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Parameters and Symbols for Use in Nuclear Magnetic Resonance (IUPAC Recommendations 1997)

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ABSTRACT: NMR is now frequently the technique of choice for the determination of chemical structure in solution. Its uses also span structure in solids and mobility at the molecular level in all phases. The research literature on the subject is vast and ever-increasing. Unfortunately, many articles do not contain sufficient information for experiments to be repeated elsewhere, and there are many variations in the usage of symbols for the same physical quantity. It is the aim of the present recommendations to provide simple check-lists that will enable such problems to be minimized in a way that is consistent with general IUPAC formulation. The area of medical NMR and imaging is not specifically addressed in these recommendations, which are principally aimed at the mainstream use of NMR by chemists (of all subdisciplines) and by many physicists, biologists, materials scientists and geologists, etc., working with NMR. The document presents recommended notation for use in journal publications involving a significant contribution of nuclear magnetic resonance (NMR) spectroscopy. The recommendations are in two parts: (A) experimental parameters which should be listed so that the work in question can be repeated elsewhere; and (B) a list of symbols (using Roman or Greek characters) to be used for quantities relevant to NMR.

A. NMR EXPERIMENTAL PARAMETERS FOR REPORTING IN PUBLICATIONS

1. Introduction

The aim of this list is to introduce a degree of uniformity in the way in which NMR results are reported in chemical journals, so as to ensure that experiments can be precisely repeated. It is to be regarded as a minimal list, though not all parameters are relevant to a given experiment. It should be noted that sample conditions (e.g. solvent, concentration) are not part of the list, although clearly it is also essential for these to be specified.

2. General

(a) The nucleus or nuclei studied.
(b) The instrument manufacturer and model.
(c) The resonance frequency or frequencies (preferably of the reference sample or samples).
(d) The magnetic field [optional if frequencies are given].
(e) The type(s) of pulse sequence.
(f) The referencing procedure for obtaining chemical shifts (and/or relative shielding constants).
(g) The size/nature of the sample tube/container.
(h) The temperature of the sample at the time of the measurement.

3. Pulse conditions

(a) The RF pulse magnetic field (or equivalent in frequency units) and/or equivalent 90° pulse duration. [Note the unambiguous word ‘duration’ rather than ‘width’ or ‘length.’]
(b) The flip (nutation) angle(s) and relative phases of all pulses.

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(c) The spectral width (or dwell time if unambiguously defined).
(d) The acquisition time (or number of acquired data points if the dwell time is given).
(e) The number of transients (acquisitions).
(f) The recycle delay. [Note: this implies the time interval following the completion of one cycle of a pulse sequence and the start of the next one, sometimes called a relaxation delay. This is distinct from a cycle time, which is the time between analogous points of successive pulse sequence cycles.]
(g) Any other relevant time intervals.
(h) The decoupling or double/multiple resonance method and conditons, including the RF magnetic field (or equivalent in frequency units and/or equivalent 90° pulse duration).
(i) Pulse shapes and relevant frequencies (for experiments with selective pulses).
(j) The magnitudes, directions, shapes and durations of any magnetic field gradients.

4. Processing parameters

(a) Zero-filling extent.
(b) Any window function (apodization, pre-acquisition delay, resolution enhancement, line broadening).
(c) Any special baseline correction or phase adjustment procedures.
(d) Any additional processing details, such as linear prediction or maximum entropy.
(e) Any special procedures for signal quantification (e.g. deconvolution).

5. Solid-state spectra (additional requirements)

(a) Contact time. [For cross-polarization operation.]
(b) Sample rotation angle.
(c) Sample rotation rate.
(d) Use of special techniques such as DOR or DAS.

6. Relaxation measurements (additional requirements)

(a) Number of measurement points used.
(b) Analysis method (exponential, etc.).
(c) Radiofrequency field magnitude (or equivalent expressed in frequency units). [For $T_{1\rho}$ measurements.]

