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PROVISIONAL RECOMMENDATIONS FOR NMR NOMENCLATURE:

NUCLEAR SPIN PROPERTIES AND CONVENTIONS FOR CHEMICAL SHIFTS

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1.   INTRODUCTION

A distinguishing feature of nuclear magnetic resonance (NMR) is that it is isotope-specific. In other words each signal can be firmly linked to a particular element and nuclide. Two features follow: Firstly there is a close connection with chemistry and, in particular, with the Periodic Table, since almost all elements can be studied. Secondly, the spin properties of each isotope need to be clearly tabulated and firmly understood. It is a principal purpose of this document to provide such information.

Any scientific discipline relies for its effectiveness upon communication of ideas and results, which can only occur if there is an agreed basis for the meaning of the terminology used. The process of communication is greatly eased if there are universally-recognised conventions for measurement and reporting of quantities with their units and symbols. The second aim of this document is to set down such a set of meanings and conventions in relation to chemical shifts (and shielding) and to list resonance frequencies for reference signals for each magnetically active nucleus observed.

Within IUPAC, Commission I.5 is responsible for Molecular Structure and Spectroscopy. Until now, this Commission has produced only three reports[1-3] specifically relating to NMR. The two earlier ones of these refer to chemical shifts. The more recent of these two publications is nearly 20 years old, and the NMR world has changed beyond recognition since then. Recently, however, conventions for chemical shifts of five nuclei of wide biochemical interest have been included in *Recommendations for the Presentation of NMR Structures of Proteins and Nuclei Acids*[4] by Commission I.7, Biophysical Chemistry. The current document extends those conventions to the entire range of NMR nuclei, provides a more comprehensive guide to the factors important in chemical shift referencing, and includes a unified list of properties of NMR-observable nuclei.

As a Provisional Recommendation, this document is open for comments from interested individuals. Proposals are made herein for a general system of chemical shift referencing, and specific numerical values are suggested. The Commission welcomes all comments but

particularly solicits views on the utility of the recommended referencing system and on the specific resonance frequencies (Ξ values) that are proposed.

2.   NUCLEAR SPIN PROPERTIES

The phenomenon of NMR is based upon the magnetic properties of various isotopes of elements in the Periodic Table.   It is therefore important to have, accessible to all NMR spectroscopists, a unified list of these properties.   These are contained in Tables 1-3 of this article which include the following for each stable or long-lived radioactive isotope with non-zero spin:

(i)   The nuclear spin quantum number, I, of the ground spin-state.

(ii)   The average mole fractional natural abundance, x, of the isotope, as a %.

(iii)   The magnetic moment, μ, of the isotope, in terms of the nuclear magneton, μ_N. It should be noted that we have chosen to use the full vectorial magnitude of μ, given by:

$$\mu / \mu_N = \gamma\hbar\sqrt{I(I+1)} \qquad (1)$$

where γ is the magnetogyric ratio and $\hbar$ is Planck's constant divided by 2π. Many lists prefer to give only the maximum value of μ, namely $\gamma\hbar I$ - frequently without explicitly stating this fact. The sign of μ given in Tables 1-3 refers to its direction compared to the related spin angular momentum vector.

(iv)   The magnetogyric ratio, γ (sometimes called the gyromagnetic ratio). The dimensions of this quantity are $T^{-1} s^{-1}$, with units normally given as radian-second^{-1} tesla^{-1}.

(v)   The receptivity, D, of a nucleus in natural abundance, which influences the NMR signal strength. A common definition involves the proportionality of D to $\gamma^3 x$. In practice it is useful to list such receptivities relative to those of the commonly-used nuclei ^{1}H and ^{13}C, giving D^p and D^C respectively. Both these quantities are given in Tables 1 and 2.

(vi)   For nuclei with spin quantum number $I > \frac{1}{2}$ the quadrupole moment, Q (Tables 2 and 3 only). These data fall naturally in the region of 10^{-28} m^2 which, as a unit, is frequently called the barn.

(vii)   The linewidth factor, ℓ, for quadrupolar nuclei. This is defined by[5]:

$$\ell = Q^2(2I + 3)/[I^2(2I - 1)] \qquad (2)$$

When taken in conjunction with the relative receptivity (e.g. as D^C/ℓ) this quantity gives a guide to the ease with which spectra can be obtained for different quadrupolar nuclei in solution for similar site symmetries and molecular mobilities. However, in practice, both symmetry and mobility may vary widely, thus introducing variations that may be several orders of magnitude.

Table 1 gives the data for the spin-½ nuclei in the Periodic Table, whereas Table 2 refers to quadrupolar nuclei. These two Tables omit the lanthanide and actinide nuclei, which are separately listed in Table 3. Many of the data in Tables 1-3 have been taken from the IUPAC "Green Book",[6] but additional information is included (particularly on resonance frequencies). A version of Tables 1-3 has been published.[7] However, the Tables given here contain revised resonance frequencies for consistency with the recommended reference, as described in Section 3.5. In addition, information about solution conditions and relevant references has been added.

3.   THE CHEMICAL SHIFT

    3.1   **Background**

    Since the discovery of the chemical shift in 1950, NMR spectroscopy has become of vital importance to chemistry and related disciplines. The chemical shift refers to a difference in resonance frequency (conventionally expressed as a fraction - see below) between nuclei in different chemical sites (or for samples under different physical conditions). Such effects are caused by variations in shielding by the electronic environment of the nuclei in question, and the concept of chemical shift is most readily based on Eq. (3):

$$\nu = \frac{\gamma}{2\pi} B_0 (1 - \sigma) \qquad (3)$$

In this equation, the resonance frequency ν (normally in the radiofrequency region) is related to the applied magnetic flux density B_0 by the magnetogyric ratio of the nucleus and the shielding constant σ. Conventionally under SI notation, ν is expressed in Hz (and is normally in the range of tens or hundreds of MHz), B_0 is in tesla and σ is a dimensionless fraction (generally reported in ppm). Equation (3) is usually applied to the situation in isotropic media (liquids, solutions and gases), for which σ may be considered as a scalar quantity. However, the value of σ depends on molecular orientation in the applied magnetic field and can be represented by a scalar quantity only because of the averaging caused by rapid isotropic molecular tumbling. Therefore, σ is a second-rank tensor and must be used in that form for many situations in the solid state and in liquid crystals (and their solutions).

Whereas frequencies can be measured very accurately, the same cannot be said of B_0. Thus, although in principle chemists would like to know the absolute value of σ, it has long been recognised that only relative values can normally be obtained with accuracy. Therefore, from the early days the concept of a standard reference signal has been developed. This requires a number of choices among which are:

(i)   whether to base chemical shifts on resonance frequencies or on shielding

(ii)   which compound to use as a reference

(iii)   what further conditions to specify for the reference situation

(iv)   whether to use separate references for different nuclei or to attempt to link them.

These matters will be dealt with in detail below.

In the early days of NMR, resonance was normally achieved by varying the applied field B_0. It therefore seemed natural for positive chemical shifts to refer to situations where the sample resonated to high field of the reference. Eq. (3) shows that this corresponds to greater

shielding for the sample than for the reference - a convention that was popular with theoreticians, who are principally concerned with σ. The first clear consensus on an experimental reference compound for proton NMR (by far the most popular nucleus at the time because of its high sensitivity) was tetramethylsilane (TMS), introduced in 1958 by Tiers.[8] However, both for proton NMR and for other nuclei various chemical shift scales were used, with some increasing in the direction of increasing magnetic field and others increasing in the direction of decreasing field (which corresponds to increasing frequency).

The convention recommended by IUPAC in the 1972 document,[1] which mostly concerned proton NMR, was that given in Equation 4:

$$\delta_{X,sample} = \left(\frac{\nu_{X,sample} - \nu_{X,reference}}{\nu_{X,reference}} \right) \qquad (4)$$

For protons referenced to TMS this convention gives positive values with increasing frequency, and most proton chemical shifts then turn out to be positive. A second IUPAC report[2] in 1976 extended the recommendations to include nuclei other than protons, always with a high-frequency-positive convention.

Of course, since σ is, in principle, a tensor quantity, so is δ. However, the present document deals only with the isotropic average value of δ, which is the usual value of relevance for solution-state NMR. Questions relating to the tensor properties of σ and δ will be the subject of a later document.

3.2   **Recommendations Endorsed**

At this point it is appropriate to list those recommendations of the previous two IUPAC reports on NMR which relate to chemical shifts[1,2] (including presentation of spectra) and which we endorse with one exception noted under item 6. These relate to notational matters and are particularly directed at publications in chemical journals. In several places we use different wording and extended meaning:-

1.   The nucleus giving rise to the spectrum concerned should always be explicitly stated in full or in abbreviation (e.g. [10]B NMR or boron-10 NMR). The isotopic mass number should be given except in cases without ambiguity. In the case of hydrogen NMR the de facto usage is proton NMR, deuterium NMR or tritium NMR, in spite of the inconsistency of the wording. Abbreviations such as PMR for proton NMR are strongly discouraged. The term multinuclear NMR is clumsy (a repeated word "nuclear") and so is also to be discouraged. Where reference to a variety of nuclei is required, multinuclear magnetic resonance should be written in full.

2.   The graphical presentation of spectra should show frequency increasing to the left and intensity increasing upwards.

3.   The dimensionless scale for chemical shifts should be tied to a reference, which should be clearly stated. The procedures used must be carefully defined.

4.   The dimensionless scale factor for chemical shifts should be expressed in parts per million, for which ppm is the appropriate abbreviation. The radiofrequency of the reference, appropriate to the nucleus in question and to the spectrometer in use, should always be quoted, with sufficient accuracy in relation to the numerical values of shifts listed. Unfortunately, older software supplied by manufacturers to convert from frequency units to ppm in FT NMR sometimes uses the carrier frequency in the denominator instead of the true frequency of the reference, which can lead to significant errors.

