NRC Publications Archive
Archives des publications du CNRC

Minimum requirements for publishing hydrogen, carbon, nitrogen, oxygen and sulfur stable-isotope delta results (IUPAC Technical Report)
Skrzypek, Grzegorz; Allison, Colin E.; Böhlke, John K.; Bontempo, Luana; Brewer, Paul; Camin, Federica; Carter, James F.; Chartrand, Michelle M. G.; Coplen, Tyler B.; Gröning, Manfred; Hélie, Jean-François; Esquivel-Hernández, Germain; Kraft, Rebecca A.; Magdas, Dana A.; Mann, Jacqueline L.; Meija, Juris; Meijer, Harro A. J.; Moossen, Heiko; Ogrinc, Nives; Perini, Matteo; Possolo, Antonio; Rogers, Karyne M.; Schimmelmann, Arndt; Shemesh, Aldo; Soto, David X.; Thomas, Freddy; Wielgosz, Robert; Winchester, Michael R.; Yan, Zhao; Dunn, Philip J. H.

This publication could be one of several versions: author's original, accepted manuscript or the publisher's version. / La version de cette publication peut être l'une des suivantes : la version prépublication de l'auteur, la version acceptée du manuscrit ou la version de l'éditeur.
For the publisher's version, please access the DOI link below./ Pour consulter la version de l'éditeur, utilisez le lien DOI ci-dessous.

Publisher's version / Version de l'éditeur:
https://doi.org/10.1515/pac-2021-1108
Pure and Applied Chemistry, 94, 11-12, pp. 1249-1255, 2022-12-16

NRC Publications Archive Record / Notice des Archives des publications du CNRC :
https://nrc-publications.canada.ca/eng/view/object/?id=f6696506-2a30-4734-bc9b-8ad029eafb42
https://publications-cnrc.canada.ca/fra/voir/objet/?id=f6696506-2a30-4734-bc9b-8ad029eafb42

Access and use of this website and the material on it are subject to the Terms and Conditions set forth at
https://nrc-publications.canada.ca/eng/copyright
READ THESE TERMS AND CONDITIONS CAREFULLY BEFORE USING THIS WEBSITE.

L'accès à ce site Web et l'utilisation de son contenu sont assujettis aux conditions présentées dans le site
https://publications-cnrc.canada.ca/fra/droits
LISEZ CES CONDITIONS ATTENTIVEMENT AVANT D'UTILISER CE SITE WEB.

Questions? Contact the NRC Publications Archive team at PublicationsArchive-ArchivesPublications@nrc-cnrc.gc.ca. If you wish to email the authors directly, please see the first page of the publication for their contact information.

Vous avez des questions? Nous pouvons vous aider. Pour communiquer directement avec un auteur, consultez la première page de la revue dans laquelle son article a été publié afin de trouver ses coordonnées. Si vous n'arrivez pas à les repérer, communiquez avec nous à PublicationsArchive-ArchivesPublications@nrc-cnrc.gc.ca.

National Research Council Canada
Conseil national de recherches Canada

DE GRUYTER Pure Appl. Chem. 2022; 94(11–12): 1249–1255

IUPAC Technical Report

Grzegorz Skrzypek*, Colin E. Allison, John K. Böhlke, Luana Bontempo, Paul Brewer, Federica Camin, James F. Carter, Michelle M. G. Chartrand, Tyler B. Coplen, Manfred Gröning, Jean-François Hélie, Germain Esquivel-Hernández, Rebecca A. Kraft, Dana A. Magdas, Jacqueline L. Mann, Juris Meija, Harro A. J. Meijer, Heiko Moossen, Nives Ogrinc, Matteo Perini, Antonio Possolo, Karyne M. Rogers, Arndt Schimmelmann, Aldo Shemesh, David X. Soto, Freddy Thomas, Robert Wielgosz, Michael R. Winchester, Zhao Yan and Philip J. H. Dunn*

Minimum requirements for publishing hydrogen, carbon, nitrogen, oxygen and sulfur stable-isotope delta results (IUPAC Technical Report)

https://doi.org/10.1515/pac-2021-1108
Received November 24, 2021; accepted October 20, 2022

Article note: Sponsoring bodies: IUPAC Inorganic Chemistry Division; Commission on Isotopic Abundances and Atomic Weights.

