

Symbols and Abbreviations

These lists contain the symbols and abbreviations most frequently used in this volume, but they are not expected to be exhaustive. Some specialized notation is only defined in the relevant chapter. An attempt has been made to standardize usage throughout the volume as far as is feasible, but it must be borne in mind that the original research literature certainly is not standardized in this way, and some difficulties may arise from this fact. Trivial use of subscripts *etc.* is not always mentioned in the symbols listed below. Some of the other symbols used in the text, *e.g.* for physical constants such as h or π , or for the thermodynamic quantities such as H or S , are not included in the list since they are considered to follow completely accepted usage.

Symbols

a_N	hyperfine (electron-nucleus) interaction constant
A	(i) hyperfine (electron-nucleus) interaction constant (ii) parameter relating to electric field effects on nuclear shielding
B	(i) magnetic induction field (magnetic flux density) (ii) parameter relating to electric field effects on nuclear shielding
B_0	static magnetic field of an n.m.r. or e.s.r. spectrometer
B_1, B_2	r.f. magnetic fields associated with ν_1, ν_2
C_X	spin-rotation coupling constant of nucleus X (used sometimes in tensor form): $C^2 = \frac{1}{3}(C_{\parallel}^2 + 2C_{\perp}^2)$.
C_{\parallel}, C_{\perp}	components of \mathbf{C} parallel and perpendicular to a molecular symmetry axis
D	(i) self-diffusion coefficient (ii) zero-field splitting constant
\mathbf{D}	rotational diffusion tensor
D_{\parallel}, D_{\perp}	components of \mathbf{D} parallel and perpendicular to a molecular symmetry axis
D_{int}	internal diffusion coefficient
D_o	overall isotropic diffusion coefficient
E	electric field
E_n	eigenvalue of $\hat{\mathcal{H}}$ (or a contribution to $\hat{\mathcal{H}}$)
g	nuclear or electronic g -factor
G	magnetic field gradient
H_{ij}	element of matrix representation of \mathcal{H}
\mathcal{H}	Hamiltonian operator – subscripts indicate its nature
I_i	nuclear spin operator for nucleus i

I_{ix}, I_{iy}, I_{iz}	components of I_i
I	(i) ionization potential (ii) moment of inertia
nJ	nuclear spin-spin coupling constant through n bonds (in Hz). Further information may be given by subscripts or in brackets. Brackets are used for indicating the species of nuclei coupled, <i>e.g.</i> $J(^{13}\text{C}, ^1\text{H})$, or, additionally, the coupling path, <i>e.g.</i> $J(\text{POCF})$
J_r	reduced splitting observed in a double resonance experiment
J	rotational quantum number
nK	reduced nuclear spin-spin coupling constant (see the notes concerning nJ)
m_i	eigenvalue of I_{iz} (magnetic component quantum number)
M_0	equilibrium macroscopic magnetization of a spin system in the presence of B_0
M_x, M_y, M_z	components of macroscopic magnetization
\bar{M}_n	the number average mol. wt.
P_A	valence p orbital of atom A
P_i	fractional population (of rotamers <i>etc.</i>)
P_{uv}	element of bond-order, charge-density matrix
q	electric field gradient
Q	(i) nuclear quadrupole moment (ii) quality factor for an r.f. coil
s_A	valence s -orbital of atom A
$S_A^2(0)$	electron density in S_A at nucleus A
S	(i) singlet state (ii) electron (or, occasionally, nuclear) spin <i>cf.</i> I (iii) ordering parameter for oriented systems (iv) overlap integral between molecular orbitals
t	elapsed time
T	(i) temperature (ii) triplet state
T_c	coalescence temperature for an n.m.r. spectrum
T_g	the glass transition temperature (of a polymer)
T_1^X	spin-lattice relaxation time of the X nuclei (further subscripts refer to the relaxation mechanism)
T_2^X	spin-spin relaxation time of the X nucleus (further subscripts refer to the relaxation mechanism)
T_2^i	inhomogeneity contribution to dephasing time for M_x or M_y
T_2^*	total dephasing time for M_x or M_y ; $(T_2^*)^{-1} = T_2^{-1} + (T_2^i)^{-1}$
T_3	decay time following $90_0\text{-}\tau\text{-}90_{90}$ pulse sequences
$T_{1\rho}^X, T_{2\rho}^X$	spin-lattice and spin-spin relaxation time of the X nuclei in the frame of reference rotating with B_1
T_{1D}	dipolar spin-lattice relaxation time
X_i	mole fraction of compound i
Z_A	atomic number of atom A
α	(i) nuclear spin wavefunction (eigenfunction of I_z) for a spin- $\frac{1}{2}$ nucleus

