IAEA
International Atomic Energy Agency

Reference Sheet for Reference Materials

(in cooperation with the U.S. National Institute for Standards and Technology (NIST))

NBS 22	Oil, liquid	(δ^2H_{VSMOW}, $\delta^{13}C_{VPDB}$)
IAEA-CH-3	Cellulose	(δ^2H_{VSMOW}, $\delta^{13}C_{VPDB}$)
IAEA-CH-6	Sucrose, granular	(δ^2H_{VSMOW}, $\delta^{13}C_{VPDB}$)
IAEA-CH-7	Polyethylene foil	(δ^2H_{VSMOW}, $\delta^{13}C_{VPDB}$)
USGS24	Graphite, powder	($\delta^{13}C_{VPDB}$)

Reference values for the relative difference in stable hydrogen isotope-amount ratio (δ^2H) in the reference materials

Table 1: Reference δ^2H values relative to VSMOW-SLAP of the reference materials NBS 22 and IAEA-CH-7. For NBS 22 the value is the statistically evaluated result of data from two studies [1, 2], see Table 3.

Name	NIST code	Material	$1000 \times \delta^2H_{VSMOW}$	$1000 \times \delta^2H_{VSMOW}$ standard uncertainty (1 sigma level)	Number of accepted results *n* (reported results)	Reference
NBS 22	RM 8539	Oil	-119.6	0.6	7(9)	[1, 2]
IAEA-CH-7	RM 8540	Polyethylene foil	-100.3	2.0	6(6)	[1]

Reference values for the relative difference in stable hydrogen isotope-amount ratio ($\delta^{13}C$) in the reference materials

Table 2: Reference $\delta^{13}C$ values relative to VPDB of the reference materials NBS 22, USGS24, IAEA-CH-3, IAEA-CH-6 and IAEA-CH-7.

Name	NIST code	Material	$1000 \times \delta^{13}C_{VPDB}$ [a]	$1000 \times \delta^{13}C_{VPDB}$ standard uncertainty (1 sigma level)	Reference
NBS 22	RM 8539	Oil	-30.03	0.05	[3]
IAEA-CH-3		Cellulose	-24.72	0.05	[3]
IAEA-CH-6	RM 8542	Sucrose	-10.45	0.04	[3]
IAEA-CH-7	RM 8540	Polyethylene foil	-32.15	0.05	[3]
USGS24	RM 8541	Graphite	-16.05	0.04	[3]

[a] Relative to VPDB using a scale normalization with $\delta^{13}C$ values for NBS 19 of +1.95‰ and for LSVEC of -46.6‰ [3].

The traceability of the δ^2H values of these reference materials to those of VSMOW and SLAP and of the $\delta^{13}C$ values to VPDB through their direct calibrations in reference to those international measurement standards justifies their status as reference materials.
The content of this reference sheet complies with the requirements of ISO Guide 31 [4].

Intended use

The reference materials listed above are intended to provide samples of well characterized relative difference in $^2H/^1H$ and $^{13}C/^{12}C$ isotope-amount ratios stated in parts per thousand (‰) from the Vienna Standard Mean Ocean Water (VSMOW) or Vienna Pee Dee Belemnite (VPDB) relative isotope-amount ratio scales, respectively.
The use of these reference materials allows comparability of δ^2H and $\delta^{13}C$ values obtained in different testing laboratories. NBS 22, IAEA-CH-3, IAEA-CH-6 and IAEA-CH-7 are intended for calibration purpose when the δ^2H and $\delta^{13}C$ are determined in organic materials. No certified δ^2H-values exist so far for IAEA-CH-3 and IAEA-CH-6. USGS24 is intended for $\delta^{13}C$ analysis of carbon bearing materials.
These materials are distributed by the International Atomic Energy Agency (IAEA), Vienna, Austria and partly by the National Institute of Standards and Technology (NIST), Gaithersburg, USA, with the NIST material codes as indicated in Tables 1 and 2.

Origin and preparation of the materials

NBS 22 was prepared by S. Silverman, Chevron Oil Company, La Habra, California. IAEA-CH-7 (its former name was PEF1) was prepared by H. Gerstenberger and M. Herrmann, Zentralinstitut für Isotopen- und Strahlenforschung, Leipzig, Germany [5]. USGS24 was prepared by T.B. Coplen, U.S. Geological Survey from Baker® technical grade graphite (96 % < 44 μm). Prior to splitting with a sample splitter, six spatially separated ~ 1 mg samples were analyzed to ensure isotopic homogeneity of the material. Peak-to-peak variation was 0.11 ‰. IAEA-CH-6 (its former name was Sucrose ANU) was supplied to the IAEA by H. Polach, Australian National University, Canberra [1]. IAEA-CH-3 was prepared at the IAEA Isotope Hydrology Laboratory, using several kilograms of cellulose sheets of the ^{14}C quality control material IAEA-C3 (separate material!) and milling it down to a grain size smaller than 100 μm. The material was subsequently homogenized by use of a tumbler. The isotopic homogeneity for $\delta^{13}C$ was checked by analyzing 30 sub-samples taken from different locations of the container. The standard deviation of 120 measurements at a sample weight of about 1 mg for $\delta^{13}C$ measurement was better than ±0.02 ‰, both for within and between bottle homogeneity.