5. The chemical shift scale should be defined with respect to resonance frequencies, with the appropriate sign convention (i.e. a positive sign should imply the sample resonates to high frequency of the reference). In order to avoid ambiguities of sign, the term "chemical shift" should *not* be used to describe variations in shielding.

6. The symbol δ (Greek delta) should be used for chemical shift scales with the sign convention given above. Such a symbol should *never* be used to refer to shielding. These recommendations cohere with the definition of the δ-scale adopted in references 1 and 2. Although, the earlier recommendations suggested that numerical values of shifts measured on such scales should not explicitly state ppm (i.e. $\delta = 5.00$ not $\delta = 5.00$ ppm), this convention is widely ignored. *We now recommend in Section 3.3 that the appropriate unit (usually ppm) be stated explicitly.*

7. The nucleus in question should be indicated as a subscript or in brackets, e.g. δ_C or $\delta(^{13}C)$, unless there is no ambiguity.

8. As far as possible full information should be given in publications regarding any factor that might influence chemical shifts, such as:

   (i) The physical state of the sample i.e. solid, liquid, solution or gas, with additional relevant facts where necessary.

   (ii) For solutions, the name of the solvent and the concentration of solute.

   (iii) The nature of the reference procedure, *e.g.* internal, external (coaxial tubes or substitution), absolute frequency. [This aspect is discussed in detail in later sections.]

   (iv) The name of the reference compound and, if used internal to a solution, its concentration.

   (v) The temperature and pressure of the sample.

   (vi) Whether oxygen and other gases have been removed from the sample.

(vii)   Any chemical present in the sample, in addition to the compound under investigation and any reference compound.

3.3   **Definition and reporting of δ scales**

As mentioned above, the IUPAC Recommendation[1] dating from 1972 defined the proton chemical shift scale such that the values appeared in ppm but suggested that the "unit" ppm should not explicitly appear with the reported number. Although there were logical reasons for this suggestion, it has not in general won approval from the NMR community and is widely ignored in practice (except in journals with punctilious editors). Moreover, it is anomalous within normal IUPAC practice to define a quantity with a restriction on the magnitude of the units to be used. Therefore it is now recommended that, to correspond to normal practice, the δ scale for nucleus X is defined by Equation 4, and that the notation ppm should appear with the appropriate numerical value, where relevant. This definition may be alternatively written:

$$\delta_{X,sample} / ppm = \left(\frac{\nu_{X,sample} - \nu_{X,reference}}{\nu_{X,reference}} \right) \times 10^6 \qquad (5)$$

or

$$\delta_{X,sample}/ppm = \frac{(\nu_{X,sample} - \nu_{X,reference})/Hz}{\nu_{X,reference}/MHz} \qquad (6)$$

This re-definition allows values to be quoted in ppb (as is appropriate for some isotope effects) or % (relevant to some heavy-metal shifts) as well as ppm (which will undoubtedly remain as the most common usage).

3.4   **Referencing Procedures**

Accurate and consistent referencing is easy to visualise but hard to implement. For mobile isotropic media (liquids, solutions and gases) there are several possible methods:

(a)   *Internal referencing*, where the reference compound is added directly to the system under study. This method is used almost universally for ^{1}H and ^{13}C NMR. However, it is clearly limited by the solubility, miscibility or mutual reactions of the sample components and may be difficult to implement for many samples in which a variety of nuclei are studied.

(b)   *External referencing*, involving sample and reference contained separately in concentric cylindrical tubes. A single spectrum is recorded, which includes signals from both the sample and the reference compound.

(c)   The use of separate cylindrical tubes for the sample and reference compound, with (in principle) spectra recorded individually for each. We shall refer to this process as the *substitution method*. It is similar to external referencing in that sample and reference materials are not mixed, but there are significant differences in the two procedures, as described later, which arise because of the use of precise field/frequency locking (usually via the ^{2}H signal of deuterated solvent).

(d)   Referencing via direct measurement of the absolute frequency of the field/frequency lock signal, usually provided by the ^{2}H resonance of an internally-contained deuterated compound (frequently the solvent). This method is discussed more fully in section 3.6.

(e)   Application of magic-angle spinning, usually with the substitution method, but also conceivably with concentric tubes — see section 3.7.

These methods all have various advantages and disadvantages. For (a) the shielding of the reference nucleus depends, to a greater or lesser extent, on the solvent, on the solute under study, and on the concentration of both solute and reference because of the effects of intermolecular interactions. These effects may be minimised by a judicious choice of solvent and reference compound, but they cannot be eliminated. External reference procedures (b) generally require corrections arising from differences in bulk magnetic susceptibility between sample and reference. These corrections depend on the geometry employed for the sample containers. For the usual coaxial cylindrical arrangement, the correction is[9]

$$(\delta_{\text{true}} - \delta_{\text{obs}}) / \text{ppm} = 10^6 \, k(\kappa_{\text{sample}} - \kappa_{\text{reference}}) \tag{7}$$

where κ refers to the relevant volume susceptibility (in rationalised units) and $k = +1/6$ for a tube perpendicular to B_{O}, $k = -1/3$ for a tube parallel to B_{O} (as is usual for a superconducting magnet), and $k = 0$ for a tube inclined at the magic angle. These theoretical factors are calculated for infinite cylinders. In practice they depend on the length of the liquid column and other geometrical factors which are not always under control. No correction is needed for spherical samples, but the production of a truly spherical sample cell is generally not feasible. [Note that the values of k are in SI units. Equation 7 is often written in cgs units, where k is multiplied by a factor of 4π, and values of κ are frequently found in compilations in cgs units.]

The substitution method uses the fact that, with the advent of stable, internally solvent-locked spectrometers, it has become feasible to obtain accurate data by measuring the spectra of sample and reference in two separate experiments. If the sample and the reference compound are each dissolved in the same solvent at low concentration, the substitution method is equivalent to use of an internal reference except that the reference substance does not contaminate the sample or interact with it, chemically or physically. If the reference compound is a nearly neat liquid with only a small amount of the deuterated solvent to serve as a lock, the measured chemical shifts may be slightly different from those obtained with an internal reference because of differing molecular interactions. It might appear that a magnetic susceptibility correction would be needed if the susceptibilities of sample and reference differ, but this is not the case. With the field/frequency lock established via the deuterated solvent, the applied magnetic field simply shifts slightly to maintain the magnetic induction inside the sample tube constant so as to keep the ^{2}H on resonance.

If the lock signal of the sample differs from that of the reference, a lock correction may need to be applied according to:

$$\delta_{\text{true}} = \delta_{\text{measured}} + \left(\delta_{\text{sample}}^{\text{lock}} - \delta_{\text{reference}}^{\text{lock}} \right) \tag{8}$$

As no primary isotope effects between proton and deuterium have been detected, the difference between deuterium lock frequencies in Eqn. (8) may be obtained from a table of proton chemical shifts. When high precision is required (or if the lock is subject to large medium shifts, as is often the case for D_2O), the measurement of the shift difference between the locks may be obtained by direct observation of the deuterium spectrum of the two solvents, placed in concentric tubes.

However, for most modern spectrometers the manufacturers have incorporated compensating procedures for lock changes, largely for the users' convenience of retaining the spectral window in the same position on the screen or chart. Unfortunately these procedures vary between manufacturers and between spectrometers of different ages from the same manufacturer, so no completely general comments on this question can be made here. NMR spectroscopists must refer to the relevant operating manual for details. In most cases with modern instruments the effect is to keep the magnetic field inside the samples constant when different lock compounds are used. In such situations the correction term in brackets in equation 8 is not necessary. Of course, the accuracy of the result clearly depends on what the manufacturers use for the term in brackets, generally present in a "look-up" table in the spectrometer software. *We recommend that manufacturers give clear, explicit and accurate guidance on their procedures in this matter and quote their "look-up" tables prominently.*

Earlier IUPAC documentation[1,2] did not suggest any specific concentration for the reference, or choice of solvents. Ideally one should use a non-polar solvent with molecules of essentially spherical shape, and measurements should be extrapolated to zero reference concentration. Clearly such procedures are not generally feasible, so that caution needs to be exercised when comparing shift data from different sources.

3.5   **A Unified Scale**

As NMR studies of various nuclei were initiated, each was, of necessity, treated independently, with some substance containing the nuclide being studied selected as a reference

compound. The result is a vast collection of data in the literature for multinuclear magnetic resonance based on a large array of references. The proliferation of reference substances is, however, unnecessary and in some ways unhelpful. In a given magnetic field all resonance frequencies form a single spectral range, and it is only because different nuclides resonate at markedly different frequencies that use of separate references has arisen. With modern instruments, in which all frequencies are derived from a single source, it is therefore possible to relate the observed frequencies of all nuclides in a particular sample to that of a single primary reference - preferably the proton resonance of TMS.[#] There are, however, two reasons for wishing to retain the concept of a separate reference for each nucleus: (*i*) It is convenient to speak of, say, an aromatic ^{13}C resonance at *x* ppm from the ^{13}C line of TMS, rather than always quoting a frequency to many significant figures. (*ii*) Many data tabulations are available with values only expressed relative to separate heteronuclear references. Thus, for a unified scale to be of practical use, there must be agreed frequency relations between a set of commonly used secondary (heteronuclear) references and the primary reference. Measurements of such relations have been reported sporadically since the time of early double resonance experiments[11], and it has been proposed to relate the separate reference frequencies to a primary standard conventionally defined for a magnetic field such that the ^{1}H TMS signal is at exactly 100 MHz. These frequencies are given[11] the symbol Ξ (Greek capital xi), and some tabulations have been reported.[12-15]

More recently, the question of a unified reference has been addressed for multinuclear studies in biomolecular NMR: Wishart et al.[16] surveyed the relevant literature, pointed out inconsistencies in existing practices, and proposed the use of a single internal reference - for their purposes, one that is highly soluble in water (sodium 2,2-dimethyl-2-silapentane-5-sulfonate, DSS). Operationally, as discussed in the following sections, it is often easier to obtain

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[#] TMS has a low boiling point (28°C), which can be advantageous in facilitating removal from non-volatile samples after use, but can in other circumstances be a severe disadvantage. To overcome this problem, a substance such as tetrakis(trimethylsilyl)methane, [(CH$_3$)$_3$Si]$_4$C (m.p. 267°C), can be used as a reference[10] and the results converted to the TMS standard.

the necessary heteronuclear frequency data directly via the lock signal than to make additional measurements with various reference materials for different nuclei.