	(ii) polarizability
β	nuclear spin wavefunction (eigenfunction of I_z) for a spin- $\frac{1}{2}$ nucleus
γ_X	magnetogyric ratio of nucleus X
δ_X	chemical shift of a nucleus of element X (positive when the sample resonates to high frequency of the reference). Usually in p.p.m.
δ_{ij}	Kronecker delta ($= 1$ if $i = j$, and $= 0$ otherwise)
$\delta(r_{KA})$	Dirac delta operator
Δ	(i) time between field gradient pulses (ii) spectral width
ΔJ	anisotropy in J ($\Delta J = J_{\parallel} - J_{\perp}$, for axial symmetry)
Δn	population difference between nuclear spin states
$\Delta\delta$	change or difference in δ
$\Delta_{\frac{1}{2}}$	full width (in Hz) of a resonance line at half-height
$\Delta\sigma$	(i) anisotropy in σ ($\Delta\sigma = \sigma_{\parallel} - \sigma_{\perp}$, for axial symmetry) (ii) differences in σ for two different situations
$\Delta\chi$	(i) susceptibility anisotropy ($\Delta\chi = \chi_{\parallel} - \chi_{\perp}$, for axial symmetry) (ii) difference in electronegativities
ϵ_r	relative permittivity
ϵ_0	permittivity of a vacuum
η	(i) nuclear Overhauser effect (ii) asymmetry factor (e.g. in e^2qQ/h) (iii) refractive index (iv) viscosity
μ	magnetic dipole moment
μ_0	permeability of a vacuum
μ_B	Bohr magneton
μ_N	nuclear magneton
ν_i	Larmor precession frequency of nucleus i (in Hz)
ν_0	(i) spectrometer operating frequency (ii) Larmor precession frequency (general, or of bare nucleus)
ν_1	frequency of 'observing' r.f. magnetic field
ν_2	frequency of 'irradiating' r.f. magnetic field
σ_i	shielding parameter of nucleus i (used sometimes in tensor form). Usually in p.p.m. Subscripts may alternatively indicate contributions to σ .
$\sigma_{\parallel}, \sigma_{\perp}$	component of σ parallel and perpendicular to a molecular symmetry axis
σ^d	diamagnetic contribution to σ
σ^p	paramagnetic contribution to σ
τ	(i) pre-exchange lifetime of molecular species (ii) time between r.f. pulses (general symbol)
τ_c	correlation time
τ_{coll}	mean time between molecular collisions in the liquid state
τ_j	angular momentum correlation time
τ_p	pulse duration
τ_t	translational magnetic relaxation correlation time

χ	(i) magnetic susceptibility (ii) electronegativity (iii) nuclear quadrupole coupling constant ($= e^2qQ/h$)
ω	carrier frequency in rad s^{-1}
$\omega_i, \omega_0, \omega_1, \omega_2$	as for $\nu_i, \nu_0, \nu_1, \nu_2$ but in rad s^{-1}
ω_m	modulation angular frequency (in rad s^{-1})
ω_r	sample rotation (rad s^{-1})

Abbreviations

(a) Physical properties

a.f.	audiofrequency
a.u.	atomic unit
a.m.	amplitude modulation
b.c.c.	body-centred cubic
c.d.	circular dichroism
c.m.c.	critical micelle concentration
e.d.	electron diffraction
e.f.g.	electric field gradient
e.s.r.	electron spin resonance
erf	the error function
f.c.c.	face-centred cubic
f.m.	frequency modulation
h.c.p.	hexagonal close-packed
h.f.	hyperfine
i.d.	inside diameter
i.f.	intermediate frequency
i.r.	infrared
l.c.	liquid crystalline
m.w.	microwave
mol. wt.	molecular weight
n.m.r.	nuclear magnetic resonance
n.q.r.	nuclear quadrupole resonance
o.d.	outside diameter
p.p.m.	parts per million
r.f.	radiofrequency
r.m.s.	root mean square
s.h.f.	super-high frequency
u.h.f.	ultra-high frequency
u.v.	ultraviolet
ADC	analog-to-digital converter
AEE	average excitation energy approximation
ARP	adiabatic rapid passage
ASIS	aromatic solvent-induced shift