Normalization

The values for δ^2H are stated here in parts per thousand difference (per mill, ‰) from the international measurement standard VSMOW. The adoption of VSMOW as zero on the δ^2H scale and of prefixed values for SLAP corresponds with the definition of the δ-value normalized on the VSMOW / SLAP scale [6, 7].

$$\delta = [(R_{sample\ /\ } R_{VSMOW}) - 1] \cdot f \qquad (1)$$

$$f = \delta°_{SLAP} / [(R_{SLAP} - R_{VSMOW}) / R_{VSMOW}] \qquad (2)$$

where R_A is the measured stable hydrogen isotope-amount ratio in substance A, $n_A(^2H)/n_A(^1H)$,
and $\delta°_{SLAP}$ is the conventionally fixed δ^2H value of -0.428 or -428.0 ‰ [6, 8].

Please note that the reporting scale for δ^2H is still denoted and referred to as VSMOW-SLAP scale, despite the exhaustion of VSMOW and SLAP and their replacement by the two international measurement standards VSMOW2 and SLAP2.

Distribution and storage

NBS 22 is issued in units of 1 mL. IAEA-CH-3, IAEA-CH-6 and IAEA-CH-7 are issued in units of 0.5 g, 1 g, and 3.6 g, respectively. USGS24 is issued in units of 0.5 g.
It is recommended that these reference materials be stored in tightly closed original containers in which they were supplied to the user.

Limit of distribution

Each set of these reference materials may be ordered only once per laboratory in a three-year period. This strategy should ensure that the materials are available for international use as long as possible.

Expiration of reference values

The reference values for relative difference in stable isotope-amount ratio of the reference materials are valid until 31 December 2017, provided they are handled and stored in accordance with the instructions given in this reference sheet.

δ^2H values as reported in selected literature

*Table 3: Calibrated δ^2H values relative to VSMOW of several studies with standard uncertainties (1σ) based on the standard deviation of individual laboratory means. *) Marked values are calculated on the raw data basis given in the respective literature. Data in 3rd row: statistical evaluation of two data sets; interquartile rejection criterion ([9], step I.). The reference value for IAEA-CH-7 based on data of [1] would not be changed significantly by the data of [5] (due to identification of outliers in the dataset when pooled) and are therefore not considered.*

Name	Material	$1000 \times \delta^2H_{VSMOW}$	$1000 \times \delta^2H_{VSMOW}$ standard uncertainty	Number of accepted results *n* (reported results)	Reference
NBS 22	Oil	-118.5*	2.8*	3(3)	[1]
NBS 22	Oil	-119.2	0.7	6(6)	[2]
NBS 22	Oil	-119.6	0.6	7(9)	This report: [1, 2]
IAEA-CH-7	Polyethylene foil	-98.8	3.4	5 (6)	[5]
IAEA-CH-7	Polyethylene foil	-100.3*	2.0*	6 (6)	[1]

$\delta^{13}C$ values as reported in selected literature

Table 4: Calibrated $\delta^{13}C$-values relative to VPDB or relative to PDB for NBS 22, USGS24, IAEA-CH-3, IAEA-CH-6 and IAEA-CH-7. The standard uncertainties (1σ) are based on the standard deviation of individual laboratory means except for the data of [3], where a Bayesian approach is used to evaluate the standard uncertainty based on data of all reference materials measured in each laboratory. For the NBS 22 measurement, the authors [10] used for the calibration of the PDB-scale NBS 20 with $\delta^{13}C_{PDB}$ = -1.06 ‰; the authors [2] used for calibration of the PDB-scale a $\delta^{13}C_{PDB}$ -value for NBS 20 of - 1.03 ‰; but we assume that their data was corrected for $\delta^{13}C$ = - 1.06 ‰..

Name	Material	$1000 \times \delta^{13}C_{PDB}$	$1000 \times \delta^{13}C_{VPDB}$	$1000 \times \delta^{13}C_{VPDB}$ standard uncertainty	Number of accepted results *n* (reported results) [preparations]	Reference
NBS 22	Oil	-29.61		0.03	1 [7]	[10]
NBS 22	Oil		-29.73	0.09	8	[1]
NBS 22	Oil	- 29.81		0.06	4 (19)	[2]
NBS 22	Oil		-30.03	0.05		[3]
USGS24	Graphite		-15.99	0.11	8 (9)	[11]
USGS24	Graphite		-16.05	0.04		[3]
IAEA-CH-3	Cellulose		-24.72	0.05		[3]
IAEA-CH-6	Sucrose		-10.47	0.13	5 (5)	[1]
IAEA-CH-6	Sucrose		-10.43	0.23	13 (13)	[12]
IAEA-CH-6	Sucrose		-10.45	0.04		[3]
IAEA-CH-7	Polyethylene foil	- 31.62		0.64	14 (16)	[5]
IAEA-CH-7	Polyethylene foil		-31.77	0.08	6 (6)	[1]
IAEA-CH-7	Polyethylene foil		-31.90	0.18	14 (14)	[12]
IAEA-CH-7	Polyethylene foil		-32.15	0.05		[3]

Legal disclaimer

The IAEA makes no warranties, expressed or implied, with respect to the data contained in this reference sheet and shall not be liable for any damage that may result from the use of such data.

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Further Information

Users of these reference materials should ensure that the reference sheet in their possession is current. This can be accomplished by contacting the IAEA reference material site at:
http://www.iaea.org/programmes/aqcs/
or the Isotope Hydrology Laboratory website at:
http://www-naweb.iaea.org/NAALIHL/reference_materials.shtml

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