***Corresponding authors: Grzegorz Skrzypek**, West Australian Biogeochemistry Centre, School of Biological Sciences, The University of Western Australia, Crawley, WA, Australia, e-mail: Grzegorz.Skrzypek@uwa.edu.au. https://orcid.org/0000-0002-5686-2393 (G. Skrzypek); and **Philip J. H. Dunn**, National Measurement Laboratory, LGC, Teddington, UK, e-mail: philip.dunn@lgcgroup.com. https://orcid.org/0000-0002-3848-6187
Colin E. Allison, Commonwealth Scientific and Industrial Research Organisation, Oceans and Atmosphere, Aspendale, VIC, Australia
John K. Böhlke and Tyler B. Coplen, United States Geological Survey, Reston, VA, USA
Luana Bontempo and Matteo Perini, Fondazione Edmund Mach, San Michele all'Adige, Italy
Paul Brewer, National Physical Laboratory, Teddington, UK
Federica Camin, Manfred Gröning and David X. Soto, International Atomic Energy Agency, Vienna, Austria
James F. Carter, Queensland Health Forensic and Scientific Services, Archerfield, Australia
Michelle M. G. Chartrand and Juris Meija, National Research Council Canada, Ottawa, ON, Canada. https://orcid.org/0000-0002-3349-5535 (J. Meija)
Jean-François Hélie, Geotop & Département des sciences de la Terre et de l'atmosphère, Université du Québec à Montréal, Montreal, Canada
Germain Esquivel-Hernández, Stable Isotopes Research Group and Water Resources Management Laboratory, Universidad Nacional Costa Rica, Heredia, Costa Rica. https://orcid.org/0000-0002-6890-6509
Rebecca A. Kraft, Jacqueline L. Mann, Antonio Possolo and Michael R. Winchester, National Institute of Standards and Technology, United States Department of Commerce, Gaithersburg, MD, USA
Dana A. Magdas, National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj-Napoca, Romania
Harro A. J. Meijer, Centre for Isotope Research, University of Groningen, Groningen, Netherlands
Heiko Moossen, Max Planck Institute for Biogeochemistry, Jena, Germany
Nives Ogrinc, Department of Environmental Sciences, J. Stefan Institute, Ljubljana, Slovenia
Karyne M. Rogers, National Isotope Centre, GNS Science, Lower Hutt, New Zealand
Arndt Schimmelmann, Department of Earth and Atmospheric Sciences, Indiana University, Bloomington, IN, USA
Aldo Shemesh, Department of Earth and Planetary Sciences, The Weizmann Institute of Science, Rehovot, Israel
Freddy Thomas, Eurofins Analytics France, Nantes, France
Robert Wielgosz, Bureau International des Poids et Mesures, Sevres Cedex, France
Zhao Yan, Institute of Quality Standard and Testing Technology for Agri-Products, Chinese Academy of Agriculture Sciences, Beijing, China

Abstract: Stable hydrogen, carbon, nitrogen, oxygen and sulfur (HCNOS) isotope compositions expressed as isotope-delta values are typically reported relative to international standards such as Vienna Standard Mean Ocean Water (VSMOW), Vienna Peedee belemnite (VPDB) or Vienna Cañon Diablo Troilite (VCDT). These international standards are chosen by convention and the calibration methods used to realise them in practice undergo occasional changes. To ensure longevity and reusability of published data, a comprehensive description of (1) analytical procedure, (2) traceability, (3) data processing, and (4) uncertainty evaluation is required. Following earlier International Union of Pure and Applied Chemistry documents on terminology and notations, this paper proposes minimum requirements for publishing HCNOS stable-isotope delta results. Each of the requirements are presented with illustrative examples.

Keywords: Isotope delta; isotope ratio; publication requirements; stable isotopes.

CONTENTS

1 Introduction

There has been a large increase of research using and reporting stable-isotope data from an increasing variety of fields including, ecology, marine sciences, earth and geosciences, forensic science, hydrology, medicine, food, and climate science. Stable-isotope data for the light elements hydrogen, carbon, nitrogen, oxygen and sulfur are commonly reported as isotope-delta values [1]. The isotope-delta of an element E in a substance P is calculated from the isotope ratio $R(^{i/j}\mathrm{E}, \mathrm{P}) = N(^{i}\mathrm{E}, \mathrm{P})/N(^{j}\mathrm{E}, \mathrm{P})$, where $N(^{i}\mathrm{E}, \mathrm{P})$ and $N(^{j}\mathrm{E}, \mathrm{P})$ are the numbers of atoms of each isotope, and $^{i}\mathrm{E}$ denotes the higher (superscript i) and $^{j}\mathrm{E}$ the lower (superscript j) atomic mass numbers of the isotopes of the element E in substance P. The isotope delta (symbol δ), of an element E in a material P is defined by the isotope ratios of an element E in substance P and in an international standard (Std) [2]:

$$\delta_{\mathrm{Std}}(^{i/j}\mathrm{E}, \mathrm{P}) = \frac{R(^{i/j}\mathrm{E}, \mathrm{P})}{R(^{i/j}\mathrm{E}, \mathrm{Std})} - 1$$

