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ScienceDirect
Journal of Magnetic Resonance 191 (2008) 340–341
JMR Journal of Magnetic Resonance
www.elsevier.com/locate/jmr

Announcement

Further conventions for NMR shielding and chemical shifts: IUPAC recommendations 2008

NMR has benefitted over the years from standardised notation recommended by the International Union of Pure and Applied Chemistry (IUPAC).[1–8] In particular, questions of referencing of chemical shifts have plagued NMR since its inception and caused numerous problems, so it is natural that IUPAC has been concerned with this area, as well as with the establishment of accurate and accepted numerical values for relevant physical quantities. The initial conventions for chemical shifts appeared[1,2] in the 1970s and were followed by two more recent documents. A joint IUPAC/IUBMB/IUPAB recommendation[7] on structural data in biopolymers included recommendations for reporting chemical shifts for several nuclides.

In 2001, a substantial document[8] updated the recommendations with regard to chemical shifts. It discussed the methods of referencing spectra and recommended that shifts of *all* nuclides be reported on a unified scale relative to the primary standard, which is the proton resonance of tetramethylsilane in dilute solution (volume fraction $\phi<1\%$) in chloroform. Such a scale is given the symbol Ξ (capital Greek xi) and is expressed as a ratio (generally in %) of the resonance frequency in question to that of the primary standard. The 2001 IUPAC document was summarised (together with two key tables of data) in an article in the *Journal of Magnetic Resonance*[9], which permitted wider dissemination of the recommendations.

Several issues that were not explored in Ref. 8 have now been addressed in some detail in a recent document[10] in the IUPAC journal *Pure and Applied Chemistry*.

Overall, there are 17 recommendations, which are not reproduced here, since they can best be appreciated in the context of the discussion in the document, but they can be summarised as follows[10]:

- Two recommendations deal with the *temperature variation* of the ^{1}H shielding in the universal reference, TMS.
- Two recommendations provide guidance on making corrections for the effect of *bulk magnetic susceptibility* (BMS) when the sample and reference are studied under conditions where BMS effects must be taken into account.
- One recommendation deals with specifications for sample *pressure* and sample deoxygenation.
- One recommendation emphasises the central role of the universal reference of TMS *in chloroform* at low concentration.
- One recommendation clarifies the *notation to be used for* Ξ when the frequencies of the heteronuclide X is obtained under various conditions relative to that of the ^{1}H reference in TMS or DSS.
- One recommendation deals with an *updated table of* Ξ *values* for all magnetic nuclides.
- Two recommendations provide guidance for referencing *chemical shifts in solids* under conditions of magic angle spinning, and include relevant data for reporting ^{13}C chemical shifts in solids relative to the universal reference of TMS in chloroform.
- Seven recommendations provide guidance for preferred notation of *chemical shift and shielding tensors*, including shielding anisotropy, asymmetry and related matters.

IUPAC is keen to see its recommendations widely publicised, and it therefore publishes these freely on the web. Thus, the key points are summarised above and reference 10 can be accessed at: http://www.iupac.org/publications/pac/80/1/0059.

 The IUPAC Task Group members responsible for preparation of this document[10] urge NMR spectroscopists to read the document and to adhere to its recommendations.

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doi:10.1016/j.jmr.2008.02.002

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