

# Symbols and Abbreviations

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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  $\pi$ , 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 $\nu_1, \nu_2$
$C_X$	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
$D_{\text{int}}$	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, e.g. $J(^{13}\text{C}, ^1\text{H})$ , or, additionally, the coupling path, e.g. $J(\text{POCF})$
$J_r$	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
$\alpha$	(i) nuclear spin wavefunction (eigenfunction of $I_z$ ) for a spin- $\frac{1}{2}$ nucleus

	(ii) polarizability
$\beta$	nuclear spin wavefunction (eigenfunction of $I_z$ ) for a spin- $\frac{1}{2}$ nucleus
$\gamma_X$	magnetogyric ratio of nucleus X
$\delta_X$	chemical shift of a nucleus of element X (positive when the sample resonates to high frequency of the reference). Usually in p.p.m.
$\delta_{ij}$	Kronecker delta ( $= 1$ if $i = j$ , and $= 0$ otherwise)
$\delta(r_{K\Lambda})$	Dirac delta operator
$\Delta$	(i) time between field gradient pulses (ii) spectral width
$\Delta J$	anisotropy in $J$ ( $\Delta J = J_{\parallel} - J_{\perp}$ , for axial symmetry)
$\Delta n$	population difference between nuclear spin states
$\Delta\delta$	change or difference in $\delta$
$\Delta_{\frac{1}{2}}$	full width (in Hz) of a resonance line at half-height
$\Delta\sigma$	(i) anisotropy in $\sigma$ ( $\Delta\sigma = \sigma_{\parallel} - \sigma_{\perp}$ , for axial symmetry) (ii) differences in $\sigma$ for two different situations
$\Delta\chi$	(i) susceptibility anisotropy ( $\Delta\chi = \chi_{\parallel} - \chi_{\perp}$ , for axial symmetry) (ii) difference in electronegativities
$\epsilon_r$	relative permittivity
$\epsilon_0$	permittivity of a vacuum
$\eta$	(i) nuclear Overhauser effect (ii) asymmetry factor (e.g. in $e^2qQ/h$ ) (iii) refractive index (iv) viscosity
$\mu$	magnetic dipole moment
$\mu_0$	permeability of a vacuum
$\mu_B$	Bohr magneton
$\mu_N$	nuclear magneton
$\nu_i$	Larmor precession frequency of nucleus $i$ (in Hz)
$\nu_0$	(i) spectrometer operating frequency (ii) Larmor precession frequency (general, or of bare nucleus)
$\nu_1$	frequency of 'observing' r.f. magnetic field
$\nu_2$	frequency of 'irradiating' r.f. magnetic field
$\sigma_i$	shielding parameter of nucleus $i$ (used sometimes in tensor form). Usually in p.p.m. Subscripts may alternatively indicate contributions to $\sigma$ .
$\sigma_{\parallel}, \sigma_{\perp}$	component of $\sigma$ parallel and perpendicular to a molecular symmetry axis
$\sigma^d$	diamagnetic contribution to $\sigma$
$\sigma^p$	paramagnetic contribution to $\sigma$
$\tau$	(i) pre-exchange lifetime of molecular species (ii) time between r.f. pulses (general symbol)
$\tau_c$	correlation time
$\tau_{\text{coll}}$	mean time between molecular collisions in the liquid state
$\tau_j$	angular momentum correlation time
$\tau_p$	pulse duration
$\tau_t$	translational magnetic relaxation correlation time

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

## 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 $\gamma$ -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.