

chemical shift, δ

in NMR

The fractional variation of the resonance frequency of a nucleus in nuclear magnetic resonance (NMR) spectroscopy in consequence of its magnetic environment. The chemical shift of a nucleus, δ , is expressed as a ratio involving its frequency, ν_{cpd} , relative to that of a standard, ν_{ref} , and defined as:

$$\delta = \frac{\nu_{\text{cpd}} - \nu_{\text{ref}}}{\nu_{\text{ref}}}$$

δ -values are normally expressed in ppm. For ^1H and ^{13}C NMR the reference signal is usually that of tetramethylsilane (TMS), strictly speaking in dilute solution in CDCl_3 . Other references are used in the older literature and for other solvents, such as D_2O . Resonance lines to high frequency from the TMS signal have positive, and resonance lines to low frequency from TMS have negative, δ -values (arising from relative deshielding and shielding respectively). The archaic terms 'downfield' and 'upfield' should no longer be used. For nuclei other than ^1H , chemical shifts are expressed either in the same manner relative to an agreed substance containing the relevant nucleus or relative to the ^1H resonance of TMS as Ξ values, defined in the references below.

Source:

PAC, 2001, 73, 1795 (*NMR nomenclature. Nuclear spin properties and conventions for chemical shifts (IUPAC Recommendations 2001)*) on page 1807

PAC, 2008, 80, 59 (*Further conventions for NMR shielding and chemical shifts (IUPAC Recommendations 2008)*) on page 61

Green Book, 3rd ed., p. 29