7. Multi-dimensional spectra

(a) The time increments and the number of data points and/or the spectral width and maximum duration of evolution periods must be given for each dimension, as well as the data size after processing.
(b) For figures of multi-dimensional spectra, each axis should be unambiguously labelled by the variable involved (e.g. δ_H, δ_C, J_{CH}) where possible, as well as by a frequency label such as F_1, F_2

8. Additional notes

(a) Figures of spectra should have an indication of the direction of increasing frequency and the captions should state the nucleus involved. Wherever feasible, assignments of chemical shifts should be indicated on illustrated spectra.
(b) Phase cycling of all r.f. pulses and of the receiver should be specified when crucial to the experiment.
(c) For novel or unusual pulse sequences a timing diagram is highly recommended. If acronyms are used instead of diagrams for established sequences, a literature reference is recommended.

B. SYMBOLS FOR NMR AND RELATED QUANTITIES

(i) Roman alphabet

a or A	Hyperfine (electron–nucleus) coupling constant
$A_q^{(l,m)}$	The mth component of an irreducible tensor of order l representing the nuclear spin operator for an interaction of type q
$\boldsymbol{B}$	Magnetic field (strictly the magnetic flux density or magnetic induction)
$\boldsymbol{B}_0$	Static magnetic field of an NMR spectrometer
$\boldsymbol{B}_1$, $\boldsymbol{B}_2$	Radiofrequency magnetic fields associated with frequencies ν_1, ν_2
$\boldsymbol{B}_L$	Local magnetic field (components B_{xL}, B_{yL}, B_{zL}) of random field or dipolar origin
$\boldsymbol{\mathsf{C}}$	Spin–rotation interaction tensor
C_X	Spin–rotation coupling constant of nuclide X
$\boldsymbol{\mathsf{D}}$	Dipolar interaction tensor
D	Dipolar coupling constant between two nuclei (say 1 and 2), $(\mu_0/4\pi)\gamma_1\gamma_2(\hbar/2\pi)r_{12}^{-3}$ in frequency units (footnote 1).
D^C	Nuclear receptivity relative to that of the carbon-13 nucleus
D^p	Nuclear receptivity relative to that of the proton (hydrogen-1 nucleus)
$\boldsymbol{E}$	Electric field strength
F	Spectral width
F_1, F_2 (or f_1, f_2)	The two frequency dimensions of a two-dimensional spectrum (use F_3, etc., for higher orders)
$\hat{\boldsymbol{F}}_G$	Nuclear spin operator for a group, G, of nuclei (components $\hat{F}_{Gx}$, $\hat{F}_{Gy}$, $\hat{F}_{Gz}$, $\hat{F}_{G+}$, $\hat{F}_{G-}$)