The international standards are chosen by convention with isotope-delta equal to zero exactly (they may be referred to as "zero points"). They can be specific reference materials (RMs) such as Vienna Standard Mean Ocean Water (VSMOW) for hydrogen- and oxygen-isotope delta, isotopically-homogenous reservoirs of the element such as atmospheric nitrogen for nitrogen-isotope delta, or hypothetical materials defined by a specific RM such as Vienna Peedee belemnite (VPDB) for carbon-isotope delta. RMs with isotope-delta values calibrated to the international standards are the source of traceability for routine measurements of isotope-delta.

The limited types and availability of internationally recognised RMs for isotope-delta measurements have led laboratories to produce their own in-house RMs (e.g., [3, 4]). Concurrently, there have been numerous changes to the values assigned to the international RMs [2], reports and guidelines on the best measurement practices (e.g., [5–7]) or conventions (e.g., [8, 9]) and even to the identities of the international standards themselves (e.g., [10]). As a result, combining stable-isotope data from various sources and over time can be challenging, even if all required information is present (e.g., [11]) but impossible when isotope-delta values are not accompanied by clear description of the traceability and calibration processes used (e.g., [12]).

As light-element (HCNOS) stable-isotope ratio data rely entirely on RMs for traceability to international standards that themselves may undergo occasional changes [2], it is essential that metadata associated with isotope-delta values are reported to ensure longevity and reusability of the published data. Therefore, a comprehensive description is required of isotope-delta values to be reported in peer-reviewed publications. Building on the FAIR (Findability, Accessibility, Interoperability, and Reusability) Data Principles laid out by Wilkinson et al. [13] and previous efforts to standardise publication guidelines for reporting of isotope-delta values (e.g., [14–18]), we present minimum requirements for reporting (1) analytical procedure, (2) traceability, (3) data processing, and (4) uncertainty evaluation. These minimum requirements have been prepared by experts participating in a virtual IAEA Technical Meeting on the Development of International Atomic Energy Agency Stable Isotope Reference Materials and Related Products (EVT1701991, 30 August–3 September 2021). The examples given below are for illustration purposes only and will vary with analytical procedure and analyte and therefore do not cover all possible circumstances.

1.1 Analytical procedure

The following information should be provided directly or by citation of previous publications: details of sample preparation procedure(s) (e.g., washing, drying, grinding, filtering, weighing, extraction, equilibration, precipitation, digestion) together with type(s) and model(s) of instrument(s) and peripheral device(s) including critical operational parameters of the measurement (e.g., gas flows, temperatures) and analytical materials (e.g., tin cups, reactor oxides, copper, water trap reagents, acids) must be reported. For stable hydrogen- and oxygen-isotope analyses of samples containing exchangeable moieties, information on operational procedures that can affect the exchangeability should be described (e.g., solvent cleaning, lipid removal, water equilibration, residual moisture drying, etc.). The frequency of quality control and RM measurements within each group of analyses also should be stated. Any software packages and their versions used to control instrumentation or to perform subsequent calculations should be specified.

> **For example:** Samples of plant leaves were washed with deionized water (*specification*), dried in the laboratory oven (*time and temperature*), and ground in a ball mill (*grain size, manufacturer*). Aliquots of X mg were placed in tin capsules (*size, type, brand*) and analysed for carbon isotope composition, using a continuous flow system consisting of a mass spectrometer connected to an elemental analyser (*type, model and brand of mass spectrometer and peripheral devices*). In the elemental analyser, each sample was combusted quantitatively at a temperature of (*temperature*) and then NO_x gases were reduced (*temperature*) to produce pure N_2. The gases produced (predominately CO_2, N_2 and H_2O) were carried through water traps (*reagent, brand*) and GC column in a stream of helium (*flow rate, gas grade and brand*), and then the CO_2 was introduced into the isotope ratio mass spectrometer via an interface (type, model, brand) for stable-isotope analysis. The instrumentation was controlled, and measurement data obtained using (*software package, version, brand*).

