14.3.1 Conventions for presentations of NMR spectra (of liquid samples)

(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 the coupling constant is *J*. The coupling between two nuclei separated by *n* chemical bonds can be indicated by the left *super*script *n*, e.g. ^{4}J denotes the coupling constant between two nuclei separated by 4 chemical bonds. Right *sub*scripts may be used to give the symbols of the coupling nuclei, e.g. the coupling constant between the phosphorus nucleus and protons in trimethylphosphite, $P(OCH_3)_3$, would bear the symbol $^{3}J_{PH}$. Alternatively a notation of the type ^{3}J(PH) or $^{3}J(^{11}BH)$ 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, δ=5.00, not δ=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 parenthesis, e.g. δ(C) or $\delta(^{11}B)$. The position of the nucleus in the structural formula could be denoted by an additional number following this symbol for the nucleus, e.g. δ(C-5) or $\delta(^{11}B\text{-}5)$.