Table of Symbols

$\langle A \rangle$	expectation value of an operator **A** [2.19], [2.47]
[**A**, **B**]	commutator of operators **A** and **B** [2.26]
A	matrix or operator **A**
$\mathbf{A}^{\dagger}$	adjoint of a matrix or operator **A**
$\mathcal{A}$	Commutation superoperator of **A**
A_{α}	axial component of the alignment tensor [2.323]
A_{kk}	principal value of the alignment tensor [2.323]
A_r	rhombicity of the alignment tensor [2.323]
A_k^q	irreducible spherical tensor of rank k [2.303]
	tensor spin operator [5.53]
A_{kp}^q	basis tensor operators of A_k^q [5.54]
$A(\omega)$	absorptive Lorentizian lineshape [3.29]
$a_{mn}(t)$	mixing coefficient for transfer of coherence from spin or site m to spin or site n [4.18], [5.19], [5.175], [5.180]
B, **B**(t)	magnetic field vector
B_0	static magnetic field strength
ΔB_0	reduced static magnetic field strength [1.19]
B_1	rf magnetic field amplitude
$\mathbf{B}_{eff}(t)$	effective magnetic field in rotating frame [1.13]
$\mathbf{B}^r$	effective magnetic field in rotating frame [1.18]
B^r	magnitude of the effective magnetic field in rotating frame [1.20]

$\mathbf{B}_{rf}(t)$	rf magnetic field [1.15]
$\mathbf{B}_j$	jth basis operator
C	capacitance [3.2]
$\mathbf{C}^{(n)}$	irreducible tensor of rank n [2.298]
$C^2_{00}(\tau)$	orientational correlation function for rotation of an isotropic sphere [5.97]
$C(\tau)$	stochastic correlation function [5.93]
$c_0(t)$	function of physical constants and spatial variables for lattice-spin system coupling [5.93]
D_{IS}	(residual) dipolar coupling constant [2.326], [2.327]
$D^2_{mn}(\alpha_{LP}, \beta_{LP}, \gamma_{LP})$	Wigner rotation matrices, Table 2.4
$D(\omega)$	dispersive Lorentzian lineshape [3.30]
$d_{\alpha N}$	sequential $^1H^{\alpha}$-$^1H^N$ NOE connectivity
$d_{\beta N}$	sequential $^1H^{\beta}$-$^1H^N$ NOE connectivity
d_{NN}	sequential $^1H^N$-$^1H^N$ NOE connectivity
d_{00}	c_0^2 [5.94]
$d^2_{mn}(\beta)$	reduced rotation matrices, Table 2.4
$\mathbf{E}$	identity matrix or operator
$\mathbf{F}^+$	observation operator [2.128]
$\mathbf{F}_z$	non-selective z-rotation [4.33]
F^q_2	components of irreducible spherical tensor of second rank [2.305]
$F^q_k(t)$	random function of spatial lattice variables [5.53]
$\mathscr{F}\{s(t)\}$	Fourier transformation of $s(t)$ [3.14]
f_c	frequency bandwidth of time-domain signal
f_n	Nyquist frequency [3.6]
$G_{x,y,z}$	pulsed field gradient strengths
$\mathscr{H}$	Hamiltonian operator
$\mathscr{H}_0$	time-independent Hamiltonian in absence of applied RF fields [2.154], [5.47]
$\mathscr{H}_1(t)$	stochastic Hamiltonian [5.47]
$\mathscr{H}_e$	effective Hamiltonian in rotating frame [2.66], [2.97]
$\mathscr{H}_J$	scalar coupling Hamiltonian [2.154]
$\mathscr{H}_{rf}(t)$	rf magnetic field Hamiltonian [2.93]
$\mathscr{H}_z$	Zeeman Hamiltonian [2.93], [2.154]
$\hbar = h/2\pi$	Planck's constant divided by 2π
I	spin angular momentum quantum number
$\mathbf{I}$	angular momentum vector [1.1]
I_x, I_y, I_z	Cartesian angular momentum operators
$I_z = m\hbar$	z-component of the angular momentum vector [1.2]
I_0, I^+, I^-	shift basis operators
$I_0\{\theta\}$	zero-order modified Bessel function [3.46]
I^{α}, I^{β}, I^+, I^-	single element basis operators
I^+, I^-	shift (raising and lowering) angular momentum operators