Ch	Cholesteric (phase)
CIDEP	chemically induced dynamic electron polarization
CIDNP	chemically induced dynamic nuclear polarization
CNDO	complete neglect of differential overlap
CP	cross polarization
CPMG	Carr–Purcell pulse sequence. Meibom–Gill modification
CSA	chemical shielding anisotropy
CW	continuous wave
DAC	digital-to-analog converter
DD	dipole–dipole (interaction or relaxation mechanism)
DEFT	driven-equilibrium Fourier transform
DNP	dynamic nuclear polarization
DSC	differential scanning calorimetry
EHMO	extended Hückel molecular orbital
ENDOR	electron–nucleus double resonance
FC	Fermi contact
FID	free induction decay
FPT	finite perturbation theory
FT	Fourier transform
GIAO	gauge-invariant atomic orbitals
INDO	intermediate neglect of differential overlap
INDOR	internuclear double resonance
La	lamellar (phase)
LCAO	linear combination of atomic orbitals
LIS	lanthanide-induced shift
LSR	lanthanide shift reagent
MASS	magic angle sample spinning
MINDO	modified INDO (MINDO/3)
MO	molecular orbital
MP	multipulse
N	nematic (phase)
NOE	nuclear Overhauser effect
NQCC	nuclear quadrupole coupling constant
OB	orbital
PRE	proton relaxation enhancement
PRFT	partially relaxed Fourier transform
QF	quadrupole moment/field gradient (interaction relaxation mechanism)
QPD	quadrature phase detection
RAM	random access memory
SCF	self-consistent field
SCPT	self-consistent perturbation theory
SD	spin-dipolar
SEFT	spin-echo Fourier transform
Sm	smectic (phase)
SOS	sum over states
S/N	signal-to-noise ratio
SPI	selective population inversion

SPT	selective population transfer
SR	spin-rotation (interaction or relaxation mechanism)
SRTA	single relaxation time approximation
STO	slater-type orbital (basis set)
VB	valence bond
WAHUHA	Wauh, Huber, and Haeberlen (cycle of pulses)

(b) *Chemical species**

acac	acetylacetonato
ACTH	adrenocorticotropic hormone (corticotropin)
ADP	adenosine diphosphate
AMP	adenosine monophosphate
ATP	adenosine triphosphate
BSA	bovine serum albumin
CMP	cytidine monophosphate
cp	cyclopentadienyl
DAP	dodecylammonium propionate
DME	1,2-dimethoxyethane
DMF	dimethylformamide
DML	dimyristoyl-lecithin
DMS	dimethylsiloxane
DMSO	dimethylsulphoxide
DNA	deoxyribonucleic acid
DPG	2,3-dipho sphoglycerate
DPL	dipalmitoyl-lecithin
dpm	dipivaloylmethanato
DPPH	diphenylpicrylhydrazyl
DSS	2,2-dimethyl-2-silapentane-5-sulphonate (usually as the sodium salt)
DTBN	di- <i>t</i> -butyl nitroxide
EBBA	<i>N</i> -(<i>p</i> -ethoxybenzylidene)- <i>p</i> -butylaniline
EDTA	ethylenediaminetetra-acetic acid
EVA	ethylene-vinyl acetate
fod	1,1,1,2,2,3,3-heptafluoro-7,7-dimethyloctane-4,6-dionato
HAB	4,4'-bis(heptyl)azoxybenzene
HMPA	hexamethylphosphoramide
HOAB	<i>p</i> - <i>n</i> -heptyloxyazoxybenzene
IHP	inositolhexaphosphate
KDP	potassium dihydrogen phosphate
MBBA	<i>N</i> -(<i>p</i> -methoxybenzylidene)- <i>p</i> -butylaniline
NADH(P)	nicotinamide adenine dinucleotide (phosphate)
NMF	<i>N</i> -methylformamide
PAA	<i>p</i> -azoxyanisole
PBA	pyrene butyric acid
PBLG	poly(L-benzyl γ -glutamate)
PC	phosphatidyl choline (lecithin)
PCB	polychlorinated biphenyl
PDMS	polydimethylsiloxane

Symbols and Abbreviations

PMA	poly(methacrylic acid)
PMMA	poly(methyl methacrylate)
POM	poly(oxymethylene)
PS	phosphatidylserine
PTFE	polytetrafluoroethylene
PVC	poly(vinyl chloride)
PVF	poly(vinyl fluoride)
PVP	poly(vinyl pyrrolidone)
RNA	ribonucleic acid (tRNA, transfer RNA)
SDS	sodium dodecyl sulphate
TAB	trimethylammonium bromide
TCNQ	tetracyanoquinodimethane
TFA	trifluoroacetic acid
THF	tetrahydrofuran
TMS	tetramethylsilane
UTP	uridine triphosphate

Amino-acid residues

Ala	alanine
Arg	arginine
Asn	asparagine
Asp	aspartic acid
Cys	cysteine
Gln	glutamine
Glu	glutamic acid
Gly	glycine
His	histidine
Hyp	hydroxyproline
Ile	isoleucine
Leu	leucine
Lys	lysine
Met	methionine
Phe	phenylalanine
Pro	proline
Ser	serine
Thr	threonine
Trp	tryptophan
Tyr	tyrosine
Val	valine

* Lower case initials are used when the species is a ligand.