F_{G}	Magnetic quantum number associated with $\hat{\boldsymbol{F}}_{\text{G}}$
g	Nuclear or electronic g factor (Landé splitting factor)
G	Magnetic field gradient amplitude
H_{ij}	Element of matrix representation of Hamiltonian operator (in energy units); superscripts indicate the nature of the operator
$\hat{\boldsymbol{I}}_j$	Nuclear spin operator for nucleus j (components $\hat{I}_{jx}, \hat{I}_{jy}, \hat{I}_{jz}$)
$\hat{I}_{j+}, \hat{I}_{j-}$	'Raising' and 'lowering' spin operators for nucleus j
I_j	Magnetic quantum number associated with $\hat{\boldsymbol{I}}_j$
$\boldsymbol{J}$	Indirect coupling tensor
^nJ	Nuclear spin–spin coupling constant through n bonds (usually given in frequency units). Parentheses may be used (for example) to indicate the species of nuclei coupled, e.g. $J(^{13}\text{C}, {}^1\text{H})$ or, additionally, the coupling path, e.g. $J(\text{POCF})$. Where no ambiguity arises, the elements involved can be, alternatively, given as subscripts, e.g. J_{CH}. The nucleus of higher mass should be given first
$J(\omega)$	Spectral density of fluctuations at angular frequency ω. Subscripts and superscripts to J may be used to indicate the relevant quantum number change (0, 1 or 2) or the order and component of the relevant tensor quantities.
^nK	Reduced nuclear spin-spin coupling constant (see the notes concerning ^nJ), $K_{jk} = 4\pi^2 J_{jk}/h\gamma_j\gamma_k$
$\boldsymbol{L}$	Angular momentum
m_j	Eigenvalue of $\hat{I}_{jz}$ (magnetic component quantum number) (footnote 2)
m_{tot}	Total magnetic component quantum number for a spin system (eigenvalue of $\Sigma_j \hat{I}_{jz}$) (footnote 2)
$m_{\text{tot}}(\text{X})$	Total magnetic component quantum number for X-type nuclei (footnote 2)
$\boldsymbol{M}_0$	Equilibrium macroscopic magnetization per volume of a spin system in the presence of $\boldsymbol{B}_0$
M_x, M_y, M_z	Components of macroscopic magnetization per volume.
M_n	nth moment of spectrum ($M_2 =$ second moment, etc.)
n_α, n_β	Populations of the α and β spin states
N	Total number of nuclei of a given type per volume in the sample
$\boldsymbol{q}$	Electric field gradient tensor in units of the elementary charge (principal components q_{XX}, q_{YY}, q_{ZZ}) (see also $\boldsymbol{V}$)
Q	eQ is the nuclear quadrupole moment, where e is the elementary charge
R_1^{X}	Spin–lattice (longitudinal) relaxation rate constant for nucleus X
R_2^{X}	Spin–spin (transverse) relaxation rate constant for nucleus X
$R_{1\rho}^{\text{X}}$	Spin–lattice relaxation rate constant in the rotating frame for nucleus X
S	Signal intensity
$\hat{\boldsymbol{S}}$	Electron (or, occasionally, nuclear) spin operator; cf. $\hat{\boldsymbol{I}}$
t_1, t_2	Time dimensions for two-dimensional NMR
T_{c}	Coalescence temperature for signals in an NMR spectrum
T_1^{X}	Spin–lattice (longitudinal) relaxation time of the X nucleus (further subscripts refer to the relaxation mechanism)
T_2^{X}	Spin–spin (transverse) relaxation time of the X nucleus (further subscripts refer to the relaxation mechanism)
T_2^*	Net dephasing time for M_x or M_y (including contribution from magnetic field inhomogeneity)
$T_{1\rho}^{\text{X}}$	Spin–lattice relaxation time of the X nucleus in the frame of reference rotating with $\boldsymbol{B}_1$
T_{d}	Pulse (recycle) delay
T_{ac}	Acquisition time
$T_q^{(l,m)}$	The mth component of an irreducible tensor of order l representing the strength of an interaction of type q
$\boldsymbol{V}$	Electric field gradient tensor. $\boldsymbol{V} = e\boldsymbol{q}$, where e is the elementary charge
$V_{\alpha\beta}$	Elements of Cartesian electric field gradient tensor
W_0, W_1, W_2	Relaxation rate constants (transition probabilities per time) between energy levels differing by 0, 1, and 2 (respectively) in m_{tot}; especially, but not uniquely, for systems of two spin-$\frac{1}{2}$ nuclei
W_{rs}	Transition probability between spin states r and s

(ii) Greek alphabet

α	Nuclear spin wavefunction (eigenfunction of $\hat{I}_{jz}$) for the $m_I = +\frac{1}{2}$ state of a spin-$\frac{1}{2}$ nucleus
α_{E}	The Ernst angle (for optimum sensitivity)
β	Nuclear spin wavefunction (eigenfunction of $\hat{I}_z$) for the $m_I = -\frac{1}{2}$ state of a spin-$\frac{1}{2}$ nucleus
γ_{X}	Magnetogyric ratio of nucleus X
δ_{X}	Chemical shift (for the resonance) of nucleus of element X (positive when the sample resonates to high fre-

