National Institute of Standards & Technology

Certificate of Analysis

Standard Reference Material® 1643f

Trace Elements in Water

This Standard Reference Material (SRM) is intended primarily for use in evaluating methods used in the determination of trace elements in fresh water. A unit of SRM 1643f consists of approximately 250 mL of acidified water in a polyethylene bottle, which is sealed in an aluminized plastic bag to maintain stability. SRM 1643f simulates the elemental composition of fresh water. The solution contains nitric acid at a volume fraction of approximately 2 %, equivalent to an amount of substance concentration (molarity) of approximately 0.32 mol/L.

Certified Values: The certified values for elements in SRM 1643f are listed in Table 1. All values are reported both as mass fractions (µg/kg) and as mass concentrations (µg/L). A NIST certified value is a value for which NIST has the highest confidence in its accuracy in that all known or suspected sources of bias have been investigated or taken into account [1]. The certified mass fraction values are consensus estimates that blend the results of the gravimetric preparation value and a value determined by either inductively coupled plasma mass spectrometry (ICP-MS) or inductively coupled plasma optical emission spectrometry (ICP-OES) [2]. The certified mass concentration values are derived from the certified mass fraction values using the measured density of SRM 1643f. Additional information about the certification of SRM 1643f is given under "Certification of Material".

The expanded uncertainty for each certified value is calculated as

$$U = ku_c$$

where k is the coverage factor for a 95 % confidence interval and u_c is the combined standard uncertainty calculated through the application of the Monte Carlo method described in the ISO/JCGM Supplement 1 [3]. The value of u_c for the certified mass fraction values is intended to represent, at the level of one standard deviation, the combined effect of uncertainty components associated with the gravimetric preparation, the ICP-MS or ICP-OES determination, method bias, and stability. Additionally, the uncertainty evaluations associated with the certified mass concentration values assume that the temperature at which the material will be measured is between 15 °C and 25 °C.

Expiration of Certification: This certification of **SRM 1643f** is valid, within the measurement uncertainty specified, until **31 October 2023**, provided the SRM is handled and stored in accordance with instructions given in this certificate (see "Instructions for Use"). This certification is nullified if the SRM is damaged, contaminated, or modified.

Maintenance of SRM Certification: NIST will monitor this SRM over the period of its certification. If substantive technical changes occur that affect the certification before the expiration of this certificate, NIST will notify the purchaser. Registration (see attached sheet or register online) will facilitate notification.

Coordination of the NIST technical measurements was under the direction of T.A. Butler, J.L. Molloy and M.R. Winchester of the NIST Chemical Sciences Division. The density, ICP-MS and ICP-OES analyses were performed by T.A. Butler and J.L. Molloy.

Statistical analysis of the experimental data was performed by A.M. Possolo of the NIST Statistical Engineering Division.

Support aspects involved in the issuance of this SRM were coordinated through the NIST Office of Reference Materials.

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Table 1. Certified Values, Expanded Uncertainties, and Coverage Factors (*k*) for Elements in SRM 1643f

Element	Mass Fraction (µg/kg)			*k*	Mass Concentration (µg/L)			*k*
Aluminum (Al)	132.5	±	1.2	1.9	133.8	±	1.2	1.9
Antimony (Sb)	54.90	±	0.39	1.9	55.45	±	0.40	2.0
Arsenic (As)	56.85	±	0.37	2.0	57.42	±	0.38	2.0
Barium (Ba)	513.1	±	7.3	2.1	518.2	±	7.3	2.1
Beryllium (Be)	13.53	±	0.11	2.1	13.67	±	0.12	2.1
Bismuth (Bi)	12.50	±	0.10	1.9	12.62	±	0.11	1.9
Boron (B)	150.8	±	6.6	2.2	152.3	±	6.6	2.2
Cadmium (Cd)	5.83	±	0.13	2.2	5.89	±	0.13	2.2
Calcium (Ca)	29 140	±	320	2.1	29 430	±	330	2.1
Chromium (Cr)	18.32	±	0.10	2.0	18.50	±	0.10	2.1
Cobalt (Co)	25.05	±	0.17	2.0	25.30	±	0.17	2.0
Copper (Cu)	21.44	±	0.70	2.1	21.66	±	0.71	2.2
Iron (Fe)	92.51	±	0.77	2.1	93.44	±	0.78	2.1
Lead (Pb)	18.303	±	0.081	2.0	18.488	±	0.084	2.1
Lithium (Li)	16.42	±	0.35	2.2	16.59	±	0.35	2.2
Magnesium (Mg)	7 380	±	58	1.9	7 454	±	60	2.0
Manganese (Mn)	36.77	±	0.58	2.1	37.14	±	0.60	2.2
Molybdenum (Mo)	114.2	±	1.7	2.1	115.3	±	1.7	2.1
Nickel (Ni)	59.2	±	1.4	2.2	59.8	±	1.4	2.2
Potassium (K)	1 913.3	±	9.0	2.0	1 932.6	±	9.4	2.1
Rubidium (Rb)	12.51	±	0.12	2.0	12.64	±	0.13	2.0
Selenium (Se)	11.583	±	0.078	2.0	11.700	±	0.081	2.0
Silver (Ag)	0.9606	±	0.0053	2.0	0.9703	±	0.0055	2.0
Sodium (Na)	18 640	±	240	2.1	18 830	±	250	2.1
Strontium (Sr)	311	±	18	2.1	314	±	19	2.2
Tellurium (Te)	0.9672	±	0.0082	2.0	0.9770	±	0.0084	2.0
Thallium (Tl)	6.823	±	0.034	1.9	6.892	±	0.035	2.0
Vanadium (V)	35.71	±	0.27	2.0	36.07	±	0.28	2.0
Zinc (Zn)	73.7	±	1.7	2.1	74.4	±	1.7	2.1

