

isotopic fractionation factor

The ratio

$$\frac{(x_1/x_2)_A}{(x_1/x_2)_B},$$

where x is the abundance, expressed as the atom fraction of the isotope distinguished by the subscript numeral, when the two isotopes are equilibrated between two different chemical species A and B (or between specific sites **A** and **B** in the same or different chemical species). The term is most commonly met in connection with deuterium solvent isotope effects, when the fractionation factor Φ expresses the ratio:

$$\Phi = \frac{(x_D/x_H)_{\text{solute}}}{(x_D/x_H)_{\text{solvent}}}$$

for the exchangeable hydrogen atoms in the chemical species (or sites) concerned. The concept is also applicable to transition states.

Source:

PAC, 1994, 66, 1077 (*Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994)*) on page 1115