The Commission on Molecular Structure and Spectroscopy recommends that a unified chemical shift scale for all nuclides be based on the proton resonance of TMS as the primary reference. This Recommendation is in line with the *Recommendations for Presentation of NMR Structures of Proteins and Nucleic Acids*, recently promulgated[4] by the IUPAC Commission on Biophysical Chemistry in conjunction with the International Union of Biochemistry and Molecular Biology and the International Union of Pure and Applied Biophysics, which includes recommended Ξ values for several nuclei of importance in such studies for aqueous solutions, but which uses the proton resonance of DSS as the primary standard because of its solubility in water (see Section 3.9).

In conformity with other areas in physical chemistry, it would be desirable to define a precise standard state - for example, pure liquid TMS or TMS at infinite dilution in $CDCl_3$ at 293 K and 1 atmosphere pressure. However, in this document we concentrate on aspects that are of immediate practical utility. Temperature and pressure effects are sufficiently small for the lighter elements to be generally ignored for most chemical usage of NMR (largely carried out at ambient probe temperature and pressure), so we make no detailed recommendations regarding these parameters. Variation of solvent and/or change in sample concentration are known to have important effects on many chemical shifts, but they should be relatively small for a symmetric, non-polarizable molecule like TMS. To assess the magnitude of the concentration effect, we measured the proton chemical shift of TMS in solutions of 0.01%, 1% and 80% by volume in $CDCl_3$ with a Varian VXR-500S spectrometer.[17] The ^{1}H NMR frequency of TMS 1 vol % in chloroform is essentially at the infinite dilution level, the value for a 0.01 vol % solution differing by less than 0.1 Hz in Ξ, which is normally reported to only 1 Hz. However, for an 80 vol % solution Ξ was found to be 9 Hz larger than for a 1 vol % solution. *Therefore, for the primary reference we recommend a dilute solution (approximately 1% or less by volume) of*

TMS in a common organic solvent (preferably CDCl$_3$ since this is the most commonly-used solvent) or of DSS in water.

Our recommendations do not in any way preclude the design and implementation of experiments to measure specific properties, such as very high precision relative frequency measurements and special sample arrangements designed to minimise certain molecular interactions. Data will continue to be reported in the most effective way for the purpose at hand, but we believe that adoption of the unified chemical shift scale will facilitate comparison of the vast majority of NMR frequency measurements. The choice of the base reference as the proton signal of TMS is in accord with the virtually universal use of this signal as a reference for proton NMR. [#]

If the recommendation for use of a unified scale is widely adopted, future measurements will be reported as Ξ values. However, to assure consistency with data already in the literature, it is important to have a set of Ξ values of sufficient accuracy to permit conversion between the primary TMS reference and at least one secondary homonuclear reference for each nuclide (other than ^{1}H). Tables 1-3 list values of Ξ for a number of commonly used secondary references, which are hereby recommended for further use. These values come from a number of sources, as indicated in the tables. For most of the nuclides listed in Table 3, there are few data available, and the values of Ξ are simply approximations based on magnetogyric ratios. However, for Tables 1 and 2, values of Ξ are stated for almost all nuclides to 1 Hz. For 55 of the most commonly studied nuclides, careful measurements of Ξ have been made specifically for the purpose of this tabulation. The frequencies of ^{13}C and [29]Si were determined for samples of TMS in dilute solution in CDCl$_3$ (^{13}C at 300 and 500 MHz,[17,21] and [29]Si at 400 MHz[22]), The remaining 53 measurements were made by the substitution method (as described above)

[#] With hindsight it might have been better to choose the [29]Si signal of TMS since that is arguably even less susceptible to outside influence than the ^{1}H resonance (silicon being at the symmetry centre of the molecule). However, because of the large amount of literature based on the proton signal, we recommend that the primary reference remain the ^{1}H signal of TMS.

with a Bruker Model MSL spectrometer operating at nominal frequency of 300 MHz for ^{1}H.[18] Since all observation frequencies and the ^{2}H lock frequency are derived from a single source, the measured frequencies (Ξ) are reproducible to better than 0.1 Hz and are reported to 1 Hz. All measurements were made at ambient temperature, approximately 27°C. The replacement reference sample used in ref. 18 was a concentrated solution (4.75 m, 80% by volume) of TMS in $CDCl_3$ but the values have been converted to refer to 1 vol % TMS in $CDCl_3$ (see above). Values of Ξ for the remaining 41 nuclides in Tables 1 and 2 are taken from published values, which have been converted to be consistent with the choice of the ^{1}H signal for TMS in very dilute solution as Ξ/MHz of exactly 100. The literature cited should be consulted for details of the experimental procedure and for estimates of experimental precision and accuracy.

For ^{1}H and ^{13}C NMR particularly, internal referencing is usually preferable in order to avoid bulk magnetic susceptibility effects, which can be of the same magnitude as some chemical shift differences that are interpretable with regard to chemical structure, and the recommended primary reference is therefore TMS in a dilute solution in $CDCl_3$. For most other nuclides, however, many of the published data have been reported relative to an external or replacement reference, often a neat liquid where feasible. To provide maximum utility, most of the entries in Tables 1 and 2 refer to such neat liquids or concentrated solutions, usually with a minimum amount of deuterated substance added to provide a stable lock. Of course, a very large number of such reference materials and lock substances could be used, but as described in Section 3.6, it is relatively simple to convert from one to another if necessary.

Values of Ξ can be determined to 1 Hz, which represents only 0.01 to 0.5 ppm. Under the unified scale, chemical shifts can thus be reported to a precision that is often dependent on linewidth or other sample-related factors, rather than instrumental factors. However, since literature data for a number of nuclides are usually referred to a secondary reference and hence

are often of considerably lower precision, small discrepancies in values of $\varXi$ may be of little practical consequence in most instances.

3.6   **Practical Application of the Unified Scale**

Modern NMR spectrometers invariably include field/frequency locking and frequency synthesisers, so that all frequencies are reliably interrelated by locking to a master clock frequency. There are two ways in which this fact can be used to determine chemical shifts, either directly on the $\varXi$ scale or with respect to a secondary reference. These two ways are equivalent to the use of the conventional internal reference and substitution methods respectively. In the former case, if a nucleus X is to be studied, and the sample can be prepared with a small amount of TMS, then two direct frequency measurements made whilst maintaining the same ^{2}H locking conditions will provide the chemical shift of X on the unified scale by the equation:

$$\varXi \,/\, \mathrm{MHz} = 100 \left(v_X^{\mathrm{obs}} \,/\, v_{\mathrm{TMS}}^{\mathrm{obs}} \right) \tag{9}$$

where $v_{\mathrm{TMS}}^{\mathrm{obs}}$ is the measured ^{1}H frequency of TMS. If this procedure is applied to a series of samples, the effect is to replace 'medium effects' on the shielding of X (given by measurements using a reference compound containing the nuclide X) by 'medium effects' on the shielding of ^{1}H in TMS. In general, this should result in a reduction of 'medium effects' due to the referencing procedure, which is desirable. Clearly, the substitution method can be used similarly and is particularly valuable when it is not convenient to add TMS to the sample. Equation (9) is still relevant. However, as noted in Section 3.4, medium effects may vary to some extent if different concentrations of sample and reference are used.

In the future, reporting of chemical shift data as $\varXi$ values may become more common and acceptable. In the meantime, conversion of $\varXi$ values to conventional chemical shifts relative to a reference of an X-containing compound requires only subtraction by the $\varXi$ value of a

suitable homonuclear reference, as given in Tables 1 and 2, followed by division by the Ξ value of the homonuclear reference. Thus:

$$\delta_X = (\Xi_{X,sample} - \Xi_{X,reference})/\Xi_{X,reference} \qquad (10)$$

The widespread use of a ^{2}H lock for NMR measurements on isotropic samples suggests a modification of the substitution approach, since the relevant reference frequency should not vary with time. Thus the chemical shifts of the X nuclei can, in principle, be determined on the unified (TMS-based) scale merely by measuring the absolute resonance frequency of the sample and using a predetermined reference frequency for the nuclide in question. Thus only one (sample) tube is required and no reference substance needs to be added. The predetermined reference frequency is obtained by measuring the proton resonance of TMS under similar conditions to the sample (i.e. with the same lock compound) in a one-off experiment for the spectrometer being used. Then the frequency of the usual secondary reference for the X nucleus can be calculated using the pre-determined value of ν_{TMS}:

$$\nu_{reference} = \nu_{TMS}\Xi_{reference}/100\,\text{MHz} \qquad (11)$$

where Ξ_{ref} takes the appropriate value given in Tables 1-3. Thence the chemical shift (or the value of Ξ_X) for the sample can be readily derived. If the lock substance in the sample solution is not the same as that of the reference solution, a lock correction must be applied (Eq. (8)).

