\sin\theta}\frac{\partial A_r}{\partial \phi} - \frac{\partial}{\partial r} r A_\phi\right), \frac{1}{r}\left(\frac{\partial}{\partial r} r A_\theta - \frac{\partial A_r}{\partial \theta}\right)\right) \\ &\quad \cdot \left(\hat{\boldsymbol{r}}, \hat{\boldsymbol{\theta}}, \hat{\boldsymbol{\phi}}\right)\end{aligned}$$

Laplacian

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

Character tables for some important symmetry groups

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	$x; y; z$	

C_s	E	σ_h			
A′	1	1	$x; y$	R_z	$x^2; y^2; z^2; xy$
A″	1	−1	z	$R_x; R_y$	$xz; yz$

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

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

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	$x; y$	

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

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)

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	$2C_3^z$	$3\sigma_v$			
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)	$(xz, yz); (x^2 - y^2, 2xy)$

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)	$(xz, yz); (x^2 - y^2, 2xy)$

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)		

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_4	E	$2C_4$	C_4^2	$2C_2$	$2C_2'$			
A_1	1	1	1	1	1			$x^2+y^2; z^2$
A_2	1	1	1	−1	−1	z	R_z	
B_1	1	−1	1	1	−1			x^2-y^2
B_2	1	−1	1	−1	1			xy
E	2	−1	−2	0	0	(x,y)	(R_x,R_y)	(xz,yz)

$D_{4\mathrm{d}}$	E	$2S_8$	$2C_4$	$2S_8^3$	C_4^2	$4C_2$	$4\sigma_\mathrm{d}$			
A_1	1	1	1	1	1	1	1			$x^2+y^2; z^2$
A_2	1	1	1	1	1	−1	−1		R_z	
B_1	1	−1	1	−1	1	1	−1			
B_2	1	−1	1	−1	1	−1	1	z		
E_1	2	$\sqrt{2}$	0	$-\sqrt{2}$	−2	0	0	(x,y)		
E_2	2	0	−2	0	2	0	0			$(x^2-y^2, 2xy)$
E_3	2	$-\sqrt{2}$	0	$\sqrt{2}$	−2	0	0		(R_x,R_y)	(xz,yz)

$D_{4\mathrm{h}}$	E	$2C_4$	C_4^2	$2C_2$	$2C_2'$	i	$2S_4$	σ_h	$2\sigma_\mathrm{v}$	$2\sigma_\mathrm{d}$		
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 $D_{4\mathrm{h}}$ 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 $\eta_+\eta_- = 1$.

$C_{5\mathrm{v}}$	E	$2C_5$	$2C_5^2$	$5\sigma_\mathrm{v}$	$\eta_\pm = \frac{1}{2}(\sqrt{5}\pm 1)$		
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			$(x^2-y^2, 2xy)$

$D_{5\mathrm{d}}$	E	$2C_5$	$2C_5^2$	$5C_2$	i	$2S_{10}^3$	$2S_{10}$	$5\sigma_\mathrm{d}$	$\eta_\pm = \frac{1}{2}(\sqrt{5}\pm 1)$		
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			

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			

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

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

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		

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

T_d	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_\mathrm{d}$			
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			$\big((2z^2-x^2-y^2),\sqrt{3}(x^2-y^2)\big)$
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	$6C_4$	$3C_4^2$	$8C_3$	$6C_2$			
A_1	1	1	1	1	1			$x^2+y^2+z^2$
A_2	1	-1	1	1	-1			
E	2	0	2	-1	0			$\big((2z^2-x^2-y^2),\sqrt{3}(x^2-y^2)\big)$
T_1	3	1	-1	0	-1	(x,y,z)	(R_x,R_y,R_z)	
T_2	3	-1	-1	0	1			(xz,xy,yz)

