United States Geological Survey

Reston Stable Isotope Laboratory

Report of Stable Isotopic Composition

Reference Material USGS76

(Hydrogen and Carbon Isotopes in Methylheptadecanoate, C_{17} Fatty Acid Methyl Ester, C_{17} FAME)

This reference material (RM) is intended for normalization of stable hydrogen (δ^2H) and carbon (δ^{13}C) measurements of unknown methylheptadecanoate ($C_{17}H_{33}OOCH_3$) and similarly-behaving hydrogen- and carbon-bearing substances. A unit consists of 50 µL sealed in a glass tube. There is no limit on distribution. This RM was prepared by A. Schimmelmann (Indiana University, Bloomington, Indiana).

Recommended values: Stable hydrogen isotopic compositions are expressed herein as delta values [1] relative to VSMOW (Vienna Standard Mean Ocean Water) on a scale normalized such that the δ^2H value of SLAP (Standard Light Antarctic Precipitation) is –428 ‰ [2,3]. Stable carbon isotopic compositions are expressed herein as delta values relative to VPDB (Vienna Peedee belemnite) on a scale normalized such that the δ^{13}C values of NBS 19 calcium carbonate and LSVEC lithium carbonate are +1.95 ‰ and –46.6 ‰, respectively [4]. The stable hydrogen- and carbon-isotope delta values of USGS76 C_{17} FAME with combined standard uncertainties are:

Reference	$\delta^2H_{VSMOW\text{-}SLAP}$	$\delta^{13}C_{VPDB\text{-}LSVEC}$	Data source
USGS76	–210.8 ± 0.9 ‰	–31.36 ± 0.04 ‰	[5]

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 value for the isotopic composition of USGS76 is valid until December 31, 2036, provided the RM is handled in accordance with the instructions given in this Report of Stable Isotopic Composition. A reference value is nullified if the RM is damaged, contaminated, or otherwise modified.

Source of the RM: The following description is taken from Schimmelmann and others [5]. This RM is a custom-synthesized C_{17} fatty acid methyl ester ($C_{18}H_{36}O_2$, CAS # 1731-92-6), which was obtained from Sigma-Aldrich with a purity of ≥99 %. The supply of 200 g was melted, subdivided as a homogeneous liquid into glass ampoules, and flame-sealed under argon. Users will receive an aliquot of this RM of 50 µL sealed in a glass tube for δ^2H and δ^{13}C normalization.

Maintenance of RM Report of Isotopic Composition: The U.S. Geological Survey RSIL will monitor these RMs and will notify the purchaser if substantive technical changes occur that affect their isotopic compositions.

Distribution and Stability: A distribution unit is available in amounts of 50 µL sealed in glass tubes. USGS76 is stable at room temperature when stored dry. It is recommended to store USGS76 in a refrigerator or freezer in the dark. Let the glass container warm to room temperature before opening in order to avoid condensation of moisture.

Reporting of Stable-isotope-delta values: The following recommendations are provided for reporting stable hydrogen and carbon isotope-delta values. It is recommended that:

- The δ^2H values of all hydrogen-bearing substances be expressed relative to VSMOW-SLAP on a scale where the δ^2H of SLAP = –428 ‰ exactly [3].
- The δ^{13}C values of all carbon-bearing substances be expressed relative to VPDB-LSVEC on a scale such that the δ^{13}C values of NBS 19 calcium carbonate and LSVEC lithium carbonate are +1.95 ‰ and –46.6 ‰, respectively [4], even though LSVEC is no longer recommended as a RM for δ^{13}C measurement [6].
- Authors report delta 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 delta 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(17), p. 2538–2560. https://doi.org/10.1002/rcm.5129

[2] Gonfiantini, R., 1978, Standards for stable isotope measurements in natural compounds: Nature, v. 271, p. 534–536. https://doi.org/10.1038/271534a0

[3] Coplen, T. B., 1994, Reporting of stable hydrogen, carbon, and oxygen isotopic abundances: Pure and Applied Chemistry, v. 66(2), p. 273–276. https://doi.org/10.1351/pac199466020273

[4] Coplen, T. B., Brand, W. A., Gehre, M., Gröning, M., Meijer, H. A. J., Toman, B., and Verkouteren, R. M., 2006, New guidelines for $\delta^{13}C$ measurements: Analytical Chemistry, v. 78(7), p. 2439–2441. https://doi.org/10.1021/ac052027c

[5] Schimmelmann, A., Qi, H., Coplen, T. B., Brand, W. A., Fong, J., Meier-Augenstein, W., Kemp, H. F., Toman, B., Ackermann, A., Assonov, S., Aerts-Bijma, A. T., Brejcha, R., Chikaraishi, Y., Darwish, T., Elsner, M., Gehre, M., Geilmann, H., Gröning, M., Hélie, J-F., Herrero-Martín, S., Meijer, H. A. J., Sauer, P. E., Sessions, A. L., and Werner, R. A., 2016, New organic reference materials for hydrogen, carbon, and nitrogen stable isotope-ratio measurements: caffeines, *n*-alkanes, fatty acid methyl esters, glycines, L-valines, polyethylenes, and oils, Analytical Chemistry, v. 88(8), p. 4294–4302. https://doi.org/10.1021/acs.analchem.5b04392

[6] Assonov, S., 2018, Summary and recommendations from the International Atomic Energy Agency Technical Meeting on the development of stable isotope reference products (21-25 November 2016): Rapid Communication in Mass Spectrometry, v. 32(10), p. 827−830. https://doi.org/10.1002/rcm.8102

[7] Coplen, T. B., 1995, Discontinuance of SMOW and PDB: Nature, v. 375, p. 285. https://doi.org/10.1038/375285a0