

INTERNATIONAL UNION OF
PURE AND APPLIED CHEMISTRY

PHYSICAL CHEMISTRY DIVISION

COMMISSION ON MOLECULAR STRUCTURE
AND SPECTROSCOPY

PRESENTATION OF NMR DATA
FOR PUBLICATION IN
CHEMICAL JOURNALS—B.
CONVENTIONS RELATING TO SPECTRA
FROM NUCLEI OTHER THAN PROTONS

(RECOMMENDATIONS 1975)

PERGAMON PRESS
OXFORD · NEW YORK · PARIS · FRANKFURT

PHYSICAL CHEMISTRY DIVISION
COMMISSION ON MOLECULAR STRUCTURE
AND SPECTROSCOPY†

PRESENTATION OF NMR DATA FOR
PUBLICATION IN CHEMICAL JOURNALS—B. CONVENTIONS
RELATING TO SPECTRA FROM NUCLEI
OTHER THAN PROTONS

(RECOMMENDATIONS 1975)

Section B constitutes the second part of the "Recommendations for the Presentation of NMR Data for Publication in Chemical Journals". Section A dealt with proton NMR spectra (*Pure Appl. Chem.* **29**, 627 (1972)). Although the present recommendations are directed toward nuclei other than protons, they are equally applicable to proton NMR.

(1) The nucleus giving rise to the spectrum should always be explicitly stated in full or in abbreviation, e.g. ^{10}B NMR spectrum (spoken: boron 10 NMR spectrum). The isotopic mass number should be stated except in cases where a single abundant isotope leads to a situation without ambiguity, e.g. NMR spectra from ^{19}F or ^{31}P .

Abbreviations such as PMR (for 'proton NMR' or 'phosphorus NMR') or CMR (for 'carbon NMR') are strongly discouraged.

(2) The dimensionless scale factor for chemical shifts should be 10^{-6} , i.e. parts per million, for which ppm is a convenient abbreviation. When large chemical shifts are given exactly, the radiofrequency of the standard substance should be reported with sufficient accuracy.

(3) The unit for spin-spin coupling constants should be hertz (cycles per second). The symbol for coupling constants is J . The coupling between two nuclei separated by n chemical bonds can be indicated by the left superscript n , e.g. 4J denotes the coupling constant between two nuclei separated by 4 chemical bonds. Right subscripts may be used to give the symbols of the coupling nuclei, e.g. the coupling constant between the phosphorus nucleus and protons in trimethylphosphite, $\text{P}(\text{OCH}_3)_3$, would bear the symbol $^3J_{\text{PH}}$. Alternatively a notation of the type $^3J(\text{PH})$ or $^3J(^{11}\text{BH})$ may be used.

(4) The graphical presentation of spectra should show the frequency decreasing to the right (applied field increasing to the right), absorption increasing upwards, and the standard sweep direction should be from high to low frequency (low to high field). Solvent and impurity bands, and spinning side-bands, should be indicated as such.

(5) Whenever possible the dimensionless scale should be tied to an internal reference, which should be explicitly stated. The dimensionless scale should be defined as

positive in the high frequency (low field) direction. The scale in parts per million should be termed the δ scale. A shift measured on this scale should be given as, for example, $\delta = 5.00$, not $\delta = 5.00$ ppm. If data from more than one nucleus are reported, the symbol δ should be used with the corresponding symbol of the element given in brackets, e.g. $\delta(\text{C})$ or $\delta(^{11}\text{B})$. The position of the nucleus in the structural formula could be denoted by an additional number following this symbol for the nucleus, e.g. $\delta(\text{C}-5)$ or $\delta(^{11}\text{B}-5)$.

(6) When the spectra are submitted for publication, additional information should include:

(a) A statement of how the spectrum was recorded, e.g. using the continuous wave (CW), pulse Fourier transform (pulse FT), or other technique. The number of spectra accumulated should be stated.

When a pulse FT technique is employed, both the duration of the pulse and the duration of a 90° pulse should be stated. These two pieces of data may be expressed in other forms, e.g. as the angle of reorientation of the magnetic vector and the duration of a 90° pulse.

(b) The name of the solvent used:

(c) The concentration of the solute.

(d) The name and concentration of the internal reference.

(e) The name of the external reference, if one is used.

(f) The diameter of the sample tube and whether or not it was rotated.

(g) The temperature of the sample.

(h) The approximate radio-frequency or magnetic field at which the measurements were made.

(i) If spectra are presented as diagrams there should be a graphical indication of the distance corresponding to a suitable range of Hz, so that fine structure spacings or widths of broad resonances can be estimated.

(k) Where relevant it should be stated whether oxygen has been removed from the sample.

(1) Other experimental information should be added where appropriate or necessary, e.g.

(i) in CW experiments the sweep rate and magnitude of the B_1 fields;‡

(ii) in double resonance experiments the magnitude of the irradiating field,‡ B_2 , whether monochromatic or noise decoupling is used, and whether CW or pulsed operation is carried out;

(iii) in cases where the experimental data are processed by a computer, all relevant information about spectral width, filtering, apodization, deconvolution processes, number of data points, etc.

†*Titular Members*: N. Sheppard (Chairman), M. A. Elyashévich (Vice-Chairman), F. A. Miller (Secretary), E. D. Becker, J. H. Beynon, E. Fluck, A. Hadni, G. Zerbi, *Associate Members*: G. Herzberg, B. Jeżowska-Trzebiatowska, Y. Morino, S. Nagakura, C. N. R. Rao, Sir Harold Thompson, D. W. Turner.

‡In contrast to the previous recommendations concerned with proton spectra the more recently adopted symbol B is used for the magnetic induction (field).