O_h	E	$8C_3$	$6C_2$	$6C_4$	$3C_4^2$	i	$6S_4$	$8S_6$	$3\sigma_\mathrm{h}$	$6\sigma_\mathrm{d}$		
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	0	0	2	2	0	-1	2	0		$\big((2z^2-x^2-y^2),\sqrt{3}(x^2-y^2)\big)$
T_{1g}	3	0	-1	1	-1	3	1	0	-1	-1	(R_x,R_y,R_z)	
T_{2g}	3	0	1	-1	-1	3	-1	0	-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	0	0	2	-2	0	1	-2	0		
T_{1u}	3	0	-1	1	-1	-3	-1	0	1	1	(x,y,z)	
T_{2u}	3	0	1	-1	-1	-3	1	0	1	-1		

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		$\Big(\sqrt{\tfrac{1}{12}}(2z^2-x^2-y^2),\ \tfrac{1}{2}(x^2-y^2), xz, xy, yz\Big)$
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		
$\cdots$		$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$		

Symmetry representations

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′ ⊕ 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′ ⊕ A″

$D_{\infty h}$ (x,y,z)	→	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 formula

$$\Gamma = a_1\Gamma^{(1)} \oplus a_2\Gamma^{(2)} \oplus \cdots \oplus a_n\Gamma^{(n)}$$
$$a_k = \frac{1}{h}\sum_R \chi^{(k)}(R)^*\chi(R)$$

Projection operator

$$\mathcal{P}^{(k)} \propto \sum_R \chi^{(k)}(R)^*\, R$$

Direct products

Generally

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

Selected tables of direct products

C_{3v}	A_1	A_2	E
A_1	A_1	A_2	E
A_2		A_1	E
E			$A_1 \oplus [A_2] \oplus E$

$C_{\infty v}$	Σ^+	Σ^-	Π	Δ
Σ^+	Σ^+	Σ^-	Π	Δ
Σ^-		Σ^+	Π	Δ
Π			$\Sigma^+ \oplus [\Sigma^-] \oplus \Delta$	$\Pi \oplus \Phi$
Δ				$\Sigma^+ \oplus [\Sigma^-] \oplus \Gamma$

T_d or O	A_1	A_2	E	T_1	T_2
A_1	A_1	A_2	E	T_1	T_2
A_2		A_1	E	T_2	T_1
E			$A_1 \oplus [A_2] \oplus E$	$T_1 \oplus T_2$	$T_1 \oplus T_2$
T_1				$A_1 \oplus E \oplus [T_1] \oplus T_2$	$A_2 \oplus E \oplus T_1 \oplus T_2$
T_2					$A_1 \oplus E \oplus [T_1] \oplus T_2$

Square brakets [ ] indicate the antisymmetrised component of the product.

