

# 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 NMR or ESR 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 $C$ parallel and perpendicular to a molecular symmetry axis
$D$	(i) self-diffusion coefficient (ii) zero-field splitting constant
$D$	rotational diffusion tensor
$D_{\parallel}, D_{\perp}$	components of $D$ parallel and perpendicular to a molecular symmetry axis
$D_{int}$	internal diffusion coefficient
$D_0$	overall isotropic diffusion coefficient
$E$	electric field
$E_n$	eigenvalue of $\mathcal{H}$ (or a contribution to $\mathcal{H}$ )
$g$	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

$M_n$	the number of average mol. wt.
$P_A$	valence $p$ orbital of atom A
$P_i$	fractional population (or 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 nuclear 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 NMR 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 $M_y$ ; $(T_2^*)^{-1} = (T_2^{-1}) + (T_2^i)^{-1}$
$T_3^X$	decay time following $90_0$ - $\tau$ - $90_{90}$ 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
$Z_A$	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 $I_x$ ) 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)
$\delta(r_{KA})$	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 states
$\Delta\delta$	change of difference in $\delta$
$\Delta_{\nu}$	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) differences in electronegativities
$\epsilon_r$	relative permittivity
$\epsilon_0$	permittivity of a vacuum
$\eta$	(i) nuclear Overhauser effect (ii) asymmetry factor ( <i>e.g.</i> 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 $\sigma$ .
$\sigma_{\parallel}, \sigma_{\perp}$	components of $\sigma$ parallel and perpendicular to a molecular symmetry axis
$\sigma^d$	diagrammatic 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
$\tau_1$	translational magnetic relaxation correlation time
$\chi$	(i) magnetic susceptibility (ii) electronegativity (iii) nuclear quadrupole coupling constant ( $= e^2qQ/h$ )
$\omega$	carrier frequency in $\text{rad s}^{-1}$
$\omega_b, \omega_0, \omega_1, \omega_2$	as for $\nu_b, \nu_0, \nu_1, \nu_2$ 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.m.c.	critical micelle concentration
e.d.	electron diffraction
e.f.g.	electric field gradient
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
l.c.	liquid crystalline
mol. wt.	molecular weight
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
ADC	analogue-to-digital converter
AEE	average excitation energy approximation
AQ	acquire
ARP	adiabatic rapid passage
BIRD	bilinear rotation decoupling
CCPPA	coupled cluster polarization propagator approximation
CH-COSY	carbon-hydrogen correlation spectroscopy
CHESS	chemical shift selection
CHF	coupled Hartree-Fock molecular orbital calculations
CIDEP	chemically induced dynamic electron polarization
CIDNP	chemically induced dynamic nuclear polarization
COSY	correlation spectroscopy

CP	cross polarization
CPMG	Carr–Purcell pulse sequence. Meiboom–Gill modification
CSA	chemical shielding anisotropy
CSI	chemical shift imaging
CW	continuous wave
DAC	digital-to-analogue converter
DD	dipole-dipole (interaction or relaxation mechanism)
DEPT	distortionless enhancement by polarization transfer
DLB	differential line broadening
DNP	dynamic nuclear polarization
DQ	double quantum
DQF	double quantum filter
ECOSY	exclusive correlation spectroscopy
EHT	extended Hückel molecular orbital theory
ENDOR	electron–nucleus double resonance
EOM	equations of motion
ESR	electron spin resonance
EXSY	exchange spectroscopy
FC	Fermi contact
FID	free induction decay
FLASH	fast low angle shot
FPT	finite perturbation theory
FT	Fourier transform
GIAO	gauge included atomic orbitals
HMQ	heteronuclear multiquantum
HOHAHA	homonuclear Hartman–Hahn
HRPA	higher random phased approximation
IDESS	improved depth selective single surface coil spectroscopy
IGLO	individual gauge for different localized orbitals
INADEQUATE	incredible natural abundance double quantum transfer experiment
INDO	intermediate neglect of differential overlap
INDO/S	intermediate neglect of differential overlap calculations for spectroscopy
INDOR	internuclear double resonance
INEPT	insensitive nuclei enhanced by polarization transfer
IR	infrared
ISIS	image selected <i>in vivo</i> spectroscopy
LIS	lanthanide induced shift
LORG	local origin
LSR	lanthanide shift reagent
MASS	magic angle sample spinning
MBPT	many body perturbation theory
MEM	maximum entropy method
MINDO	modified INDO
MQ	multiple quantum
MQC	multiple quantum coherence
MQF	multiple quantum filter
NMR	nuclear magnetic resonance
NOE	nuclear Overhauser enhancement
NOESY	nuclear Overhauser enhancement spectroscopy
NQCC	nuclear quadrupole coupling constant
NQR	nuclear quadrupole resonance
PFG	pulsed field gradient
PRE	proton relaxation enhancement
QF	quadrupole moment/field gradient
QPD	quadrature phase detection
REX	relativistically extended Hückel molecular orbital theory
ROESY	rotating frame Overhauser enhancement spectroscopy
RPA	random phase approximation
SCPT	self consistent perturbation theory
SD	spin dipolar
SECSY	spin echo correlation spectroscopy

SEFT	spin echo Fourier transform
SLITDRESS	slice interleaved depth resolved surface coil spectroscopy
SOPPA	second order polarization propagator approach
SPI	selective population inversion
SPT	selective population transfer
SR	spin rotation (interaction or relaxation mechanism)
TART	tip angle reduced $T_1$ imaging
TOCSY	total correlation spectroscopy
UV	ultraviolet
WAHUHA	Waugh, Huber and Häberlen (cycle of pulses)
ZQ	zero quantum
ZQC	zero quantum coherence

(b) *Chemical species\**

acac	acetylacetonato
ACTH	adrenocorticotrophic 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	dimethyl sulfoxide
DNA	deoxyribonucleic acid
DPG	2,3-diphosphoglycerate
DPI	dipalmitoyl-lecithin
dpm	dipivaloylmethanato
DPPH	diphenylpicrylhydrazyl
DSS	2,2-dimethyl-2-silapentane-5-sulfonate (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 $\mu$ -glutamate)
PC	phosphatidyl choline (lecithin)
PCB	polychlorinated biphenyl
PDMS	polydimethylsiloxane
PMA	poly(methacrylic acid)
PMMA	poly(methyl methacrylate)
POM	poly(oxymethylene)
PS	phosphatidylserine
PTFE	polytetrafluoroethylene
PVC	poly(vinyl chloride)

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

PVF	poly(vinyl fluoride)
PVP	poly(vinyl pyrrolidone)
RNA	ribonucleic acid (tRNA, transfer RNA)
SDS	sodium dodecyl sulfate
TAB	trimethylammonium bromide
TCNQ	tetracyanoquinodimethane
TFA	trifluoroacetic acid
THF	tetrahydrofuran
TMS	tetramethylsilane
UTP	uridine triphosphate

*Amino-acid residues*

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