1.2 Metrological traceability

Isotope-delta values for hydrogen, carbon, nitrogen, oxygen and sulfur are traceable to international standards [1, 19]. Traceability of isotope-delta values is assured by calibration of measurement results using RMs that are traceable to the international standards (a process often referred to as normalisation). Publications must list the identity of the RMs used to normalise the isotope delta results, as well as the values and uncertainties assigned to these RMs. The identity of the international standard (e.g., material with isotope-delta equal to zero) should also be stated.

> **For example:** Measured nitrogen isotope-delta values were calibrated with respect to atmospheric nitrogen (Air-N_2) using *RMs (names, their values associated standard or expanded uncertainties)*. Each RM was measured in duplicate at the start and end of each daily group of analyses of samples (*number of repeated measurements on each sample*).

If in-house RMs were used, additional information about those RMs, including how they were calibrated, must be provided [4]. Without this information, traceability to the international standards might be compromised. Where experimental analysis used isotopic abundances of the stable isotopes (such as when applying isotopically enriched materials, or when using, e.g., Nuclear Magnetic Resonance, or Inductively Coupled Plasma Mass Spectrometry), it must be made clear how these abundances were obtained [20].

1.3 Data processing

Publications should disclose how stable-isotope measurement results were normalised [7] by either providing the measurement model equation or describing the basic principles used (e.g., linear ordinary least squares regression, quadratic errors-in-variables regression or other). All other corrections applied to instrumental readings should also be stated. These include corrections for the blank, memory effects, drift, linearity/mass effects, isobaric and other interferences. Results of analyses of samples with exchangeable hydrogen or oxygen, should be accompanied by details on water equilibration with non-exchangeable RMs or comparative equilibration with matrix matched RMs [21–23].

> **For example:** Care was taken to ensure that the measured aliquots of RMs and samples yielded a similar amount of gas; minor differences were adjusted using a linearity correction based on the signal recorded for measured isotopomers (*range of values*). A linear drift correction was applied using the results of the quality control (QC) material run regularly throughout each sample group of analyses in duplicate after measurement of every *X* samples. Isotope-delta values for the CO_2 gas derived from the samples relative to a working gas, which was introduced from a high-pressure cylinder (*grade, producer*) directly into the mass spectrometer, were obtained using the instrumental software (*software, version, producer*) using the ^{17}O correction for CO_2 [5]. The isotope-delta values in the samples were calibrated using linear multi-point normalisation whose parameters were obtained using the errors-in-variables regression method [24].

For compound-specific stable-isotope analyses, peak detection and integration parameters and corrections for baseline and for the presence of derivative contributions when applied should also be reported (*e.g.*, [25]).

1.4 Uncertainty evaluation

Each reported isotope-delta value needs to be accompanied by a standard uncertainty or expanded uncertainty with coverage factor and coverage probability. The procedure used to evaluate the uncertainty should be described explicitly or by citation of previous research. Simple uncertainty evaluations can be obtained from the standard deviation of a stated number of analyses of each RM, sample, or a matrix-matched QC material.

> **For example:** The uncertainty of the reported isotope-delta values was evaluated as the standard deviation of the mean of repeated (n = 4) measurements of each material within a single group of analyses.

Such simple estimates will inevitably neglect various sources of uncertainty including the contributions introduced by reference material calibration, data normalisation or other corrections. More comprehensive methods to evaluate uncertainty (e.g., methods listed in the Guide to the Expression of Uncertainty in Measurement (GUM) [26] or in the Eurachem/CITAC guide: Quantifying Uncertainty in Analytical Measurement [27] including Monte Carlo, Bayesian or Kragten approaches) can capture the additional contributions arising from the various corrections applied to measurement results, particularly normalisation, and use more complex procedures.

> **For example:** The standard uncertainty of the results was evaluated by propagating the contributions arising from measurement of the samples, measurement of the RMs as well as the uncertainties in the assigned isotope delta values of those RMs through the multi-point errors-in-variables regression using a Monte Carlo method as described in detail elsewhere [24]. The reported combined uncertainty corresponds to 95 % confidence and was calculated using a coverage factor k = 2.