[a] The measurand is the total mass fraction for each element. Metrological traceability is to the SI unit for mass, expressed as micrograms per kilogram and micrograms per liter.

Preparation of Material: SRM 1643f was prepared at NIST using only high purity reagents. A polyethylene cylindrical tank was filled with deionized water and sufficient nitric acid to bring the nitric acid amount of substance concentration (molarity) to approximately 0.32 mol/L. Known masses of the matrix elements (sodium, potassium, calcium, and magnesium) were added to the tank as solutions prepared from the same materials used to prepare the SRM 3100 series of single element solutions. Known masses of the other elements were then added to the tank solution using weighed aliquots of the SRM 3100 series. After mixing thoroughly, the tank solution was transferred into the acid-cleaned, 250 mL, polyethylene, SRM bottles and immediately sealed in individual aluminized plastic bags.

Certification of Material: Each of the certified elements was determined using either ICP-MS or ICP-OES. The final total mass of the tank solution prior to bottling was determined from the sum of the mass fraction values of the elements in Table 1 and the sum of the known masses of those elements added to prepare the solution, therefore allowing calculation of the gravimetric preparation mass fraction for each element. Certified mass fraction values were calculated by combining the gravimetric preparation values with the ICP-MS or ICP-OES values, as described under Certified Values. Certified mass concentration values were calculated using the measured density of 1.0101 g/mL ± 0.0012 g/mL, where the uncertainty is expressed at a confidence level of approximately 95 %, within the temperature range of 15 °C to 25 °C.

INSTRUCTIONS FOR USE

Precautions: The SRM should be shaken before use because of possible water condensation on the inner surfaces of the bottle. To prevent possible contamination of the SRM, **DO NOT** insert pipettes into the bottle. Samples should be decanted at a room temperature of 15 ºC to 25 ºC. After use, the bottle should be recapped tightly and returned to the aluminized plastic bag, which should be folded and sealed with sealing tape. This safeguard will protect the SRM from possible environmental contamination and long-term evaporation.

The accuracy of trace element determinations, especially at the micrograms per liter level, is limited by contamination. Apparatus should be scrupulously cleaned and only high purity reagents employed. Sampling and manipulations, such as evaporations, should be done in a clean environment, such as a Class-100 clean hood.

REFERENCES

[1] May, W.; Parris, R.; Beck, C.; Fassett, J.; Greenberg, R.; Guenther, F.; Kramer, G., Wise; S., Gills, T.; Colbert, J.; Gettings, R.; MacDonald, B.; *Definition of Terms and Modes Used at NIST for Value-Assessment of Reference Materials for Chemical Measurements*; NIST Special Publication 260-136, U.S. Government Printing Office: Washington, DC (2000); available at http://www.nist.gov/srm/publications.cfm (accessed Aug 2015).

[2] DerSimonian, R.; Laird, N.; *Meta-Analysis in Clinical Trials*; Control. Clin. Trials, Vol. 7, pp. 177–188 (1986).

[3] JCGM 101:2008; *Evaluation of Measurement Data — Supplement 1 to the "Guide to the Expression of Uncertainty in Measurement" — Propagation of Distributions using a Monte Carlo Method*; Joint Committee for Guides in Metrology (JCGM) (2008); available at http://www.bipm.org/utils/common/documents/jcgm/JCGM_101_2008_E.pdf (accessed Aug 2015).

Users of this SRM should ensure that the Certificate of Analysis in their possession is current. This can be accomplished by contacting the SRM Program: telephone (301) 975-2200; fax (301) 948-3730; e-mail srminfo@nist.gov; or via the Internet at http://www.nist.gov/srm.