

chemical shift (in NMR), δ

The 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 in ppm by its frequency, ν_{cpd} , relative to a standard, ν_{ref} , and defined as:

$$\delta = \frac{\nu_{\text{cpd}} - \nu_{\text{ref}}}{\nu_0} \times 10^6$$

where ν_0 is the operating frequency of the spectrometer. For ^1H and ^{13}C NMR the reference signal is usually that of tetramethylsilane (SiMe_4). Other references are used in the older literature and in other solvents, such as D_2O .

If a resonance signal occurs at lower frequency or higher applied field than an arbitrarily selected reference signal, it is said to be upfield, and if resonance occurs at higher frequency or lower applied field, the signal is downfield. Resonance lines upfield from SiMe_4 have positive, and resonance lines downfield from SiMe_4 have negative, δ -values.

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