The uncertainty for all results obtained using a particular method protocol may also be estimated from the results of well-planned method validation studies [28]. Conformity of results to the method performance characteristics obtained during validation studies need to be demonstrated for each group of analyses.

> **For example:** The standard uncertainty of the results was estimated to be 0.04 ‰ based on the historic performance from various interlaboratory comparisons.

Provision of an uncertainty budget providing the magnitude of each contribution considered is recommended.

2 Summary

These guidelines provide an outline for data reporting that will facilitate intercomparison and reuse of stable-isotope delta measurement results produced independently by different laboratories over time. They also simplify adjustment of the results if values assigned to RMs are revised. To further improve communication, consistent terminology and notation are critical. Therefore, authors are encouraged to adhere to the basic nomenclature principles as outlined in the SI Brochure [29] and IUPAC Green Book [30], in addition to any other technical reports and guidelines (e.g., [5]). Authors should also maximize the accessibility and reusability of the data by providing their data in a format that can be efficiently extracted by others, e.g., in plain text digital formats. This should include each separate analysis for samples, quality control materials and RMs. While there are a variety of ways one can present the data, a key principle is to capture all the variables that are deemed important and to annotate them in a manner that is largely self-explanatory. Storage of unprocessed data (e.g., data without application of any corrections or calibrations) can also facilitate recalculation of results should there be changes to reporting conventions.

> **Example text following this advice suitable for inclusion within the methods section of a manuscript (mention of any product or brand does not reflect use or endorsement by the authors):**

Analytical procedure: Samples of plant leaves were washed with deionized water (deionised water 0.05 $\mu S\ cm^{-1}$), dried in the laboratory oven at 50 °C over 48 h, and ground in a ball mill (Fritsch, Idar-Oberstein, Germany) to fine powders. Aliquots of (1.0 ± 0.1) mg were placed in tin capsules (8 mm × 5 mm, IVA Analysentechnik, Meerbusch, Germany) and analysed for stable carbon isotope composition, using a continuous-flow system consisting of an elemental analyser (Thermo Flash 1112) connected via a Conflo IV peripheral to a Delta V Plus mass spectrometer (Thermo-Finnigan, Germany). In the elemental analyser, each sample was combusted quantitatively with oxygen added to the helium stream at a temperature of 1000 °C in a reactor comprised of Cr_2O_3 (IVA) and silvered oxides of cobalt (IVA) and then NO_x gases were reduced at 650 °C with electrolytic copper (IVA) to produce N_2. The gases obtained were carried through water traps (granular magnesium perchlorate, Sercon, UK) and GC column in a stream of helium (grade 99.999 % purity; BOC, Australia, 100 mL/min), then CO_2 was introduced into the isotope ratio mass spectrometer.
Traceability: Results are reported in permille (‰) using the delta $\delta(^{13}C)$ notation and were normalised to VPDB using NBS 22 (IAEA, Vienna, Austria), USGS40, USGS24 (US Geological Survey, Reston, VA, USA) with assigned carbon isotope-delta values and standard uncertainties of (−30.03 ± 0.05) ‰, (−26.39 ± 0.04) ‰, (−16.05 ± 0.04) ‰, respectively [1]. Each RM was measured in duplicate at the beginning and the end of each daily group of analyses.
Data processing: Isotope-delta values for the CO_2 gas derived from the samples relative to working gas introduced from a high-pressure cylinder (99.995 % purity; BOC, Australia) directly into the mass spectrometer were obtained using the instrumental software (Isodat 2.5, Thermo Scientific, Bremen, Germany) "SSH" ^{17}O correction for CO_2 [31]. A drift correction was applied using the results of quality control (QC) material run regularly throughout each sample group of analyses in duplicate after every 10 sample measurements. Special care was taken to ensure that the amount of yield gas for RMs and samples was the same but minor differences

were adjusted using a linearity correction based upon the signal recorded for measured masses (<0.020 ‰ V^{-1}), quantified at the beginning of each run. The isotope delta results were normalised to VPDB by multi-point normalisation [7] and the errors-in-variables regression method [24].

Uncertainty: The combined standard measurement uncertainty, associated with the stable-isotope analyses including contributions from both known and measured isotope-delta values of RMs used for normalisation as well as measured isotope-delta values of samples, was calculated according to Gröning [32] and does not exceed 0.10 ‰ (1σ). All isotope delta results are included in … [provide reference to Electronic Supplementary Materials file].

