Summary of Nomenclature and Formulas for use with Stable Isotopes

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Isotopic Abundance

Note that all measures of isotopic abundance and fractionation are dimensionless and have no units. They are often expressed with the addition of the modifier ‰ (permil, or parts per thousand), by analogy to % (percent, parts per hundred). Both % and ‰ are dimensionless, and are not units!

Isotope ratio: $^{13}R = [^{13}\mathrm{C}]/[^{12}\mathrm{C}]$ $\quad$ $^{2}R = [^{2}\mathrm{H}]/[^{1}\mathrm{H}]$ $\quad$ etc. for each isotope system

Fractional abundance: $^{15}F = \dfrac{[^{15}\mathrm{N}]}{[^{15}\mathrm{N}]+[^{14}\mathrm{N}]}$

Useful conversions: $^{13}R = \dfrac{^{13}F}{1-{}^{13}F}$ $\quad$ $^{18}F = \dfrac{^{18}R}{1+{}^{18}R}$

Delta value: $\delta^{13}C_{PDB} = \dfrac{^{13}R_{samp} - {}^{13}R_{PDB}}{^{13}R_{PDB}}$ $\quad$ $\delta^{2}\mathrm{H}_{SMOW} = \dfrac{^{2}R_{samp}}{^{2}R_{SMOW}} - 1$ $\quad$ (usually expressed as ‰)

Isotopic Mass Balance

$$^{13}F_{tot} = X_1\,{}^{13}F_1 + X_2\,{}^{13}F_2 + etc\ldots$$

(exact; 1,2,… are components of the mixture; *X* is mole fraction of C in each component; *F* is fractional abundance of ^{13}C in each component)

$$n_{tot}\delta^{18}O_{tot} = n_1\delta^{18}O_1 + n_2\delta^{18}O_2 + etc\ldots$$

(approximate; *n* can be any conserved measure of amount, *e.g.* moles, atoms, grams, liters, etc.; δ can be expressed as ‰)

Isotopic Fractionation

The most frequent point of confusion here is failure to specify the order of comparison (A/B versus B/A).

Fractionation factor: $^{18}\alpha_{A/B} = \dfrac{^{18}R_A}{^{18}R_B} = \dfrac{\delta^{18}O_A + 1}{\delta^{18}O_B + 1}$ $\quad$ (varies around 1.0; δnot as‰)

$$^{18}\alpha_{A/B} = \frac{\delta^{18}O_A + 1000}{\delta^{18}O_B + 1000}$$

(δexpressed as ‰; useful, but strictly incorrect)

Enrichment factor: $^{13}\varepsilon_{A/B} = {}^{13}\alpha_{A/B} - 1$ $\quad$ (varies around 0; usually expressed as ‰)

More useful forms: $\delta^{2}\mathrm{H}_A = {}^{2}\alpha_{A/B}\delta^{2}\mathrm{H}_B + \left({}^{2}\alpha_{A/B} - 1\right)$ $\quad$ (exact; δ without ‰ units)

$\delta D_A = \delta D_B + \varepsilon_{A/B}$ $\quad$ (approximate; δ and ε both as ‰)

Rayleigh Distillation

Fractional distillation of a product from a closed system reservoir (A→B).
General equation is $R = R_0 f^{\alpha-1}$ (but not a practical form for common use).

Reactant (A): $\delta_{Af} = \varepsilon_{A/B} \ln(1 - f_B) + \delta_{Ao}$ (approximate; δ and ε both as ‰)

δ_{Af}	isotopic composition of A when reaction has yielded f_B fraction of B
$\varepsilon_{A/B}$	isotopic enrichment factor for reaction of A→B
f_B	fractional yield of product B (f=0 at start, =1 at completion)
δ_{Ao}	Isotopic composition of A at beginning of reaction

Instantaneous Product (B'): $\delta_{B'f} = \varepsilon_{A/B} \ln(1 - f_B) + \delta_{Ao} + \varepsilon_{A/B}$ (approximate; δ and ε both as ‰)

$\delta_{B'f}$	Isotopic composition of B forming instantaneously when reaction has reached f_B

Pooled Product (B): $\delta_{Bf} = \delta_{Ao} - \frac{\varepsilon_{A/B}(1 - f_B)\ln(1 - f_B)}{f_B}$ (approximate; δ and ε both as ‰)

$\delta_{B'f}$	Isotopic composition of pooled B (sum of all product) formed by the reaction up to the point f_B