

Guidelines for Reporting Certain Isotopic Values Relevant to Ground-Water Studies

by Tyler B. Coplen, U.S. Geological Survey, Reston, VA 22092

As Secretary of the Commission on Atomic Weights and Isotopic Abundances of the International Union of Pure and Applied Chemistry (IUPAC), I would like to point out recent recommendations regarding the reporting of certain isotopic values relevant to ground-water studies. These recommendations stem from the observation that isotopic values of many elements are not presently comparable between laboratories. For example, the measurement of $\delta^{13}\text{C}$ of atmospheric CO_2 is normally reported to 0.01 per mil ($^0_{/00}$) relative to PDB (Peedee belemnite). Yet the difference between the reference material NBS 19 calcite (+1.95 $^0_{/00}$) relative to the reference material PDB at different laboratories varies by as much as 0.38 $^0_{/00}$. This situation occurred because as the supply of PDB became exhausted, different laboratories used different materials for calibration. The following are the new guidelines.

Guidelines

Hydrogen

Water. Relative $^2\text{H}/^1\text{H}$ values ($\delta^2\text{H}$) of water should be expressed in $^0_{/00}$ relative to VSMOW water ($0^0_{/00}$) on a scale normalized such that the $\delta^2\text{H}$ of SLAP water is $-428^0_{/00}$ exactly and so stated in author's report.

Other substances. Relative $^2\text{H}/^1\text{H}$ values ($\delta^2\text{H}$) of other substances should be expressed in $^0_{/00}$ relative to VSMOW water ($0^0_{/00}$) on a scale normalized such that the $\delta^2\text{H}$ of SLAP water is $-428^0_{/00}$ exactly and so stated in author's report. It is recommended that the author's measured $\delta^2\text{H}$ of NBS 22 oil, NBS 30 biotite, or other internationally distributed reference material be reported, as appropriate to the analytical method.

Carbon

Carbonate. Relative $^{13}\text{C}/^{12}\text{C}$ values ($\delta^{13}\text{C}$) of carbonate should be expressed in $^0_{/00}$ relative to VPDB by assigning a value of +1.95 $^0_{/00}$ exactly to NBS 19 calcite.

Other substances. Relative $^{13}\text{C}/^{12}\text{C}$ values ($\delta^{13}\text{C}$) of other substances should be expressed in $^0_{/00}$ relative to VPDB by assigning a value of +1.95 $^0_{/00}$ exactly to NBS 19 calcite. It is recommended that the author's measured $\delta^{13}\text{C}$ of NBS 22 oil, USGS24 graphite, or other internationally distributed reference material be reported, as appropriate to the analytical method.

Oxygen

Water. Relative $^{18}\text{O}/^{16}\text{O}$ values ($\delta^{18}\text{O}$) of water should be expressed in $^0_{/00}$ relative to VSMOW water ($0^0_{/00}$) on a scale normalized such that the $\delta^{18}\text{O}$ of SLAP water is $-55.5^0_{/00}$ exactly and so stated in author's report.

Carbonate. Relative $^{18}\text{O}/^{16}\text{O}$ values ($\delta^{18}\text{O}$) of carbonate should be expressed in $^0_{/00}$ (on a scale normalized such that the $\delta^{18}\text{O}$ of SLAP water is $-55.5^0_{/00}$ exactly relative to VSMOW water, and so stated in author's report) either

1. relative to VPDB on a scale such that the $\delta^{18}\text{O}$ of NBS 19 calcite is $-2.2^0_{/00}$ exactly, stating the value of the oxygen isotopic fractionation factor used to calculate the $\delta^{18}\text{O}$ of the carbonate sample and NBS 19 if they are not identical, or

2. relative to VSMOW water ($0^0_{/00}$), stating the values of all isotopic fractionation factors upon which the $\delta^{18}\text{O}$ measurement depends.

If $\delta^{18}\text{O}$ values cannot be reported on a normalized scale (perhaps because of the inability to measure water samples), then the author's measured $\delta^{18}\text{O}$ of NBS 18 carbonatite or other internationally distributed reference material should be reported, as appropriate.

Other substances (oxygen gas, sulfate, silicate, phosphate, etc.). Relative $^{18}\text{O}/^{16}\text{O}$ values ($\delta^{18}\text{O}$) of all other oxygen-bearing substances should be expressed in $^0_{/00}$ relative to VSMOW water ($0^0_{/00}$) on a scale normalized such that the $\delta^{18}\text{O}$ of SLAP water is $-55.5^0_{/00}$ exactly and so stated in author's report, stating either

1. the values of all isotopic fractionation factors upon which a $\delta^{18}\text{O}$ value depends, or

2. the author's measured $\delta^{18}\text{O}$ of NBS 28 quartz, NBS 30 biotite, NBS 127 barium sulfate, or other internationally distributed reference material.

If $\delta^{18}\text{O}$ values cannot be reported on a normalized scale (perhaps because of the inability to measure water samples), then the author's measured $\delta^{18}\text{O}$ of NBS 28 quartz, or other internationally distributed reference material should be reported, as appropriate to the analytical method.

Editor's Note — These are reasonable recommendations and GROUND WATER will inform and encourage all authors reporting isotopic values to follow these conventions.