

United States Geological Survey

Reston Stable Isotope Laboratory

Report of Stable Isotopic Composition

Reference Material W-67400-S

Water

(Hydrogen and Oxygen Isotopes in Water)

This reference material (RM) is intended for daily normalization of stable hydrogen ($\delta^2\text{H}$) and oxygen ($\delta^{18}\text{O}$) measurements of unknown waters with an isotope-ratio mass spectrometer or a laser absorption spectrometer. A unit of this RM consists of 8 autoclaved glass ampoules of reference water. Each glass ampoule contains 7 mL of water.

Recommended Values: Stable hydrogen and oxygen isotopic compositions are expressed herein as delta values [1] relative to VSMOW (Standard Mean Ocean Water) on scales normalized such that the $\delta^2\text{H}$ and $\delta^{18}\text{O}$ values of SLAP (Standard Light Antarctic Precipitation) are -428‰ and -55.5‰ , respectively [2,3]. Each stable isotopic composition is given as a reference isotope-delta value with an estimated expanded uncertainty ($U = 2u_c$) about the reference value that provides an interval that has about a 95-percent probability of encompassing the true value.

Stable hydrogen isotopic composition: $\delta^2\text{H}_{\text{VSMOW-SLAP}} = +1.2 \pm 1.0\text{‰}$

Stable oxygen isotopic composition: $\delta^{18}\text{O}_{\text{VSMOW-SLAP}} = -1.97 \pm 0.08\text{‰}$

Technical coordination for this RM was provided by Arndt Schimmelmann of Indiana University and Haiping Qi of the U.S. Geological Survey Reston Stable Isotope Laboratory (RSIL).

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Expiration of Reference Value: The reference values for the isotopic composition of W-67400-S are valid until December 31, 2039, provided the RM is handled in accordance with the instructions given in this Report of Stable Isotopic Composition (see “Instructions for Use”). The reference value is nullified if the glass ampoule containing the RM is inadvertently broken.

Source of the RM: Tap water was obtained from Puerto Rico and homogenized. About 7 mL was loaded into each glass ampoule and sealed with a torch. Each ampoule was inverted and autoclaved at about 120 °C for a minimum of 20 minutes to terminate biological activity. Each ampoule was weighed to identify and eliminate any leaking ampoules.

Stability: W-67400-S is stable at normal room temperatures. The reference values in this Report of Investigation apply only to freshly opened ampoules.

Instructions for Use: This RM is intended for daily calibration of instrumentation and for calibrating unknown waters by interspersing aliquots of the RM among water sample unknowns. The unused fraction of this RM should be discarded after opening an ampoule due to the strong possibility of evaporative losses causing significant isotopic fractionation. It is envisioned that laboratory personnel will open an aliquot of W-67400-S daily and they analyze their unknown waters. Laboratory personnel can use two different water RMs (others include USGS46 and USGS47) and then normalize isotopic measurement results to the VSMOW-SLAP scale [4]. Many users employ LIMS for Light Stable Isotopes for their normalization [5].

Reporting of Stable-isotope-delta Values: The following recommendations are provided for reporting stable hydrogen and oxygen isotope-delta values [3]. It is recommended that:

- The $\delta^2\text{H}$ values of all hydrogen-bearing substances be expressed relative to VSMOW-SLAP on a scale where $\delta^2\text{H}_{\text{SLAP}} = -428 \text{‰}$ exactly or $\delta^2\text{H}_{\text{SLAP2}} = -427.5 \text{‰}$ [6].
- The $\delta^{18}\text{O}$ values of all oxygen-bearing substances be expressed relative to VSMOW-SLAP or relative to Vienna Peedee belemnite (VPDB; for carbonates) on a scale such that the $\delta^{18}\text{O}$ of SLAP = -55.5‰ relative to VSMOW, and for carbonates, such that $\delta^{18}\text{O}$ of NBS 19 calcium carbonate = -2.2‰ .
- Authors report δ values of international distributed (secondary) isotopic reference materials as though they had been interspersed among and used for normalization of unknowns, as appropriate, for the measurement method. In this manner, measurement results can be adjusted in the future as analytical methods improve and consensus values of internationally distributed isotopic reference materials change.
- Reporting of δ values relative to SMOW and PDB (Peedee belemnite) be discontinued [7].

REFERENCES

- [1] Coplen, T. B., 2011, Guidelines and recommended terms for expression of stable-isotope-ratio and gas-ratio measurement results: Rapid Communications in Mass Spectrometry, v. 25, 2538–2560, (last accessed August 2012 at <http://onlinelibrary.wiley.com/doi/10.1002/rcm.5129/abstract>).
- [2] Gonfiantini, R., 1978, Standards for stable isotope measurements in natural compounds: Nature, v. 271, p. 534–536.

- [3] Coplen, T. B., 1994, Reporting of stable hydrogen, carbon, and oxygen isotopic abundances: Pure and Applied Chemistry, v. 66, p. 273–276.
- [4] Coplen, T. B., 1988, Normalization of oxygen and hydrogen isotope data: Chemical Geology (Isotope Geosciences Section), v. 72, p. 293–297.
- [5] LIMS for Light Stable Isotopes, <http://isotopes.usgs.gov/research/topics/lims.html> .
- [6] International Atomic Energy Agency (IAEA), Reference Sheet for International Measurement Standards, http://nucleus.iaea.org/rpst/Documents/VSMOW2_SLAP2.pdf (last accessed August 2012).
- [7] Coplen, T. B., 1995, Discontinuance of SMOW and PDB: Nature, v. 375, 285.