

# 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 list below. Some of the other symbols used in the text, *e.g.* for physical constants such as  $h$  or  $\pi$ , or for thermodynamic quantities such as  $H$  or  $S$ , are not included in the list since they are reckoned to follow completely accepted usage (see M. L. McGlashan, 'Physico-Chemical Quantities and Units', Royal Institute of Chemistry Monographs for Teachers, No. 15, second edition, 1971). The spin-system notation used in the present volume of Specialist Periodical Reports on n.m.r. is that suggested by Haigh [*J. Chem. Soc. (A)*, 1970, 1682].

## Symbols

$a$	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
$\bar{C}$	one third of the trace of $\mathbf{C}$ : $\bar{C} = \frac{1}{3}(C_{\parallel} + 2C_{\perp})$
$D$	(i) self-diffusion coefficient (ii) doublet state
$\mathbf{D}$	rotational diffusion tensor
$D_{\parallel}, D_{\perp}$	components of $\mathbf{D}$ parallel and perpendicular to a molecular symmetry axis
$e$	magnitude of the charge on the electron

$E$	electric field
$E_n$	eigenvalue of $\hat{\mathcal{H}}$ (or of a contribution to $\hat{\mathcal{H}}$ )
$f$	modulation frequency
$F_G$	nuclear spin operator for a group, $G$ , of nuclei
$\hat{F}_{Gx}, \hat{F}_{Gy}, \hat{F}_{Gz}$	components of $\hat{F}_G$
$F_G$	magnetic quantum number associated with $\hat{F}_G$
$g$	nuclear or electronic $g$ -factor
$G$	magnetic field gradient
$H_{ij}$	element of matrix representation of $\hat{\mathcal{H}}$
$\hat{\mathcal{H}}$	Hamiltonian operator (in energy units) – subscripts indicate the nature of the operator
$\hat{I}_i$	nuclear spin operator for nucleus $i$
$\hat{I}_{ix}, \hat{I}_{iy}, \hat{I}_{iz}$	components of $\hat{I}_i$
$\hat{I}_{i+}, \hat{I}_{i-}$	‘raising’ and ‘lowering’ spin operators for nucleus $i$
$I_i$	magnetic quantum number associated with $\hat{I}_i$
$I$	(i) ionization potential (ii) moment of inertia
$\mathcal{I}_{mn}$	intensity of a transition between nuclear states $m$ and $n$
${}^nJ$	nuclear spin–spin coupling constant through $n$ bonds (in Hz). Further information may be given by subscripts or in brackets. Normally subscripts are only used for algebraic symbols for nuclei in spectral analysis cases, e.g. $J_{Ax}$ . 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. $J(\text{POCF})$
$J$	rotational quantum number
$\mathcal{J}$	electron exchange interaction
${}^nK$	reduced nuclear spin–spin coupling constant (see the notes concerning ${}^nJ$ )
$K$	Knight shift
$m_l$	eigenvalue of $\hat{I}_{iz}$ (magnetic component quantum number)
$m_T$	total magnetic quantum number for a spin system (eigenvalue of $\sum_i \hat{I}_{iz}$ )
$M_0$	equilibrium macroscopic magnetization of a spin system in the presence of $B_0$
$M_x, M_y, M_z$	components of macroscopic magnetization
$M_n$	moment of a spectrum ( $M_2 =$ second moment, <i>etc.</i> )
$p_A$	valence $p$ orbital of atom A
$P_i$	fractional population (of rotamers <i>etc.</i> )
$P_{s_A s_B}$	molecular orbital bond order between $s_A$ and $s_B$
$\mathcal{P}$	probability of a transition between two nuclear levels
$q$	electric field gradient
$Q$	(i) McConnell’s constant relating to $a$ (ii) nuclear quadrupole moment (iii) quality factor for an r.f. coil
$R$	(i) Redfield relaxation matrix (ii) magnitude of reaction electric field
$s_A$	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
$t_{cp}$	180° pulse separation in a Carr–Purcell sequence
$T$	(i) temperature (ii) triplet state
$T_c$	(i) coalescence temperature for an n.m.r. spectrum (ii) critical solution temperature (iii) phase transition temperature
$T_1^X$	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)
$T_2'$	inhomogeneity contribution to dephasing time for $M_x$ or $M_y$
$T_2^*$	total dephasing time for $M_x$ or $M_y$ ; $(T_2^*)^{-1} = T_2^{-1} + (T_2')^{-1}$
$T_3$	decay time following 90 <sub>0</sub> - $\tau$ -90 <sub>90</sub> 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
$T_d$	pulse delay time (in FT n.m.r.)
$T_{ac}$	acquisition time (in FT n.m.r.)
$T_p$	period for repetitive pulses ( = interpulse time = $T_{ac} + T_d$ if $\tau_p$ is negligible)
$T_N$	Néel temperature
$X_i$	mole fraction of compound $i$
$Z_A$	atomic number of atom A
$\alpha$	(i) nuclear spin wavefunction (eigenfunction of $\hat{I}_z$ ) for a spin- $\frac{1}{2}$ nucleus (ii) polarizability
$\alpha_A^2$	$s$ -character of hybrid orbital at atom A
$\beta$	nuclear spin wavefunction (eigenfunction of $\hat{I}_z$ ) for a spin- $\frac{1}{2}$ nucleus
$\gamma_X$	(i) magnetogyric ratio of nucleus X (ii) activity coefficient of compound X
$\Gamma_N, \Gamma_M$	polarization (net or multiplet, respectively) in Kaptein's rules for CIDNP
$\delta_X$	chemical shift (for the resonance) of nucleus of element X (positive when the sample resonates to high frequency of the reference). Usually in p.p.m. Further information regarding solvent, references, or nucleus of interest may be given by superscripts or subscripts or in brackets.
$\delta_{ij}$	Kronecker delta ( = 1 if $i = j$ , and = 0 otherwise)
$\Delta$	(i) time between field gradient pulses (ii) spectral width
$\Delta C$	anisotropy in <b>C</b> ( $\Delta C = C_{  } - C_{\perp}$ )

