

Making an imPACT

interesting perspectives for increasing environmental realism in chemical risk assessment. The legislation and regulation of various groups of biologically active substances, such as pesticides, biocides, and pharmaceuticals, and the new chemical regulation (REACH) emphasizes the need to have available well-defined reference matrices. This need parallels the need to test environmental fate and effects and new materials (e.g., artificially produced nanomaterials).

The concept that we outline provides suitable guidelines for selecting reference matrices. However, we note that agreement on optimal application of reference matrices and interpretation of results obtained in tests using reference matrices needs to be reached between scientists, risk assessors, reference laboratories, and international standard organizations.

For more information and comments, contact Werner Kördel <werner.koerdel@ime.fraunhofer.de>; Willie Peijnenburg <wjgm.peijnenburg@rivm.nl>; or Bernd Gawlik <bernd.gawlik@jrc.it>.

 www.iupac.org/web/ins/2001-026-1-600

Comprehensive Inter-Laboratory Calibration of Reference Materials for $\delta^{18}\text{O}$ Versus VSMOW Using Various On-Line High-Temperature Conversion Techniques

W.A. Brand, T.B. Coplen, A.T. Aerts-Bijma, J.K. Böhlke, M. Gehre, H. Geilmann, M. Gröning, H.G. Jansen, H.A. J. Meijer, S.J. Mroczkowski, H. Qi, K. Soergel, H. Stuart-Williams, S.M. Weise, and R.A. Werner

Rapid Comm. Mass Spectrom. 2009
Vol. 23, Issue 7, pp. 999-1019
doi:10.1002/rcm.3958

Internationally distributed organic and inorganic oxygen isotopic reference materials have been calibrated by six laboratories carrying out more than 5 300 measurements using a variety of high-temperature conversion techniques (HTC) in an evaluation sponsored by IUPAC. To aid in the calibration of these reference materials, which span more than 125 per mille, an artificially enriched reference water ($\delta^{18}\text{O}$ of +78.91 per mille) and two barium sulfates (one depleted and one enriched in ^{18}O) were prepared and calibrated relative to VSMOW2* and SLAP reference waters. These materials were used to calibrate the other isotopic reference materials in this study, which yielded:

Isotopic reference material	$10^3 \delta(^{18,16}\text{O}_{\text{VSMOW-SLAP}})$ reference value
IAEA-602 benzoic acid	+71.28
USGS35 sodium nitrate	+56.81
IAEA-NO-3 potassium nitrate	+25.32
IAEA-601 benzoic acid	+23.14
IAEA-SO-5 barium sulfate	+12.13
NBS 127 barium sulfate	+8.59
VSMOW water	0
IAEA-600 caffeine	-3.48
IAEA-SO-6 barium sulfate	-11.35
USGS34 potassium nitrate	-27.78
SLAP water	-55.5

A primary conclusion of this study is that nitrate samples analyzed for $\delta(^{18,16}\text{O})$ should be analyzed with internationally distributed isotopic nitrates, and likewise for sulfates and organics. Authors reporting relative differences of oxygen-isotope ratios [$\delta(^{18,16}\text{O})$] of nitrates, sulfates, or organic material should explicitly state in their reports the $\delta(^{18,16}\text{O})$ values of two or more internationally distributed nitrates (USGS34, IAEA-NO-3, and USGS35), sulfates (IAEA-SO-5, IAEA-SO-6, and NBS 127), or organic material (IAEA-601 benzoic acid, IAEA-602 benzoic acid, and IAEA-600 caffeine), as appropriate to the material being analyzed, had these reference materials been analyzed with unknowns. This procedure ensures that readers will be able to normalize the $\delta(^{18,16}\text{O})$ values at a later time should it become necessary. The high-temperature reduction technique for analyzing $\delta(^{18,16}\text{O})$ and $\delta(^2\text{H})$ is not as widely applicable as the well-established combustion technique for carbon and nitrogen stable isotope determination. To obtain the most reliable stable isotope data, materials should be treated in an identical fashion; within the same sequence of analyses, samples should be compared with working reference materials that are as similar in nature and in isotopic composition as feasible.

*In 2007, VSMOW2 replaced the almost exhausted VSMOW as the primary reference material and anchor to the VSMOW scale (for details, see <<http://www.naweb.iaea.org/NAALHIL/>> and <http://www.naweb.iaea.org/NAALHIL/docs/ref_mat/InfoSheet-VSMOW2-SLAP2.pdf>). For ^{18}O , VSMOW2 and VSMOW are indistinguishable. The scale itself remains unaltered and keeps its name ("VSMOW").

 www.iupac.org/web/ins/2005-022-1-200