3 Membership of sponsoring bodies

Membership of the Inorganic Chemistry Division Committee for the period 2020–2021 was as follows:

President: L.R. Öhrström (Sweden); **Vice President:** L. Armelao (Italy); **Secretary:** D. Rabinovich (USA); **Titular members**: J. Colón (Puerto Rico), M. Hasegawa (Japan), P. Knauth (France), M.H. Lim (South Korea), R. Macaluso (USA), J. Meija (Canada), X.K. Zhu (China); **Associate members:** M. Diop (Senegal), J. Galamba Correia (Portugal), P. Gómez-Sal (Spain), P. Karen (Norway), A. Powell (Germany), T. Walczyk (Singapore); **National representatives:** F. Abdul Aziz (Malaysia), Y. Gorbunova (Russia), M. Gruden-Pavlovic (Serbia), P.J. Kulesza (Poland), G.J. Leigh (UK), O. Metin (Turkey), K. Sakai (Japan), V. Stilinović (Croatia), Y.-C. Tsai (China/Taipei), M. Wieser (Canada).

Membership of the Commission on Isotopic Abundances and Atomic Weights for the period 2020–2021 was as follows:

Chair: J. Meija (Canada); **Secretary**: T. Prohaska (Austria); **Titular Members**: M. Gröning (Austria), J. Irrgeher (Germany), J. Vogl (Germany), H.A.J. Meijer (The Netherlands); **Associate Members**: A. Possolo (USA), J. Wang (China), P.J.H. Dunn (UK), H. Moossen (Germany), Y. Takahashi (Japan).

Acknowledgments: We gratefully acknowledge the support of the IUPAC and its funding bodies. The following IUPAC project contributed to this Technical Report: 2020-013-1-200. We acknowledge the valuable comments from Jan Kaiser and the other nine anonymous reviewers. Any use of trade, firm, or product names is for descriptive purposes only and does not imply endorsement by the U.S. Government or other listed organisation.

References

[1] CIPM, Decision CIPM/104-26, Traceability Exception: Delta Value Isotope Ratio Measurements (2015), https://www.bipm.org/documents/20126/48101963/Traceability-Exception-QM1.pdf/ca63c530-c553-60a1-9111-406c66de4c4d (accessed Nov 18, 2021).

[2] W. A. Brand, T. B. Coplen, J. Vogl, M. Rosner, T. Prohaska. *Pure Appl. Chem.* **86**, 425 (2014), https://doi.org/10.1515/pac-2013-1023.

[3] J.-F. Hélie, C. Hillaire-Marcel. *Rapid Commun. Mass Spectrom.* **35**, e9008 (2021), https://doi.org/10.1002/rcm.9008.

[4] P. J. H. Dunn, D. Malinovsky, G. Holcombe, S. Cowen, H. Goenaga-Infante. *Rapid Commun. Mass Spectrom.* **35**, e9177 (2021), https://doi.org/10.1002/rcm.9177.

[5] W. A. Brand, S. S. Assonov, T. B. Coplen. *Pure Appl. Chem.* **82**, 1719 (2010), https://doi.org/10.1351/pac-rep-09-01-05.

[6] P. J. H. Dunn, J. F. Carter (Eds.). *FIRMS Good Practice Guide for IRMS*, 2nd ed. (2018), https://www.forensic-isotopes.org/gpg.html (accessed Nov 18, 2021).

[7] G. Skrzypek. *Anal. Bioanal. Chem.* **405**, 2815 (2013), https://doi.org/10.1007/s00216-012-6517-2.

[8] T. B. Coplen, W. A. Brand, M. Gehre, M. Gröning, H. A. J. Meijer, B. Toman, R. M. Verkouteren. *Anal. Chem.* **78**, 2439 (2006), https://doi.org/10.1021/ac052027c.

[9] S. Assonov, A. Fajgelj, C. Allison, M. Gröning. *Rapid Commun. Mass Spectrom.* **35**, e9018 (2021), https://doi.org/10.1002/rcm.9014.

[10] T. B. Coplen. *Pure Appl. Chem.* **66**, 273 (1994), https://doi.org/10.1351/pac199466020273.

[11] S. Magozzi, C. P. Bataille, K. A. Hobson, M. B. Wunder, J. D. Howa, A. Contina, H. B. Vander Zanden, G. J. Bowen. *Methods Ecol. Evol.* **12**, 732 (2021), https://doi.org/10.1111/2041-210x.13556.