As an example, suppose that a ^{77}Se resonance has been measured on a compound dissolved in acetone-d_6 resulting in a value:

$$\nu_{sample} = 76344378\,\text{Hz}$$

On this spectrometer, the ^{1}H resonance of the TMS dissolved in CDCl$_3$ has been found at 400103342 Hz when the spectrometer was installed. The reference frequency of selenium is then, from Table 1:

$$400103342 \times 19.071535/100 = 76305849\,\text{Hz}$$

The proton chemical shifts of the locks are:

$$\delta_H(CHCl_3) = 7.27\,\text{ppm and } \delta_H(acetone) = 2.17\,\text{ppm}$$

Then:

$$\delta_{Se,\ sample} = (76344378 - 76305849)/76.305849 + (2.17 - 7.27) = 499.8\ \text{ppm}$$

Since this is still basically a substitution method, an error will arise if the ^{2}H frequency of the solvent has been influenced by the particular sample used. For many samples that consist of dilute solutions the error is small, and for many nuclei with large chemical shift ranges the error introduced in this way is probably smaller than would occur if a homonuclear (X) reference were used in the conventional manner.

Reporting of Ξ_X and δ_X measurements in future heteronuclear magnetic resonance studies will ultimately lead to a large set of consistent data, provided that values of $\Xi_{X,ref}$ are established and used consistently in all future work. Therefore, particularly for comparison with chemical shifts reported relative to a homonuclear (X) reference via conventional internal referencing procedures, it is essential that the values of Ξ in Tables 1 and 2 represent the accepted values for the substances listed (which are the "best" available at the present time). *We therefore recommend that the defined local chemical shift scale zero values are established as those listed in Tables 1 and 2, and that such definitions are not subject to future change arising from remeasurement even where this results in increasing accuracy for the reference compound in question.* [However, these values will be subject to correction during the period when these *Provisional Recommendations* are open for public comment before being published in final form.]

The Unified Scale offers many advantages over other methods of referencing. However, serious errors can occur in reading and displaying frequencies in some spectrometers unless care is taken. The software in NMR spectrometers is continually evolving, and even some spectrometers of relatively recent vintage are configured to display frequencies that are rounded off or that appear with many figures that do not correctly represent the frequency of a peak indicated by the cursor. The correct information is available in the appropriate parameter tables, but the authors of this document have found that in instruments which are several years old it

may be necessary to seek the correct file and not rely on what appears to be an "obvious" display. Although the situation has improved with the latest version of commercial instruments, *we strongly recommend that each user verify that his/her own instrument correctly determines one or more values of Ξ as given in Tables 1-3.*

3.7 **Alternative Reference Compounds**

Most of the elements have more than one proposed reference for the chemical shift scale mentioned in the literature. The majority are secondary standards chosen for convenience. Although our recommendation stands for the compounds listed in Tables 1 and 2, there are some situations where an alternative reference has to be used. One of these cases occurs when ^{1}H, ^{13}C, ^{15}N, [29]Si and other nuclei have to be referenced in highly polar solvents such as water, where TMS is only very sparingly soluble. For those situations, sodium 2,2-dimethyl-2-silapentane-5-sulfonate (DSS) or its partially deuterated form, $Me_3SiCD_2CD_2CD_2SO_3Na$, is the recommended primary reference.[16,49] [3-(trimethylsilyl) sodium propionate (TSP) is another salt that has also been suggested.[50]] When DSS is used as a reference, it has been recommended[4] that ^{1}H chemical shifts be denoted by the symbol δ_{DSS} to distinguish them from those referenced to TMS. However, the resonances of DSS and TMS, *both dissolved in the same solvent*, are found to be very close: On the scale with TMS as zero, DSS has a chemical shift of $\delta = 0.0173$ ppm in dilute aqueous solution, while in dilute solution in dimethylsulfoxide-d_6, the chemical shift of DSS is $\delta = -0.0246$ ppm[4]. For most purposes these differences are negligible (falling well below the anticipated range of solvent effects), and *data from the TMS and DSS scales may be validly compared without correction for the different ^{1}H reference.*

Table 4 repeats the recommended values of Ξ from Reference 4, along with data for additional references proposed for nitrogen, and compares them with our recommendations in Tables 1 and 2. For ^{13}C studies in aqueous solution, Reference 4 recommends using the ^{13}C methyl resonance of DSS, rather than that of TMS, as the secondary reference. Carbon-13

chemical shifts based on DSS and TMS differ by about 2 ppm, which can cause confusion if not clarified. *We recommend that when ^{13}C chemical shifts are referenced to DSS, that point should be made clear by using a notation such as $\delta_{DSS}(^{13}C)$.*

Reference 4 recommends use of trimethylphosphate (internal) as a secondary reference for ^{31}P studies in aqueous solution, whereas Table 1 recommends 85% phosphoric acid (external), which has been used more widely, particularly for chemical systems where use of an internal reference is not feasible. The two secondary references differ by about 3 ppm, so *it is important to specify which is being used.*

Several references have been used historically for nitrogen NMR, partly resulting from the very different properties and natural abundances of the two nuclides (^{14}N and ^{15}N). Nitromethane as either an internal or external reference has been the most widely used for ^{14}N and to some extent for ^{15}N, while liquid ammonia has been a popular external reference for ^{15}N. Ammonium and tetramethylammonium salts have been used as internal references for both ^{14}N and ^{15}N. Reference 4 recommends liquid NH$_3$ as a secondary reference for ^{15}N in aqueous solutions, since most biochemical applications of ^{15}N NMR have used this reference. In Tables 1 and 2 *we recommend nitromethane as a reference*, in line with common usage in many other applications. The values of Ξ are compared in Table 4, along with those for tetramethylammonium iodide, which has been suggested as an internal reference for both ^{14}N and ^{15}N since the tetrahedral geometry results in sharp lines for both isotopomers.

For most of the nuclei listed in Tables 1 and 2 we give Ξ values for only one homonuclear (X) reference, since conversions to other reference compounds can be made readily from literature values. During the period that these Recommendations are in Provisional form, the Commission will be glad to consider the inclusion of additional values of Ξ for which a need can be demonstrated.

3.8 **Magic-angle Spinning**

It has been shown[53,54] that bulk isotropic magnetic susceptibility effects are eliminated by spinning an infinitely-long cylindrical sample with its axis at the magic angle (54.7°) to the static magnetic field of an NMR spectrometer. Therefore, in principle, magic-angle spinning (MAS) can be used in the external referencing method to obtain chemical shifts free from bulk susceptibility problems. Whereas this technique was proposed in the context of solid-state NMR (see below), its utility applies equally well to the solution state[55,56]. In practice an infinitely long cylinder is not necessary to reduce bulk susceptibility effects on chemical shifts to an acceptable level. Strictly speaking, to correct for <u>isotropic</u> bulk susceptibility effects, it is also not necessary to spin at the magic angle, but merely to orient the cylinder containing the sample at the magic angle (see Eq. (7)). However, spinning may narrow the lines significantly (especially for solids) and so is essential for accurate chemical shift measurement.

3.9 **Solids**

Sample-handling procedures differ substantially for solids from those appropriate for solutions, and there are clear advantages to using suitable solids as secondary references. This is almost always done using sample replacement. However, the spectrometers are generally used without field/frequency locking, so that the resulting chemical shifts are inevitably less accurate than those for solutions. This is not a significant problem, because linewidths are usually substantially greater than those for solutions and they impose an upper limit to accuracy. High-resolution NMR of solids almost invariably relies on magic-angle spinning, and, as discussed in section 3.7, this eliminates the effects of differences in bulk isotropic magnetic susceptibilities. The early paper by Earl and VanderHart[53] addressed this matter, and a recent review by Vanderhart[9], which refers to both liquids and solutions, further discusses the influence of MAS for referencing spectra. Unfortunately, the situation is only simple for systems with isotropic magnetic susceptibility. VanderHart[9] discusses the case of anisotropic susceptibility, but there is to date little experimental work in this area. However, in general it may be taken that, within the

accuracy of measurement, referencing by sample replacement under MAS conditions in an unlocked but stable spectrometer is to a good approximation equivalent to the substitution method as described in section 3.5.

Several papers[57-59] take advantage of the MAS technique to suggest secondary solid standards for practical use in solid-state NMR. For example the ^{13}C signals of solid adamantane, glycine, hexamethylbenzene and tetrakis (trimethylsilyl) silane have been referenced to those for liquids and solutions using MAS, and data were reported to accuracies in the region of 0.004 - 0.04 ppm.

Chemical shift referencing for solid-state NMR is not yet at the stage where much further discussion is warranted here, so the only recommendation that we make is for referencing procedures to be always clearly and carefully stated in publications.

4. SUMMARY OF RECOMMENDATIONS

In addition to the endorsements of earlier Recommendations stated in Section 3.2 above, the Commission recommends the following:

(a)   Equation (4) (with alternative presentations as in equations (5) and (6)) should be used to define chemical shift scales, with ppm (or ppb or %, as appropriate) explicitly quoted with numerical values.

(b)   The ^{1}H signal of tetramethylsilane in dilute solution (ca. 1% by volume in CDCl$_3$ for preference) should be used as the primary *internal* or substitution reference for the resonance frequencies (and hence chemical shifts) for *all* nuclei. However, for aqueous solutions the recommendations of ref. 38 are supported.

(c)   The secondary references listed in Tables 1 and 2 may be used for the nuclei of the various elements, with their absolute frequencies taking the fixed values

given (not subject to revision after these Recommendations are adopted in final form).

(d)   Internal referencing may be used for solutions but its limitations should be recognised.

(e)   For solution-state measurements, referencing via an internal ^{2}H lock signal may be used, either to give the value of $\varXi$ directly or to calculate the chemical shift with respect to the relevant secondary reference (via equation (8) where relevant).

(f)   Referencing by the substitution method with field/frequency lock spectrometers may also be used for solutions.

(g)   External referencing for either liquids or solids may be carried out with magic-angle spinning.

(h)   External referencing by means other than (f) and (g) is to be discouraged unless corrections are applied for bulk susceptibility effects.

(i)   In all circumstances, and especially where strict adherence to these Recommendations is not feasible, details of experimental procedures should be given clearly so that results may be validly intercompared.

REFERENCES

1.   "Recommendations for the Presentation of NMR Data for Publication in Chemical Journals", *Pure Appl. Chem.* **29**, 627 (1972).