$I^+(rs)$, $I^-(rs)$	single transition shift operators
i	$\sqrt{-1}$
i	unit vector along Cartesian x-axis
J	scalar coupling tensor
$\mathbf{J}(t)$	bulk angular momentum vector [1.10]
$^nJ_{ij}$, J_{ij}	n-bond scalar coupling constant between spins I_i and I_j
$J(\omega)$	orientational spectral density function [5.95]
j	unit vector along Cartesian y-axis
$j(\omega)$	spectral density function for isotropic phase in the high temperature limit [5.90]
$j^q(\omega)$	spectral density function [5.63]
$j^q_{mn}(\omega)$	cross spectral density function for the mth and nth relaxation interactions [5.77]
k	unit vector along Cartesian z-axis
k_{ij}	microscopic rate constant for exchange between the ith and jth chemical species [5.165]
k_B	Boltzmann constant
k_{ex}	$k_1 + k_{-1}$
k_1	forward microscopic rate constant for two-site chemical exchange [5.156]
k_{-1}	reverse microscopic rate constant for two-site chemical exchange [5.156]
L	inductance [3.1]
$\hat{L}(t)$	Liouvilian superoperator [5.48]
M_0	equilibrium magnetization [1.7]
M_r	molecular mass
M_x, M_y, M_z	Cartesian component of the magnetization vector
$\mathbf{M}(t)$	bulk magnetic moment or magnetization vector [1.11]
$\mathbf{M}^r(t)$	bulk magnetization vector in the rotating frame [1.17]
$M^+(t)$	complex magnetization [1.40]
m	magnetic quantum number [1.2]
$\mathcal{N}$	number of spins per unit volume
N_A	Avogadro's number
$\mathbf{n}_\chi$	unit vector directed along a rotation axis χ
P	projection operator [2.40]
$P_n(\cos\theta)$	Legendre polynomials
$P_{nm}(\cos\theta)$	associated Legendre polynomials
$\mathrm{P}_\phi(\alpha)$	rf pulse with phase ϕ and on-resonance rotation angle α [3.96], [3.106]
$P(t)$	probability density [2.3]
$P_{\alpha\alpha}$, $P_{\alpha\beta}$, $P_{\beta\alpha}$, $P_{\beta\beta}$	spin state populations
$\mathscr{P}(\Psi)$	probability density for lattice-spin system coupling [2.45]
$p(\alpha, \beta, \gamma)$	orientational probability distribution [2.314]
R	resistance [3.1] pulse element for composite pulse decoupling

$\mathbf{R}$	relaxation rate matrix [5.14]
R_{ex}	contribution to transverse relaxation from chemical exchange
$R_I(\theta)$	relaxation rate constant for spin I in a tilted rotating frame [5.138]
R_1	spin-lattice or longitudinal relaxation rate constant [1.24]
$R_{1\rho}$	rotating-frame autorelaxation rate constant
R_2	spin-spin or transverse relaxation rate constant [1.26]
R_2^*	inhomogeneously broadened transverse relaxation rate constant
R_{2MQ}	relaxation rate constant for heteronuclear multiple quantum coherence [7.9]
R_C	cross rate constant [5.21]
$R_\chi(\alpha)$	rotation matrix for rotation around the χ axis by an angle α [1.34], [2.102]
R_{inhom}	inhomogeneous line broadening constant
R_{IS} (θ_I, θ_S)	cross-relaxation rate constant for spins I and S in a tilted rotating frame [5.140]
R_L	leakage rate constant [5.21]
r_{ij}	distance between spins i and i
r_H	hydrodynamic radius [1.44]
r_w	thickness of hydration layer [1.45]
SW	spectral width [3.9]
$S_c(t_1,t_2)$	cosine-modulated signal [4.44]
S_m	order parameter [2.319], [2.321]
$S_N(t_1,t_2)$	N-type signal [4.47]
$S_P(t_1,t_2)$	P-type signal [4.46]
$S_s(t_1,t_2)$	sine-modulated signal [4.45]
S^2	square of generalized order parameter [5.103]
S/N	signal-to-noise ratio
$S(\omega)$, $S(\nu)$	frequency domain signal
$s_e(t)$	signal envelope function
$s(t)$	time-domain signal
$\mathbf{T}$	inversion operator [2.110]
$\mathrm{Tr}\{\mathbf{A}\}$	trace of $\mathbf{A}$
$T_1 = 1/R_1$	spin-lattice or longitudinal time constant
$T_2 = 1/R_2$	spin-spin or transverse relaxation time constant
Δt	sampling interval [3.6]
t_0	initial sampling delay [3.27]
t_{max}	maximum acquisition time for 1D NMR
t_1, t_2, ...	direct acquisition time or indirect evolution time
$t_{1,max}$, $t_{2,max}$, ...	maximum value of t_1, t_2, ...
$\mathbf{U}$	unitary operator, matrix or propagator
$\mathbf{u}$	vector
$u(\omega)$	imaginary part of complex frequency domain spectrum [1.43]
V	voltage [3.180] volume
$\bar{V}$	specific volume [1.45]
$\mathbf{v}$	vector
$v(\omega)$	real part of complex frequency domain spectrum [1.42]