$\Delta J$	anisotropy in $J$ ( $\Delta J = J_{\parallel} - J_{\perp}$ )
$\Delta n$	population difference between nuclear states
$\Delta\delta$	change or difference in $\delta$
$\Delta\nu_{\frac{1}{2}}$	full width (in Hz) of a resonance line at half-height
$\Delta\sigma$	(i) anisotropy in $\sigma$ ( $\Delta\sigma = \sigma_{\parallel} - \sigma_{\perp}$ ) (ii) differences in $\sigma$ for two different situations
$\Delta\chi$	(i) susceptibility anisotropy ( $\Delta\chi = \chi_{\parallel} - \chi_{\perp}$ ) (ii) difference 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
$\mu$	(i) magnetic dipole moment (ii) electric 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
$\Xi_X$	resonance frequency for the nucleus of element X in a magnetic field such that the protons in TMS resonate at exactly 100 MHz
$\Pi_{s_A s_B}$	mutual polarizability of $s_A$ and $s_B$
$\rho_{s_A}^2$	spin density in $s_A$
$\sigma_i$	(i) shielding constant of nucleus $i$ (used sometimes in tensor form). Usually in p.p.m. Subscripts may alternatively indicate contributions to $\sigma$ . (ii) collision cross-section (iii) spin density matrix
$\sigma_{\parallel}, \sigma_{\perp}$	components of $\sigma$ parallel and perpendicular to a molecular symmetry axis
$\tau$	(i) pre-exchange lifetime of molecular species (ii) cage lifetime (in CIDNP work) (iii) time between r.f. pulses (general symbol)
$\tau_c$	correlation time
$\tau_{coll}$	mean time between molecular collisions in the liquid state
$\tau_1, \tau_2$	correlation time for the spherical harmonics $Y_{1m}, Y_{2m}$
$\tau_{\parallel}, \tau_{\perp}$	correlation time for molecular rotation parallel and perpendicular to a molecular symmetry axis
$\tau_J$	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 ( $= e^2qQ/h$ )
$\omega_c$	carrier frequency in $\text{rad s}^{-1}$
$\omega_l, \omega_0, \omega_1, \omega_2$	as for $\nu_l, \nu_0, \nu_1, \nu_2$ but in $\text{rad s}^{-1}$
$\omega_m$	modulation angular frequency (in $\text{rad s}^{-1}$ )

## *Abbreviations*

### *(a) Physical properties*

a.c.	alternating current
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
d.c.	direct current
e.d.	electron diffraction
e.f.g.	electric field gradient
e.s.r.	electron spin resonance
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
ARP	adiabatic rapid passage
ASIS	aromatic solvent-induced shift
BCD	binary coded decimal
CAT	computer of average transients