	quency of the reference). Usually in ppm (footnote 3). Further information regarding solvent, references or nucleus of interest may be given by superscripts or subscripts or in parentheses.
Δn	Population difference between nuclear states (Δn_0 at Boltzmann equilibrium)
$\Delta\delta$	Change or difference in δ
$\Delta\nu_{1/2}$	Full width in frequency units of a resonance line at half-height
$\Delta\sigma$	Anisotropy in $\boldsymbol{\sigma}$ $[\Delta\sigma = \sigma_{ZZ} - \frac{1}{2}(\sigma_{XX} + \sigma_{YY})]$ (footnote 4). (See also ζ)
$\Delta\chi$	(i) Susceptibility anisotropy ($\Delta\chi = \chi_{\parallel} - \chi_{\perp}$); (ii) difference in electronegativities
ε_0	Permittivity of a vacuum
ζ	Anisotropy in shielding (footnote 4), expressed as $\sigma_{ZZ} - \sigma_{\mathrm{iso}}$. (see also $\Delta\sigma$)
η	(i) Nuclear Overhauser enhancement (so that the nuclear Overhauser effect is $1 + \eta$); (ii) tensor asymmetry factor (e.g. in σ); (iii) viscosity
κ	Skew of a tensor. (See also footnote 7)
θ	Angle, especially for that between a given vector and $\boldsymbol{B}_0$
$\boldsymbol{\mu}$	(i) Magnetic dipole moment (component μ_z along $\boldsymbol{B}_0$); (ii) electric dipole moment
μ_0	Permeability of a vacuum
μ_{B}	Bohr magneton
μ_{N}	Nuclear magneton
ν_j	Larmor precession frequency of nucleus j (usually given in MHz)
ν_0	(i) Spectrometer operating frequency; (ii) Larmor precession frequency (general, or of bare nucleus)
ν_1	Frequency of 'observing' RF magnetic field B_1 (to be distinguished from its strength, γB_1, for which the symbol Ω_1 is recommended)
ν_2	Frequency of 'irradiating' RF magnetic field B_2 (to be distinguished from its strength, γB_2, for which the symbol Ω_2 is recommended)
Ξ_{X}	Resonance frequency for the nucleus of element X in a magnetic field such that the protons in tetramethylsilane (TMS) resonate at exactly 100 MHz
ρ	Density matrix
$\hat{\rho}$	Density operator
ρ_{ij}	Element of matrix representation of $\hat{\rho}$
$\boldsymbol{\sigma}$	Shielding tensor (footnotes 5 and 6)
σ_j	(Isotropic) shielding constant of nucleus j. Usually given in ppm. Subscripts may alternatively indicate contributions to σ
$\sigma_{\parallel}, \sigma_{\perp}$	Components of shielding tensor $\boldsymbol{\sigma}$ parallel and perpendicular to the symmetry axis (axially-symmetric case) (footnote 5)
$\hat{\sigma}$	Reduced density operator
τ	(i) Time between RF pulses (general symbol); (ii) lifetime in dynamic NMR usage
τ_{c}	Correlation time for molecular-level motion, especially for isotropic molecular tumbling
τ_{d}	Dwell time
τ_{null}	Recovery time sufficing to give zero signal after a 180° pulse
τ_{p}	Pulse duration
τ_{sc}	Correlation time for relaxation by the scalar mechanism
τ_{sr}	Correlation time for spin–rotation relaxation
$\tau_{\parallel}, \tau_{\perp}$	Correlation times for molecular tumbling parallel and perpendicular to the symmetry axis (axially symmetric case)
χ	(i) Magnetic susceptibility (footnote 7); (ii) nuclear quadrupole coupling constant ($\chi = e^2 q_{ZZ} Q/h$)
$\omega_j, \omega_0, \omega_1, \omega_2$	As for ν_j, ν_0, ν_1, ν_2 but for angular frequencies
Ω	Span of a tensor
Ω_1, Ω_2	R.f. magnetic fields, expressed in angular frequency units for a nucleus of magnetogyric ratio γ ($\Omega_1 = -\gamma\boldsymbol{B}_1$, $\Omega_2 = -\gamma\boldsymbol{B}_2$)

Notes

1. Note that confusion might arise when the so-called alphabet expansion is used for $\boldsymbol{D}$, since this includes a term D which is not the dipolar coupling constant.
2. M rather than m is frequently recommended, but most NMR practitioners use m so as to avoid confusion with magnetization.
3. Whereas earlier IUPAC recommendations give a definition of δ which requires that the 'unit' ppm is not stated when values are quoted, this is largely ignored and a change of recommendation is under consideration.
4. $\zeta = 2\Delta\sigma/3$.
5. The symbols $\boldsymbol{\sigma}$ (and related terms for components), σ_j, $\sigma_{\parallel}$, $\sigma_{\perp}$ should refer to shielding on an absolute scale (for theoretical work). For shielding relative to a reference, symbols such as $\sigma_{\parallel} - \sigma_{\mathrm{ref}}$ should be used.
6. For tensors, doubled subscript *capital* letters X, Y and Z should generally be used for principal components, e.g. σ_{XX}, σ_{YY} and σ_{ZZ} for shielding. Alternatively, numerical subscripts may be used (e.g. σ_{11}, σ_{22}, σ_{33}).
7. The symbol κ may also be used for magnetic susceptibility, some authors reserving χ for unrationalized units.

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