2.   "Presentation of NMR Data for Publication in Chemical Journals – B. Conventions relating to Spectra from Nuclei other than Protons", *Pure Appl. Chem.* **45**, 217 (1976).

3.   R.K. Harris, J. Kowalewski and S.C. de Menezes, "Parameters and Symbols for Use in Nuclear Magnetic Resonance", *Pure Appl. Chem.* **69**, 2489 (1997).

4.   J.L. Markley, A. Bax, Y. Arata, C.W. Hilbers, R. Kaptein, B.D. Sykes, P.E. Wright and K. Wüthrich, "Recommendations for the Presentation of NMR Structures of Proteins and Nucleic Acids", *Pure Appl. Chem.*, **70**, 117 (1998).

5.   "NMR and the Periodic Table", Eds. R.K. Harris and B.E. Mann, Academic Press (1978).

6.   "Quantities, Units and Symbols in Physical Chemistry", I. Mills, T. Cvitas, K. Homann, N. Kallay and K. Kuchitsu, published for IUPAC by Blackwell Scientific Publications, 1993.

7.   R.K. Harris, "*Encyclopedia of Nuclear Magnetic Resonance*", Eds.-in-Chief D.M. Grant and R.K. Harris **5**, 3301 (1996), John Wiley & Sons Ltd. (Chichester).

8.   G.V.D. Tiers, *J. Phys. Chem.* **62**, 1151 (1958).

9.   D.L. VanderHart, "*Encyclopedia of Nuclear Magnetic Resonance*", Eds-in-Chief D.M. Grant and R.K. Harris **5**, 2938 (1996), *John Wiley & Sons Ltd. (Chichester)*.

10.   N.N. Zemlyanskii and O.K. Sokolikova, *Russ. J. Anal. Chem.* **36**, 1421 (1981).

11.   W. McFarlane, *Proc. Roy. Soc. (London)* A **306**, 185 (1968).

12.   W. McFarlane, *Ann. Rev. NMR Spectrosc.* **1**, 135 (1968).

13.   R.K. Harris and B.J. Kimber, *J. Magn. Reson.* **17**, 174 (1975).

14.   D. Canet, C. Goulon-Ginet and J.P. Marchal, *J. Magn. Reson.* **22**, 537 (1976).

15.   S. Brownstein and J. Bornais, *J. Magn. Reson.* **38**, 131 (1980).

16.   D.S. Wishart, C.G. Bigam, J. Yao, F. Abildgaard, H.J. Dyson, E. Oldfield, J.L. Markley and B.D. Sykes, *J. Biomol. NMR,* **6**, 135 (1995).

17.   H.J.C. Yeh, previously unpublished work.

18.   P. Granger, measurements (as described in section 3.5), previously unpublished in the primary literature, but presented in preliminary form in ref. 7.

19.   J.P. Bloxsidge, J.A. Elvidge, J.R. Jones, R.B. Mane and M. Saljoughian, *Magn. Reson. Chem.* **12**, 574 (1979).

20. H.L. Anderson, *Phys. Rev.* **76**, 1460 (1949).

21. A.M. Kenwright, previously unpublished work.

22. B. Ancian, previously unpublished work.

23. H.T. Edzes, *Magn. Reson. Chem.* **30**, 850 (1992).

24. C. Brevard, previously unpublished work.

25. P.L. Goggin, R.J. Goodfellow and F.J.S. Reed, *J. Chem. Soc. Dalton*, 576 (1974); S.J. Anderson, J.R. Barnes, P.L. Goggin and R.J. Goodfellow, *J. Chem. Res. (M)*, 3601 (1978).

26. R. Benn and A. Rufinska, *Angew. Chem. (Int)*. **25**, 861 (1986).

27. J.D. Kennedy and W. McFarlane, *J.C.S. Perkin II*, 1187 (1977).

28. T.H. Brows, E.B. Whipple and P.H. Verdier, *J. Chem. Phys.* **38**, 3029 (1963).

29. G.A. Schumacker and G.J. Schrobilgen, *Inorg. Chem.* **23**, 2923 (1984).

30. J.F. Hinton, G.L. Turner, G. Young and K.R. Metz, *Pure Appl. Chem.* **54**, 2359 (1982).

31. J.F. Hinton and R.W. Briggs, *J. Magn. Reson.* **25**, 556 (1997).

32. P. Pyykko, *Z. Naturforsch.* **47**A, 189 (1992).

33. P. Raghavan, *At. Data Nucl. Data Tables* **42**, 189 (1989).

34. J.D. Kennedy in "Multinuclear NMR", Ed. J. Mason, Plenum Press, Ch. 8, p.221 (1987).

35. J.T. LaTourrette, W.E. Quinn and R.F. Ramsey, *Phys. Rev.* **107**, 1202 (1957).

36. W. Sahm and A. Schwenk, *Z. Naturforsch.* **29a**, 1754 (1974).

37. W. Sahm and A. Schwenk, *Z. Naturforsch*, **29a**, 1763 (1974).

38. O. Lutz, A. Schwenk and A. Uhl, *Z. Naturforsch*, **30a**, 1122 (1975).

39. N. Hao, M.J. McGlinchey, B.G. Sayer and G.J. Schrobilgen, *J. Magn. Reson.* **46**, 158 (1982).

40. J. Kodweiss, O. Lutz, W. Messner, K.R. Mohn, A. Nolle, B. Stütz and D. Zepf, *J. Magn. Reson.* **43**, 495 (1981).

41. J. Kaufmann, W. Sahm and A. Schwenk, *Z. Naturforsch.* **26A**, 1384 (1971).

42. D. Brinkman, *Helv. Phys. Acta*, **41**, 367 (1968).

43. O. Lutz and H. Oehler, *Z. Physik A*, **288**, 11 (1978).

44.   O. Lutz and H. Oehler, *J. Magn. Reson.* **37**, 261 (1980).

45.   C. Brevard and P. Granger, "Handbook of High Resolution Multinuclear NMR", Wiley (1981).

46.   G. Wu and R.E. Wasylishen, Magn. Reson. Chem. **31**, 537 (1993).

47.   A.G. Avent, M.F. Lappert and G.A. Lawless, *J. Amer. Chem. Soc*. **111**, 3423, (1989).

48.   H. LeBail, C. Chachaty, P. Rigny and R. Bougon, *C.R. Acad. Sci*. **297**, 451 (1983).

49.   G.V.D. Tiers and A. Kowalewsky, paper presented to the Division of Physical Chemistry, 137th National Meeting ACS, Cleveland, Ohio, 1960; Abstracts, p.1712; G.V.D. Tiers and R.I. Coon, *J. Org. Chem.* **26**, 2097 (1961).

50.   G.V. Tiers and A. Kowalewsky, Division of Physical Chemistry, 137th ACS National Meeting, Cleveland, Ohio, 1960; L. Pohl and M. Ecke, *Angew Chem. Internat. Ed*. **8**, 381 (1969); D.H. Live and S.I. Chan, *Org. Magn. Reson.*, **5**, 275 (1973).

51.   E.D. Becker, *J. Magn. Reson.,* **4**, 142(1971).

52.   E.D. Becker, R.B. Bradley and T. Axenrod, *J. Magn. Reson.* **4**, 136 (1971).

53.   W.L. Earl and D.L. VanderHart, *J. Magn. Reson.* **48**, 35 (1982).

54.   D. Doskočilová, D.D. Tao and B. Schneider, *Czech. J. Phys.* B**25**, 202 (1975); D. Doskočilová and B. Schneider, *Macromol.*, **5**, 125 (1972).

55.   A.N. Garroway, *J. Magn. Reson.* **49**, 168 (1982).

56.   S. Hayashi, M. Yanagisawa and K. Hayamizu, *Anal. Sci.* **7**, 955 (1991).

57.   S. Hayashi and K. Hayamizu, *Bull. Chem. Soc. Jpn.* **62**, 2429 (1989).

58.   S. Hayashi and K. Hayamizu, *Bull. Chem. Soc. Jpn.* **64**, 685 (1991).

59.   S. Hayashi and K. Hayamizu, *Bull. Chem. Soc. Japan* **64**, 688 (1991).

Table 1 The Spin Properties of the Spin-½ Nuclei[a]

