**isotopic fractionation factor**

The ratio

\[
\frac{(x_i/x_j)_A}{(x_i/x_j)_B},
\]

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 \( \Phi \) 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