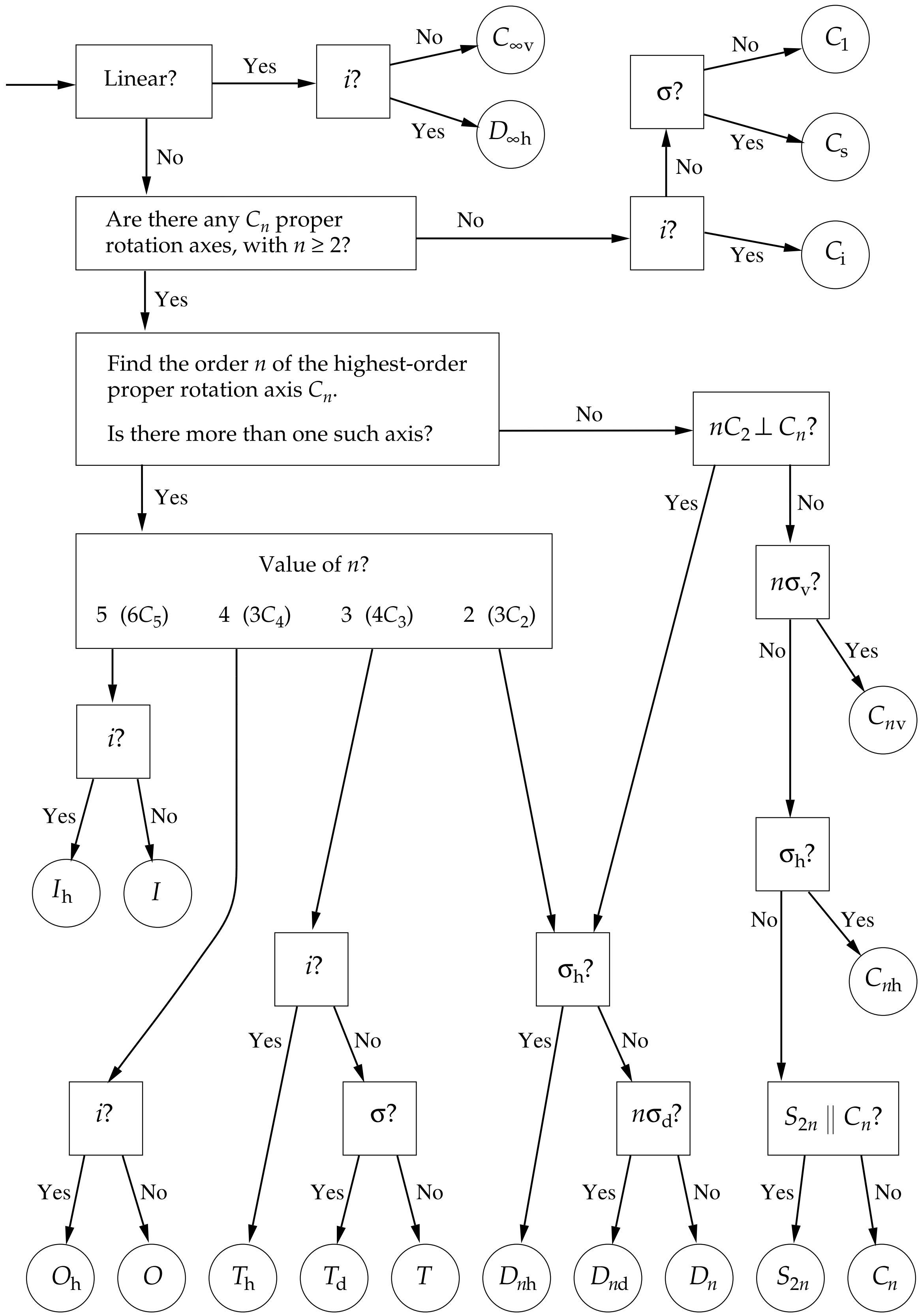
For point groups with a centre of inversion,

$$\mathrm{g}\otimes\mathrm{g} = \mathrm{g} \qquad \mathrm{u}\otimes\mathrm{u} = \mathrm{g} \qquad \mathrm{g}\otimes\mathrm{u} = \mathrm{u}.$$

For point groups with a horizontal mirror plane,

$$'\otimes\,' = \,' \qquad ''\otimes\,'' = \,' \qquad '\otimes\,'' = \,''.$$

Flow chart for determining molecular point groups



Space groups

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

P2$_1$

GEPs:

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

SEPs:

None

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

P2$_1$2$_1$2$_1$

GEPs:

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

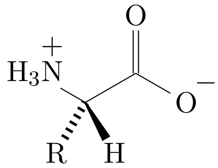
SEPs:

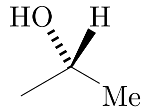
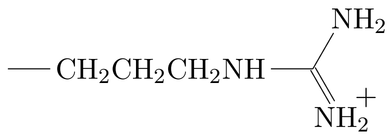
None

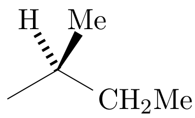
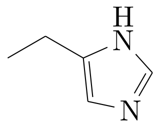
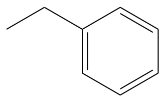
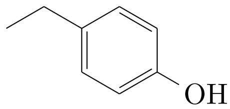
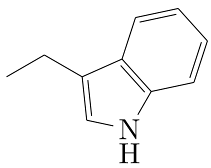
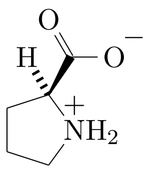
Parameters for selected magnetic nuclei