Isotope[b]	Natural abundance,[c] C /%	Magnetic moment,[d] μ/μ_N	Magnetogyric ratio,[d] $\gamma/10^7$ rad T^{-1} s^{-1}	NMR frequency,[e] Ξ/MHz	Reference compound	Sample conditions[f]	Literature	Relative receptivity[g]	
								D^p	D^C
^{1}H	99.985	4.837353570	26.7522128	100.000000[h]	Me$_4$Si	CDCl$_3$, 1% v/v		1.000	5.71×10^3
^{3}H[i]	-	5.159714367	28.5349779	106.663984	Me$_4$Si-t_1	[j]	19	-	-
^{3}He	1.37×10^{-4}	-3.685154336	-20.3801587	76.178972	He	gas[j]	20	6.06×10^{-7}	3.46×10^{-3}
^{13}C	1.10	1.216613	6.728284	25.145020	Me$_4$Si	CDCl$_3$, 1% v/v	17,21	1.75×10^{-4}	1.00
^{15}N	0.366	-0.49049746	-2.71261804	10.136784	MeNO$_2$	neat/CDCl$_3$ [k]	18	3.82×10^{-6}	2.18×10^{-2}
^{19}F	100	4.553333	25.18148	94.094008	CCl$_3$F	[j]	15	0.834	4.77×10^3
^{29}Si	4.67	-0.96179	-5.3190	19.867187	Me$_4$Si	CDCl$_3$, 1% v/v	22	3.67×10^{-4}	2.10
^{31}P	100	1.95999	10.8394	40.480742	H$_3$PO$_4$	[j]	23	0.0665	3.80×10^2
^{57}Fe	2.2	0.1569636	0.8680624	3.237778	Fe(CO)$_5$	C$_6$D$_6$ [ℓ]	24	7.52×10^{-7}	4.30×10^{-3}
^{77}Se	7.63	0.92677577	5.1253857	19.071537	Me$_2$Se	neat/C$_6$D$_6$ [k]	18	5.37×10^{-4}	3.07
^{89}Y	100	-0.23801049	-1.3162791	4.900200	Y(NO$_3$)$_3$	H$_2$O/D$_2$O [m]	18	1.19×10^{-4}	0.681
^{103}Rh	100	-0.1531	-0.8468	3.186447[n,o,p]	Rh(acac)$_3$	CDCl$_3$, sat.	26	3.17×10^{-5}	0.181
(^{107}Ag)	51.839	-0.19689893	-1.0889181	4.047819[o]	AgNO$_3$	D$_2$O, sat.	18	3.50×10^{-5}	0.200
^{109}Ag	48.161	-0.22636279	-1.2518634	4.653533[o]	AgNO$_3$	D$_2$O, sat.	18	4.94×10^{-5}	0.282
(^{111}Cd)	12.80	-1.0303729	-5.6983131	21.215480	CdMe$_2$	neat[j]	27	1.24×10^{-3}	7.07
(^{113}Cd)[q]	12.22	-1.0778568	-5.9609155	22.193175	CdMe$_2$	neat[j]	27	1.35×10^{-3}	7.72
(^{115}Sn)	0.34	-1.5915	-8.8013	32.718749	Me$_4$Sn	neat/C$_6$D$_6$ [k]	18	1.21×10^{-4}	0.694
(^{117}Sn)	7.68	-1.73385	-9.58879	35.632259	Me$_4$Sn	neat/C$_6$D$_6$ [k]	18	3.54×10^{-3}	20.2
^{119}Sn	8.59	-1.81394	-10.0317	37.290632	Me$_4$Sn	neat/C$_6$D$_6$ [k]	18	4.53×10^{-3}	25.9
(^{123}Te)	0.908	-1.276431	-7.059098	26.169767	Me$_2$Te	neat/C$_6$D$_6$ [k]	18	1.67×10^{-4}	0.953
^{125}Te	7.139	-1.5389360	-8.5108404	31.549789	Me$_2$Te	neat/C$_6$D$_6$ [k]	18	2.30×10^{-3}	13.1
^{129}Xe	26.4	-1.347494	-7.452103	27.811008[o,r,s]	XeOF$_4$	neat[j]	28	5.71×10^{-3}	32.6
^{183}W	14.3	0.20400919	1.1282403	4.166398	Na$_2$WO$_4$	D$_2$O, 1M	24	1.07×10^{-5}	6.13×10^{-2}
^{187}Os	1.6	0.1119804	0.6192895	2.282331	OsO$_4$	CCl$_4$, 0.98M	24	1.99×10^{-7}	1.13×10^{-3}
^{195}Pt	33.8	1.0557	5.8385	21.496752[n,o]	[PtCl$_6$]$^{2-}$	D$_2$O, 1.2M	18	3.51×10^{-3}	20.1
^{199}Hg	16.87	0.87621937	4.8457916	17.910325	Me$_2$Hg[t]	neat/C$_6$D$_6$ [k]	18	1.00×10^{-3}	5.73
(^{203}Tl)	29.524	2.80983305	15.5393338	57.123200[u]	Tl(NO$_3$)$_3$	[j]	-	0.0578	3.31×10^2
^{205}Tl	70.476	2.83747094	15.6921808	57.683838[o]	Tl(NO$_3$)$_3$	[j]	31	0.142	8.13×10^2
^{207}Pb	22.1	1.00906	5.58046	20.920599	Me$_4$Pb	neat/C$_6$D$_6$ [k]	18	2.01×10^{-3}	11.5

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^a A complete list for stable nuclei, but excluding the lanthanides and actinides and most radioactive isotopes.
^b Nuclei in parentheses are considered to be not the most favourable of the element concerned for NMR.
^c Data from Mills et al.,[6] pp. 98-104. For the error limits, see Mills et al.[6]
^d Data derived from the compilation in Mills et al.,[6] pp. 98-104, which lists values of $\mu_{max}/\mu_N = \gamma\hbar I/\mu_N$. For the error limits, see Mills et al.[6]
^e Resonance frequency in a magnetic field such that the protons of TMS at infinite dilution (in practice at 1% v/v) in CDCl$_3$ resonate at exactly 100 MHz.
^f M ≡ molarity in mol dm^{-3} (solution); m ≡ molality in mol kg^{-1} (solvent). Results from ref. 18 were initially referenced[7] to a TMS concentration of 4.75 m in CDCl$_3$, but the values are corrected to refer to a dilute (1% v/v) solution of TMS in CDCl$_3$.
^g D^P is the receptivity relative to that of ^{1}H whereas D^C is relative to ^{13}C.
^h Value by definition (see the text).
ⁱ Radioactive (half-life 12 y).
^j See literature cited.
^k Small amount of lock substances (<10% v/v) in neat liquid.
^ℓ 20% by volume C$_6$D$_6$ in Fe(CO)$_5$.
^m H$_2$O/D$_2$O solution, concentration not reported.
ⁿ Alternatively, the precise values 3.160000 MHz and 21.400000 have been suggested[25] as the references for ^{103}Rh and ^{195}Pt, respectively.
^o Value revised from that given in the Encyclopedia[7] (in addition to the conversion from 4.75 m TMS/CDCl$_3$ to 1% v/v TMS/CDCl$_3$ as the standard).
^p Subject to considerable variation with temperature.
^q Long-lived radioactive isotope.
^r Data converted by Granger to the reference recommended herein.
^s Calculated from ref. 28 using information from ref. 29.
^t The high toxicity of this compound means its direct use should be strongly discouraged.
^u Deduced from refs. 30 and 31.

Table 2 The Spin Properties of Quadrupolar Nuclei[a]

Isotope[b]	Spin[c]	Natural abundance,[c] $C/\%$	Magnetic moment,[d] μ/μ_N	Magnetogyric ratio,[d] $\gamma/10^7$ rad T^{-1}s^{-1}	Quadrupole moment[e] Q/barn	NMR frequency,[f] Ξ/MHz	Reference sample	Sample conditions[g]	Literature	Linewidth factor,[h] $10^{56}\,\ell/\text{m}^4$	D^p	D^C
^{2}H[j]	1	0.015	1.21260077	4.10662791	2.860×10^{-3}	15.350609	$(CD_3)_4Si$	neat	18	4.1×10^{-5}	1.45×10^{-6}	8.27×10^{-3}
^{6}Li	1	7.5	1.1625637	3.9371709	-8.2×10^{-4}	14.716106	LiCl	D_2O, 9.7m	18	3.4×10^{-6}	6.38×10^{-4}	3.64
^{7}Li	3/2	92.5	4.20407505	10.3977013	-4.01×10^{-2}	38.863790	LiCl	D_2O, 9.7m	18	2.1×10^{-3}	0.272	1.55×10^3
^{9}Be	3/2	100	-1.520136	-3.759666	5.288×10^{-2}	14.051820[k]	$BeSO_4$	D_2O, 0.43m	18	3.7×10^{-3}	1.39×10^{-2}	79.3
^{10}B	3	19.9	2.0792055	2.8746786	8.459×10^{-2}	10.743658	$BF_3.Et_2O$	$CDCl_3{}^{\ell}$	34	1.4×10^{-3}	3.95×10^{-3}	22.6
^{11}B	3/2	80.1	3.4710308	8.5847044	4.059×10^{-2}	32.083974[k]	$BF_3.Et_2O$	$CDCl_3{}^{\ell}$	34	2.2×10^{-3}	0.132	7.56×10^2
^{14}N[j]	1	99.634	0.57100428	1.9337792	2.01×10^{-2}	7.226330	CH_3NO_2	neat/CDCl$_3{}^m$	18	2.0×10^{-3}	1.00×10^{-3}	5.73
^{17}O	5/2	0.038	-2.24077	-3.62808	-2.558×10^{-2}	13.556430	D_2O	neat	18	2.1×10^{-4}	1.11×10^{-5}	6.32×10^{-2}
^{21}Ne	3/2	0.27	-0.854376	-2.11308	0.10155	7.894530[k,n]	Ne	gas		1.4×10^{-2}	6.65×10^{-6}	3.80×10^{-2}
^{23}Na	3/2	100	2.8629811	7.0808493	0.1006	26.451921[k]	NaBr	D_2O, 9.9m	18	1.3×10^{-2}	9.27×10^{-2}	5.30×10^2
^{25}Mg	5/2	10.00	-1.01220	-1.63887	0.1994	6.121643	$MgCl_2$	D_2O, 15m	18	1.3×10^{-2}	2.68×10^{-4}	1.53
^{27}Al	5/2	100	4.3086865	6.9762715	0.1403	26.056890	$Al(NO_3)_3$	D_2O, 1.1m	18	6.3×10^{-3}	0.207	1.18×10^3
^{33}S	3/2	0.75	0.8311696	2.055685	-6.78×10^{-2}	7.676020[k]	$(NH_4)_2SO_4$	D_2O, sat.	18	6.1×10^{-3}	1.70×10^{-5}	9.72×10^{-2}
^{35}Cl	3/2	75.77	1.061035	2.624198	-8.11×10^{-2}	9.797931	KCl	D_2O, 2.2m	18	8.8×10^{-2}	3.58×10^{-3}	20.4
^{37}Cl	3/2	24.23	0.8831998	2.184368	-6.39×10^{-2}	8.155764	KCl	D_2O, 2.2m	18	5.4×10^{-3}	6.60×10^{-4}	3.77
^{39}K	3/2	93.2581	0.50543376	1.2500608	5.9×10^{-2}	4.666423	KI	D_2O, 3.8m	18	4.6×10^{-3}	4.76×10^{-4}	2.72
$(^{40}$K)	4	0.0117	-1.4513203	-1.5542854	-7.3×10^{-2}	5.801987[k,o]	KI	D_2O		5.2×10^{-4}	6.12×10^{-7}	3.50×10^{-3}
$(^{41}$K)	3/2	6.7302	0.27739609	0.68606808	7.2×10^{-2}	2.561332[p]	KI	D_2O		6.9×10^{-3}	5.68×10^{-6}	3.24×10^{-2}
^{43}Ca	7/2	0.135	-1.494067	-1.803069	-4.09×10^{-2}	6.729996[q]	$CaCl_2$	D_2O		2.3×10^{-4}	8.68×10^{-6}	4.96×10^{-2}
^{45}Sc	7/2	100	5.3933489	6.5087973	-0.22	24.291702	$ScCl_3$	D_2O, 1M	24	6.6×10^{-3}	0.302	1.73×10^3
^{47}Ti	5/2	7.3	-0.93294	-1.5105	0.29	5.637587	$TiCl_4$	neat^r	18	2.7×10^{-2}	1.53×10^{-4}	0.876
^{49}Ti	7/2	5.5	-1.25201	-1.51095	0.24	5.639095	$TiCl_4$	neat^r	18	7.8×10^{-3}	2.08×10^{-4}	1.19
$(^{50}$V)^s	6	0.250	3.6137570	2.6706490	0.209	9.970315	$VOCl_3$	neat/C$_6$D$_6{}^m$	18	1.7×10^{-3}	1.39×10^{-4}	0.796
^{51}V	7/2	99.750	5.8380835	7.0455117	-5.2×10^{-2}	26.302963	$VOCl_3$	neat/C$_6$D$_6{}^m$	18	3.7×10^{-4}	0.383	2.19×10^3
^{53}Cr	3/2	9.501	-0.61263	-1.5152	-0.15	5.652511[k]	$(NH_4)_2CrO_4$	D_2O, 1M	18	3.0×10^{-2}	8.63×10^{-5}	0.493
^{55}Mn	5/2	100	4.1042437	6.6452546	0.33	24.789062	$KMnO_4$	D_2O, 0.82m	18	3.5×10^{-2}	0.179	1.02×10^3
^{59}Co	7/2	100	5.247	6.332	0.404	23.727074	$K_3[Co(CN)_6]$	D_2O, 0.56m	18	2.2×10^{-2}	0.278	1.59×10^3
^{61}Ni	3/2	1.140	-0.96827	-2.3948	0.162	8.936051	$Ni(CO)_4$	neat/C$_6$D$_6{}^m$	39	3.5×10^{-2}	4.09×10^{-5}	0.234
^{63}Cu	3/2	69.17	2.8754908	7.1117890	-0.211	26.515473[k]	$[Cu(CH_3CN)_4][ClO_4]$	CH$_3$CN, sat.^{t}	18	5.9×10^{-2}	6.50×10^{-2}	3.71×10^2
^{65}Cu	3/2	30.83	3.07465	7.60435	-0.195	28.403661	$[Cu(CH_3CN)_4][ClO_4]$	CH$_3$CN, sat.^{t}	18	5.1×10^{-2}	3.54×10^{-2}	2.02×10^2
^{67}Zn	5/2	4.1	1.035556	1.676688	0.150	6.256820	$Zn(NO_3)_2$	D_2O, sat.	18	7.2×10^{-3}	1.18×10^{-4}	0.673
$(^{69}$Ga)	3/2	60.108	2.603405	6.438855	0.168	24.001255	$Ga(NO_3)_3$	D_2O, 1.1m	40	3.8×10^{-2}	4.19×10^{-2}	2.39×10^2
^{71}Ga	3/2	39.892	3.307871	8.181171	0.106	30.496579	$Ga(NO_3)_3$	D_2O, 1.1m	40	1.5×10^{-2}	5.71×10^{-2}	3.26×10^2
^{73}Ge	9/2	7.73	-0.9722881	-0.9360303	-0.173	3.488315	$(CH_3)_4Ge$	neat	41^u	2.2×10^{-3}	1.09×10^{-4}	0.624