[12] R. A. Werner, W. A. Brand. *Rapid Commun. Mass Spectrom.* **15**, 501 (2001), https://doi.org/10.1002/rcm.258.

[13] M. D. Wilkinson, M. Dumontier, I. J. Aalbersberg. *Sci. Data* **3**, 160018 (2016).

[14] A. L. Bond, K. A. Hobson. *Waterbirds* **35**, 324 (2012), https://doi.org/10.1675/063.035.0213.

[15] T. B. Coplen. *Rapid Commun. Mass Spectrom.* **25**, 2538 (2011), https://doi.org/10.1002/rcm.5129.

[16] W. Meier-Augenstein, A. Schimmelmann. *Isot. Environ. Health Stud.* **55**, 113 (2019).

[17] P. Roberts, R. Fernandes, O. E. Craig, T. Larsen, A. Lucquin, J. Swift, J. Zech. *Rapid Commun. Mass Spectrom.* **32**, 361 (2017), https://doi.org/10.1002/rcm.8044.

[18] P. Szpak, J. Z. Metcalfe, R. A. MacDonald. *J. Archaeol. Sci. Rep.* **13**, 609 (2017), https://doi.org/10.1016/j.jasrep.2017.05.007.

[19] P. De Bièvre, R. Dybkaer, A. Fajgelj, D. B. Hibbert. *Pure Appl. Chem.* **83**, 1873 (2011).

[20] G. Skrzypek, P. J. H. Dunn. *Rapid Commun. Mass Spectrom.* **34**, e8892 (2020), https://doi.org/10.1002/rcm.8892.

[21] D. X. Soto, G. Koehler, L. I. Wassenaar, K. A. Hobson. *Rapid Commun. Mass Spectrom.* **31**, 1193 (2017), https://doi.org/10.1002/rcm.7921.

[22] L. I. Wassenaar, K. A. Hobson. *Isot. Environ. Health Stud.* **39**, 211 (2003), https://doi.org/10.1080/1025601031000096781.

[23] H. Qi, M. Gröning, T. B. Coplen, B. Buck, S. J. Mroczkowski, W. A. Brand, H. Geilmann, M. Gehre. *Rapid Commun. Mass Spectrom.* **24**, 1821 (2010), https://doi.org/10.1002/rcm.4559.

[24] J. Meija, M. M. G. Chartrand. *Anal. Bioanal. Chem.* **410**, 1061 (2018), https://doi.org/10.1007/s00216-017-0659-1.

[25] M. Pilecky, K. Winter, L. I. Wassenaar, M. J. Kainz. *Rapid Commun. Mass Spectrom.* **35**, e9135 (2021), https://doi.org/10.1002/rcm.9135.

[26] Joint Committee for Guides in Metrology. International Bureau of Weights and Measures (BIPM) JCGM 102. *Evaluation of Measurement Data – Supplement 2 to the "Guide to the Expression of Uncertainty in measurement" – Extension to Any Number of Output Quantities* (2011), https://www.bipm.org/en/committees/jc/jcgm/publications (accessed Jan 25, 2021).

[27] S. L. R. Ellison, A. Williams (Eds.). *Eurachem/CITAC Guide: Quantifying Uncertainty in Analytical Measurement*, 3rd ed. Eurachem, (2012). ISBN 978-0-948926-30-3.

[28] V. J. Barwick, S. L. R. Ellison. *Accred. Qual. Assur.* **5**, 47 (2000), https://doi.org/10.1007/s00769-017-1286-4.

[29] BIPM. *The International System of Units (SI)*, 9th ed. (2019), https://www.bipm.org/en/publications/si-brochure (accessed Nov 18, 2021).

[30] E. R. Cohen, T. Cvitas, J. G. Frey, B. Holmstrom, K. Kuchitsu, R. Marquardt, I. Mills, F. Pavese, M. Quack, J. Stohner, H. Strauss, M. Takami, A. J. Thor. *Quantities, Units, and Symbols in Physical Chemistry, IUPAC Green Book*, The Royal Society of Chemistry, UK, 3rd ed. (2007). https://doi.org/10.1039/978184755.

[31] J. Santrock, S. A. Studley, J. M. Hayes. *Anal. Chem.* **57**, 1444 (1985), https://doi.org/10.1021/ac00284a060.

[32] M. Gröning. *Rapid Commun. Mass Spectrom.* **25**, 2711 (2011).