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	$\frac{1}{2}$

Amino acids

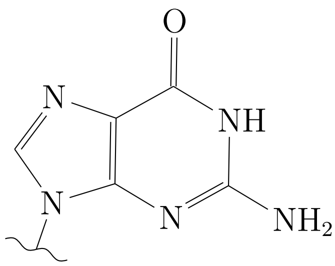
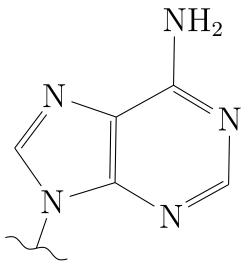
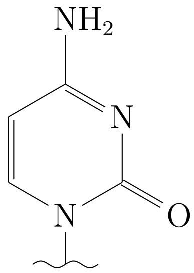
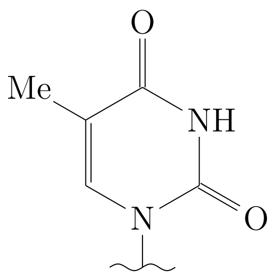
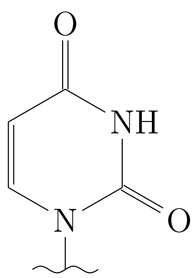


Name	Three-letter code	Single-letter code	Side chain, R =
Serine	Ser	S	$-CH_2OH$
Threonine	Thr	T	
Cysteine	Cys	C	$-CH_2SH$
Methionine	Met	M	$-CH_2CH_2SMe$
Aspartic acid	Asp	D	$-CH_2COO^-$
Asparagine	Asn	N	$-CH_2CONH_2$
Glutamic acid	Glu	E	$-CH_2CH_2COO^-$
Glutamine	Gln	Q	$-CH_2CH_2CONH_2$
Lysine	Lys	K	$-CH_2CH_2CH_2CH_2NH_3^+$
Arginine	Arg	R	
Glycine	Gly	G	$-H$
Alanine	Ala	A	$-Me$

Name	Three-letter code	Single-letter code	Side chain, R =
Leucine	Leu	L	$—CH_2CHMe_2$
Isoleucine	Ile	I	
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	

DNA codon table

First position	Second position: T		Second position: C		Second position: A		Second position: G		Third position
T	TTT	Phe	TCT	Ser	TAT	Tyr	TGT	Cys	T
T	TTC	Phe	TCC	Ser	TAC	Tyr	TGC	Cys	C
T	TTA	Leu	TCA	Ser	TAA	Stop	TGA	Stop	A
T	TTG	Leu	TCG	Ser	TAG	Stop	TGG	Trp	G
C	CTT	Leu	CCT	Pro	CAT	His	CGT	Arg	T
C	CTC	Leu	CCC	Pro	CAC	His	CGC	Arg	C
C	CTA	Leu	CCA	Pro	CAA	Gln	CGA	Arg	A
C	CTG	Leu	CCG	Pro	CAG	Gln	CGG	Arg	G
A	ATT	Ile	ACT	Thr	AAT	Asn	AGT	Ser	T
A	ATC	Ile	ACC	Thr	AAC	Asn	AGC	Ser	C
A	ATA	Ile	ACA	Thr	AAA	Lys	AGA	Arg	A
A	ATG	Met	ACG	Thr	AAG	Lys	AGG	Arg	G
G	GTT	Val	GCT	Ala	GAT	Asp	GGT	Gly	T
G	GTC	Val	GCC	Ala	GAC	Asp	GGC	Gly	C
G	GTA	Val	GCA	Ala	GAA	Glu	GGA	Gly	A
G	GTG	Val	GCG	Ala	GAG	Glu	GGG	Gly	G