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^{75}As	3/2	100	1.858354	4.596163	0.314	17.122712	NaAsF$_6$	CH$_3$CN^{v,w}	18	0.13	2.54×10^{-2}	1.45×10^2
(^{79}Br)	3/2	50.69	2.719351	6.725616	0.331	25.054454	NaBr	D$_2$O, 9.9m	18	0.15	4.03×10^{-2}	2.30×10^2
^{81}Br	3/2	49.31	2.931283	7.249776	0.276	27.007028	NaBr	D$_2$O, 9.9m	18	0.10	4.91×10^{-2}	2.80×10^2
^{83}Kr	9/2	11.5	-1.07311	-1.03310	0.253	3.847600^{k,x}	Kr	gas	42	4.7×10^{-3}	2.19×10^{-4}	1.25
(^{85}Rb)	5/2	72.165	1.6013071	2.5927050	0.228	9.655173	RbCl	D$_2$O, 5.7m	18	1.7×10^{-2}	7.66×10^{-3}	43.8
^{87}Rb^s	3/2	27.835	3.552582	8.786400	0.132	32.721218	RbCl	D$_2$O, 5.7m	18	2.3×10^{-2}	4.93×10^{-2}	2.82×10^2
^{87}Sr	9/2	7.00	-1.2090236	-1.1639376	0.335	4.333800	SrCl$_2$	D$_2$O, 0.5M	24	8.3×10^{-3}	1.90×10^{-4}	1.09
^{91}Zr	5/2	11.22	-1.54246	-2.49743	-0.206	9.296298	Zr(C$_5$H$_5$)$_2$Cl$_2$	CH$_2$Cl$_2$, sat.^{t}	18	1.4×10^{-2}	1.07×10^{-3}	6.09
^{93}Nb	9/2	100	6.8217	6.5674	-0.32	24.476195	K[NbCl$_6$]	CH$_3$CN, sat.^{w}	18	7.6×10^{-3}	0.488	2.79×10^3
^{95}Mo	5/2	15.92	-1.082	-1.751	2.2×10^{-2}	6.516943	Na$_2$MoO$_4$	D$_2$O, 2M^y	18	1.5×10^{-4}	5.21×10^{-4}	2.98
(^{97}Mo)	5/2	9.55	-1.105	-1.788	0.255	6.653712	Na$_2$MoO$_4$	D$_2$O, 2M^y	18	2.1×10^{-3}	3.33×10^{-4}	1.90
^{99}Tc^s	9/2	-	6.281	6.046	0.3	22.508316	NH$_4$TcO$_4$	D$_2$O^z	18	6.7×10^{-3}	-	-
^{99}Ru	5/2	12.7	-0.7588	-1.229	7.9×10^{-2}	4.605151	K$_4$[Ru(CN)$_6$]	D$_2$O, 0.3M	18	2.0×10^{-3}	1.44×10^{-4}	0.821
^{101}Ru	5/2	17.0	-0.8505	-1.377	0.457	5.161369	K$_4$[Ru(CN)$_6$]	D$_2$O, 0.3M	18	6.7×10^{-2}	2.71×10^{-4}	1.55
^{105}Pd	5/2	22.33	-0.760	-1.23	0.660	4.576100	K$_2$PdCl$_6$	D$_2$O, sat.	24	0.14	2.53×10^{-4}	1.45
(^{113}In)	9/2	4.3	6.1124	5.8845	0.799	21.865656	In(NO$_3$)$_3$	D$_2$O, 0.1M^A	40	4.7×10^{-2}	1.51×10^{-2}	86.3
^{115}In^s	9/2	95.7	6.1256	5.8972	0.810	21.912527	In(NO$_3$)$_3$	D$_2$O, 0.1M^A	40	4.9×10^{-2}	0.338	1.93×10^3
^{121}Sb	5/2	57.36	3.9796	6.4435	-0.36	23.930601	KSbCl$_6$	CH$_3$CN, sat.^{w}	18	4.1×10^{-2}	9.35×10^{-2}	5.34×10^2
(^{123}Sb)	7/2	42.64	2.8912	3.4892	-0.49	12.958903	KSbCl$_6$	CH$_3$CN, sat.^{w}	18	3.3×10^{-2}	1.99×10^{-2}	1.14×10^2
^{127}I	5/2	100	3.328710	5.389573	-0.78	20.008632	KI	D$_2$O, 5.7m	18	0.19	9.54×10^{-2}	5.45×10^2
^{131}Xe^j	3/2	21.2	0.8931899	2.209076	-0.12	8.244885^{k,B}	XeOF$_4$	neat		1.9×10^{-2}	5.97×10^{-4}	3.41
^{133}Cs	7/2	100	2.9277407	3.5332539	-3.71×10^{-3}	13.116208	CsNO$_3$	D$_2$O, 1.7m	18	1.9×10^{-6}	4.84×10^{-2}	2.76×10^2
(^{135}Ba)	3/2	6.592	1.08178	2.67550	0.16	9.934415	BaCl$_2$	D$_2$O, 0.5M	43	3.4×10^{-2}	3.30×10^{-4}	1.88
^{137}Ba	3/2	11.23	1.21013	2.99295	0.245	11.112890	BaCl$_2$	D$_2$O, 0.5M	43	8.0×10^{-2}	7.86×10^{-4}	4.49
^{138}La^s	5	0.0902	4.068095	3.557239	0.45	13.194268	LaCl$_3$	D$_2$O/H$_2$O^C	44	1.2×10^{-2}	8.48×10^{-5}	0.485
^{139}La	7/2	99.9098	3.1556770	3.8083318	0.20	14.125606	LaCl$_3$	D$_2$O/H$_2$O^C	44	5.4×10^{-3}	6.05×10^{-2}	3.46×10^2
^{177}Hf	7/2	18.606	0.8997	1.086	3.365	(4.007)^{k,D}	-	-		1.5	2.61×10^{-4}	1.49
^{179}Hf	9/2	13.629	-0.7085	-0.6821	3.793	(2.517)^{k,D}	-	-		1.1	7.46×10^{-5}	0.426
^{181}Ta	7/2	99.988	2.6879	3.2438	3.28	11.989601	KTaCl$_6$	CH$_3$CN, sat.	45	1.5	3.74×10^{-2}	2.14×10^2
(^{185}Re)	5/2	37.40	3.7710	6.1057	2.18	22.524602^E	KReO$_4$	D$_2$O	45	1.5	5.19×10^{-2}	2.96×10^2
^{187}Re^s	5/2	62.60	3.8096	6.1682	2.07	22.751602^E	KReO$_4$	D$_2$O	45	1.4	8.95×10^{-2}	5.12×10^2
^{189}Os^j	3/2	16.1	0.851970	2.10713	0.856	7.765401	OsO$_4$	CCl$_4$, 0.98M	24	0.98	3.93×10^{-4}	2.25
(^{191}Ir)	3/2	37.3	0.1946	0.4812	0.816	(1.718)^{k,D}	-	-		0.89	1.09×10^{-5}	6.20×10^{-2}
^{193}Ir	3/2	62.7	0.2113	0.5227	0.751	(1.871)^{k,D}	-	-		0.75	2.34×10^{-5}	0.134
^{197}Au	3/2	100	0.191271	0.473060	0.547	(1.729)^{k,D}	-	-		0.29	2.77×10^{-5}	0.158
^{201}Hg^j	3/2	13.18	-0.7232483	-1.788769	0.385	6.611400^F	(CH$_3$)$_2$Hg^G	neat		0.20	1.97×10^{-4}	1.13
^{209}Bi^s	9/2	100	4.5444	4.3750	-0.37	16.069288	Bi(NO$_3$)$_2$	D$_2$O^H	18	1.0×10^{-2}	0.144	8.25×10^2

