chemical shift, $\delta$

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, $\delta$, is expressed as a ratio involving its frequency, $\nu_{\text{cpd}}$, relative to that of a standard, $\nu_{\text{ref}}$, and defined as:

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

$\delta$-values are normally expressed in ppm. For $^1\text{H}$ and $^{13}\text{C}$ 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$_2$O. Resonance lines to high frequency from the TMS signal have positive, and resonance lines to low frequency from TMS have negative, $\delta$-values (arising from relative deshielding and shielding respectively). The archaic terms 'downfield' and 'upfield' should no longer be used. For nuclei other than $^1\text{H}$, chemical shifts are expressed either in the same manner relative to an agreed substance containing the relevant nucleus or relative to the $^1\text{H}$ resonance of TMS as $\varepsilon$ 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