W_0, W_I, W_S, W_2	transition frequencies [5.10], [5.118]
$W(\alpha, \beta, \gamma)$	potential of mean force [2.314]
$Y_2^q[\Omega(t)]$	modified spherical harmonic function (Table 5.1)
Z	complex impedence [3.2]
α	pulse rotation angle [1.23]
$\lvert\alpha\rangle$	spin state with $m = 1/2$
$\{\alpha, \beta, \gamma\}$	Euler angles
a_e	Ernst angle [3.189]
$\lvert\beta\rangle$	spin state with $m = -1/2$
γ	magnetogyric ratio [1.3]
$\hat{\boldsymbol{\Gamma}}$	relaxation superoperator [5.68]
Γ_{rs}	rate constant for cross-relaxation between basis operators B_r and B_s [5.73]
$\Delta\nu_{FWHH}$	full-width-at-half-height linewidth in Hertz
$\Delta\omega$	resonance frequency difference between chemical species in two-site exchange process
$\Delta\omega_{FWHH}$	full-width-at-half-height linewidth
δ	chemical shift (ppm) [1.51]
δ_{ij}	Kronecker delta function [2.16]
η	asymmetry of the shielding tensor [1.50]
η_{IS}	NOE enhancement [5.150]
η_w	viscosity of the solvent [1.44]
η_{xy}	transverse interference relaxation rate constant [5.145]
η_z	longitudinal interference relaxation rate constant [5.144]
θ	tilt angle [1.21] or strong coupling parameter [2.157]
θ_0	zero-order phase correction
θ_1	first-order phase correction
$\theta\{\omega\}$	frequency-dependent phase correction
$\boldsymbol{\mu}$	nuclear magnetic moment vector [1.3]
μ_x, μ_y, μ_z	Cartesian components of the magnetic moment [1.3], [2.28]-[2.30]
μ_0	permeability of free space
ν	frequency in units of Hertz
ρ_I	spin-lattice relaxation rate constant for spin I [5.10]
σ	isotropic nuclear shielding [1.48]
$\boldsymbol{\sigma}$	Cartesian nuclear shielding tensor [2.299]
$\sigma(t)$, σ	density operator [2.46]
$\Delta\sigma$	nuclear shielding anisotropy [1.49]
σ^{eq}	equilibrium spin density operator or matrix [2.123]
σ_{IS}, σ_{IS}^{NOE}	cross-relaxation rate constant between spins I and S [5.10], [5.150]
σ_{IS}^{ROE}	rotating frame cross-relaxation rate constant for spins I and S [5.141]

σ_{ij}	components of nuclear shielding tensor [1.46], [2.299]
$\sigma_{\parallel} = \sigma_{zz}$	parallel component of nuclear shielding tensor
$\sigma_{\perp} = (\sigma_{xx} + \sigma_{yy})/2$	perpendicular component of nuclear shielding tensor
τ_c	rotational correlation time of a molecule [1.44]
τ_e	effective correlation time for internal motions
τ_m	mixing time
τ_p	pulse length
τ_{RD}	radiation damping time constant [3.162]
$\{\phi,\psi\}$	backbone dihedral angles
$\phi(t)$	time-dependent phase of wavefunction [2.6]
$\Psi(t)$	wavefunction or state function [2.1]
$\psi(\tau)$, ψ	basis function, eigen-function, or stationary state function
ψ^*	complex conjugate of ψ
Ω	offset or chemical shift
$\mathbf{\Omega}$	diagonal matrix of chemical shift frequencies $d_{ij}\Omega_i$
$\mathbf{\Omega}(t) = \{\theta(t), \phi(t)\}$	polar angles
$\boldsymbol{\chi}$	magnetic susceptibility tensor [2.329]
χ_1	side-chain dihedral angle
$\boldsymbol{\omega}$	angular velocity
ω	frequency in angular units, s^{-1}
ω_e	effective frequency in rotating frame
ω_0	Larmor resonance frequency [1.14]
ω_1	rf magnetic field strength
ω^r	effective angular frequency in rotating frame [1.22]
ω_{NR}	non-resonance frequency shift [3.86]
ω_{pivot}	pivot frequency for phase correction
ω_{rf}	rf magnetic field frequency
Ξ	relative resonance frequency for an X spin [3.194]