^a Excluding the lanthanides and actinides.

^b Nuclei in parentheses are considered to be not the most favourable of the element concerned for NMR.

^c Data from Mills et al.,[6] pp. 98-104. For the error limits on the natural abundances, see Mills et al.[6]

^d Data derived from the compilation in Mills et al.,[6] pp. 98-104, which lists values of $\mu_{ma}/\mu_N = \gamma \hbar I/\mu_N$. For the error limits, see Mills et al.[6]

^e Data from Mills et al.,[6] pp. 98-104 (taken mostly from Pyykko[32] and Raghavan[33]). It should be noted that reported values of Q may be in error by as much as 20-30%. For the error limits, see Mills et al.[6]

^f Resonance frequency in a magnetic field such that the protons of TMS at infinite dilution (in practice at 1% v/v) in $CDCl_3$ resonate at exactly 100 MHz.

^g M $\equiv$ molarity in mol dm^{-3} (solution); m $\equiv$ molality in mol kg^{-1} (solvent). Results from ref. 18 were initially referenced[7] to a TMS concentration of 4.75 m in $CDCl_3$, but the values are corrected to refer to a dilute (1% v/v) solution of TMS in $CDCl_3$.

^h $\ell = (2I + 3)Q^2/I^2(2I - 1)$ (Harris and Mann[5]).

ⁱ D^p is receptively relative to that of ^1H whereas D^C is relative to ^{13}C. The values are given to three significant figures only.

^j A useful isotope of $I = ½$ exists.

^k Value revised from Encyclopedia[7] (in addition to the conversion from 4.75 m TMS/$CDCl_3$ to 1% v/v TMS/$CDCl_3$ as the standard).

^ℓ 15% by volume of $BF_3.Et_2O$ in $CDCl_3$.

^m Small amount of lock substance ($\leq$ 10% v/v) in neat liquid, except for ^{61}Ni (where ca. 20% v/v C_6D_6 is involved).

ⁿ Deduced from a ratio given in ref. 35.

^o Deduced from data in ref. 36.

^p Deduced from a ratio given in ref. 37.

^q Deduced from a ratio given in ref. 38.

^r External $CDCl_3$ lock, corrected for magnetic susceptibility.

^s Radioactive, with a long half-life.

^t Containing a little C_6D_6 (<10% by volume).

^u With conversion factors applied by Granger.

^v Semi-saturated solution.

^w In CH_3CN/CD_3CN for ^{93}Nb, ^{121}Sb and ^{123}Sb; in CH_3CN with an internal capillary of C_6F_6 (suitable corrections being applied) for ^{75}As.

^x The data in ref. 42 are only accurate to 4 decimal places. The proposal herein is that $\Xi\,(^{83}Kr)$ is defined to the 6 decimal places given.

^y Plus a small quantity of NaOH.

^z Semi-saturated in H_2O/D_2O.

^A Plus 0.5M DNO_3.

^B Calculated from the value for ^{129}Xe via the ^{129}Xe:^{131}Xe frequency ratio, measured by P. Granger on a sample of Xe gas.

^C For the solution conditions, see the reference.

^D Value calculated from literature data on nuclear magnetic moments.

^E The proposal herein is to define to 6 decimal places, but linewidths are generally such that this is unnecessarily accurate.

^F Deduced from the ^{201}Hg:^{199}Hg ratio given in ref. 46.

^G The high toxicity of this compound means its direct use should be strongly discouraged.

^H Saturated in conc. HNO_3, then diluted with an equal volume of D_2O.

Table 3:   The spin properties of lanthanide and actinide nuclei[e]

Isotope	Spin	Natural abundance $C/\%$	Magnetic moment[d] μ/μ_N	Magnetogyric ratio $\gamma/10^7$ rad T^{-1} s^{-1}	Quadrupole moment[d] $Q/$barn	NMR frequency[f] $\Xi/$MHz
^{141}Pr	$\frac{5}{2}$	100	5.0587	8.1907	-5.89×10^{-2}	(30.62)
^{143}Nd	$\frac{7}{2}$	12.18	-1.208	-1.457	-0.63	(5.45)
^{145}Nd	$\frac{7}{2}$	8.30	-0.744	-0.898	-0.33	(3.36)
^{147}Sm[a]	$\frac{7}{2}$	15.0	-0.9239	-1.115	-0.259	(4.17)
^{149}Sm	$\frac{7}{2}$	13.8	-0.7616	-0.9192	7.5×10^{-2}	(3.44)
^{151}Eu	$\frac{5}{2}$	47.8	4.1078	6.6510	0.903	(24.86)
^{153}Eu	$\frac{5}{2}$	52.2	1.8139	2.9369	2.412	(10.98)
^{155}Gd	$\frac{3}{2}$	14.80	-0.33208	-0.82132	1.30	(3.07)
^{157}Gd	$\frac{3}{2}$	15.65	-0.43540	-1.0769	1.36	(4.03)
^{159}Tb	$\frac{3}{2}$	100	2.600	6.431	1.432	(24.04)
^{161}Dy	$\frac{5}{2}$	18.9	-0.5683	-0.9201	2.507	(3.44)
^{163}Dy	$\frac{5}{2}$	24.9	0.7958	1.289	2.648	(4.82)
^{165}Ho	$\frac{7}{2}$	100	4.732	5.710	3.49	(21.34)
^{167}Er	$\frac{7}{2}$	22.95	-0.63935	-0.77157	3.565	(2.88)
^{169}Tm	$\frac{1}{2}$	100	-0.4011	-2.218	-	(8.29)
^{171}Yb	$\frac{1}{2}$	14.3	0.85506	4.7288	-	17.499306[b]
^{173}Yb	$\frac{5}{2}$	16.12	-0.80446	-1.3025	2.80	(4.821)
^{175}Lu	$\frac{7}{2}$	97.41	2.5316	3.0552	3.49	(11.404)
^{176}Lu[a]	7	2.59	3.3880	2.1684	4.92	(8.131)
^{235}U[a]	$\frac{7}{2}$	0.7200	-0.43	-0.52	4.55	1.841400[c]

[a] Long-lived radioactive isotope

[b] Reference: Yb(η-C$_5$Me$_5$)$_2$(THF)$_2$ 0.171M in THF solution[47]

[c] Reference: UF$_6$ neat (+ 10% C$_6$D$_6$).[48] Value revised from Encyclopedia.

[d] For the limits of accuracy, see Ref. 6, pp. 98-104

[e] These nuclides are sufficiently little used that values for linewidth factors and relative receptivities are not listed here. However, for ^{169}Tm, $D^P = 5.70 \times 10^{-4}$ and $D^C = 3.26$, while for ^{171}Yb, $D^P = 7.90 \times 10^{-4}$ and $D^C = 4.51$

[f] Values in brackets are approximate (calculated from the magnetogyric ratios). The values from ^{173}Yb, ^{175}Lu and ^{176}Lu are revised from those in the Encyclopedia.

Table 4 Alternative Secondary References

Isotope	Alternative Secondary References				Recommended Secondary References[a]		
	Reference Compound	Sample Conditions	NMR Frequency Ξ / MHz	Literature	Reference Compound	Sample Conditions	NMR Frequency Ξ / MHz
^{1}H	DSS	Internal	100.000000	4	TMS	Internal[b]	100.000000
^{2}H	DSS	Internal	15.350608	4	TMS	Internal[b]	15.350609
^{13}C	DSS	Internal	25.144953	4	TMS	Internal[b]	25.145020
^{31}P	$(CH_3O)_3PO$	Internal	40.480864	4	H_3PO_4 (85%)	External	40.480737
^{15}N	NH_3 (liquid)	External	10.132912	4	CH_3NO_2	External	10.136784
^{15}N	$(CH_3)_4N^+I^-$	Internal[c]	10.133356	51, 52			
^{14}N	$(CH_3)_4N^+I^-$	Internal[c]	7.223885	51	CH_3NO_2	External	7.226330

[a] See Tables 1 and 2.

[b] Infinite dilution (in practice 1% v/v) in $CDCl_3$.

[c] 0.075 M in DMSO-d_6