CHF	coupled Hartree-Fock
CIDEP	chemically induced dynamic electron polarization
CIDNP	chemically induced dynamic nuclear polarization
CNDO	complete neglect of differential overlap
CPMG	Carr–Purcell pulse sequence, Meibom–Gill modification
CSA	chemical shift (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
EHMO	extended Hückel molecular orbital
ENDOR	electron–nucleus double resonance
FC	Fermi contact
FET	field-effect transistor
FID	free induction decay
FPT	finite perturbation theory
FT	Fourier transform
GIAO	gauge-invariant atomic orbitals
HR	high resolution
HSP	homogeneity-spoiling pulse
INDO	intermediate neglect of differential overlap
INDOR	internuclear double resonance
LCAO	linear combination of atomic orbitals
LIS	lanthanide-induced shift
LSR	lanthanide shift reagent
MO	molecular orbital
MOSFET	metal oxide silicon FET (q.v.)
NOE	nuclear Overhauser effect
NQCC	nuclear quadrupole coupling constant
OB	orbital (contribution to scalar coupling)
PRE	proton relaxation enhancement
PRFT	partially relaxed Fourier transform
QF	quadrupole moment/field gradient (interaction or relaxation mechanism)
QPD	quadrature phase detection
RPFT	repetitively pulsed Fourier transform
SC	scalar (interaction or relaxation mechanism)
SCF	self-consistent field
SD	spin-dipolar (contribution to scalar coupling)
SEFT	spin-echo Fourier transform
S/N	signal-to-noise ratio
SOS	sum over states
SPI	selective population inversion
SPT	selective population transfer
SR	spin-rotation (interaction or relaxation mechanism)
UCHF	uncoupled Hartree-Fock

VB	valence bond
WAHUHA	Waugh, Huber, and Haeberlen (cycle of pulses)
WEFT	water-eliminated Fourier transform

(b) *Chemical species\**

acac	acetyl acetonato
ADP	adenosine diphosphate
AMP	adenosine monophosphate
ATP	adenosine triphosphate
bhmc	3- <i>t</i> -butylhydroxymethylene- <i>d</i> -camphorato
BSA	bovine serum albumin
CMP	cytidine monophosphate
cp	cyclopentadienyl
DAP	dodecylammonium propionate
DDT	1,1,1-trichloro-2,2-bis( <i>p</i> -chlorophenyl)ethane
DME	1,2-dimethoxyethane
DMF	dimethylformamide
DML	dimyristoyl lecithin
DMSO	dimethylsulphoxide
DNA	deoxyribonucleic acid
DPG	2,3-diphosphoglycerate
DPL	dipalmitoyl lecithin
DPPH	diphenyl picryl hydrazyl
DSS	2,2-dimethyl-2-silapentane-5-sulphonate (usually as the sodium salt)
EBBA	<i>N</i> -( <i>p</i> -ethoxybenzylidene)- <i>p</i> -butylaniline
EDTA	ethylenediaminetetra-acetic acid
facam	3-trifluoroacetyl- <i>d</i> -camphorato
fod	1,1,1,2,2,3,3-heptafluoro-7,7-dimethyl-4,6-octanedionato
HAB	4,4'-bis(heptyl)azoxybenzene
hfbc	3-heptafluorobutyryl- <i>d</i> -camphorato
HOAB	<i>p</i> - <i>n</i> -heptyloxyazoxybenzene
IHP	inositol hexaphosphate
KDP	potassium dihydrogen phosphate
MBBA	<i>N</i> -( <i>p</i> -methoxybenzylidene)- <i>p</i> -butylaniline
MMA	methyl methacrylate
NADH	nicotinamide adenine dinucleotide
OMTS	octamethyltetrasiloxane
PAA	<i>p</i> -azoxyanisole
PBA	pyrene butyric acid
PBLG	poly( $\alpha$ -benzyl L-glutamate)
PMAA	poly(methacrylic acid)
PMMA	poly(methyl methacrylate)
PSA	pyrene sulphonic acid
PTFE	polytetrafluoroethylene
PVC	poly(vinyl chloride)

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

PVP	poly(vinyl pyrrolidone)
py	pyridine
RNA	ribonucleic acid
SDS	sodium dodecyl sulphate
TBBA	terephthal-bis-4-(4-n-butylaniline)
TCNQ	tetracyanoquinodimethane
TFA	trifluoroacetic acid
THF	tetrahydrofuran
tmhd†	2,2,6,6-tetramethylheptane-3,5-dionato
TMS	tetramethylsilane

† This ligand is sometimes referred to as dpm, dipivaloylmethanato.