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Reference Material 8690

Per- and Polyfluoroalkyl Substances (PFAS) in Aqueous Film-Forming Foams (AFFF) Formulation I

REFERENCE MATERIAL INFORMATION SHEET

Purpose: This Reference Material (RM) is intended for the identification and quantification of per- and polyfluoroalkyl substances (PFAS) in aqueous film-forming foams (AFFFs).

Description: A unit of RM 8690 consists of four 2 mL ampoules. Each ampoule contains approximately 1.2 mL of methanol solution.

Non-Certified Values: Non-certified values are suitable for use in method development, method harmonization, and process control but do not provide metrological traceability to the International System of Units (SI) or other higher-order reference system [1]. Non-certified mass fraction values are provided in Table 1 below.

Table 1. Non-Certified Values for RM 8690

Measurand	Common Acronym	Mass Fraction (as-received)[(a)] (µg/g)	
Perfluorobutanoic Acid	PFBA	0.104	± 0.016
Perfluorohexanoic Acid	PFHxA	0.295	± 0.026
Perfluoroheptanoic Acid	PFHpA	0.0918	± 0.0370
Perfluorooctanoic Acid	PFOA	0.317	± 0.078
Perfluoropropanesulfonic Acid	PFPrS	0.302	± 0.016
Perfluorobutanesulfonic Acid	PFBS	0.473	± 0.032
Perfluoropentanesulfonic Acid	PFPeS	0.409	± 0.085
Perfluorohexanesulfonic Acid	PFHxS	2.64	± 0.12
Perfluoroheptanesulfonic Acid	PFHpS	0.315	± 0.225
Perfluorooctanesulfonic Acid	PFOS	19.4	± 0.4
Perfluorobutane Sulfonamide	PFBSA	0.0356	± 0.0065
Perfluorohexane Sulfonamide	PFHxSA	0.035	± 0.013
6:2 Fluorotelomer Sulfonic Acid	6:2 FTS	0.222	± 0.066
Perfluorohexane Sulfonamido Amine	N-AP-FHxSA	9.12	± 1.71
N-[3-(perfluoro-1-hexanesulfonamido)propan-1-yl]-N,N,N-trimethylammonium	N-TAmP-FHxSA	0.293	± 0.023
6:2 Fluorotelomer Sulfonamide Propyl Betaine	6:2 FTAB	2.50	± 0.5

[(a)] Values are expressed as $x \pm U(x)$, where x is the value and $U(x)$ is the expanded uncertainty of the value. The expanded uncertainty is calculated as $U(x) = ku_c$ where u_c is the standard uncertainty and k is the coverage factor. For values shown, $k = 2$. While the best estimate of the mass fraction for the measurand lies within the interval $x \pm U(x)$, this interval may not include the true value.

Period of Validity: The non-certified values are valid within the measurement uncertainty specified until **31 January 2033.** The value assignments are nullified if the material is stored or used improperly, damaged, contaminated, or otherwise modified.

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Maintenance of Non-Certified Values: NIST will monitor this material to the end of its period of validity. If substantive technical changes occur that affect the non-certified values during this period, NIST will update this Reference Material Information Sheet and notify registered users. RM users can register online from a link available on the NIST SRM website or fill out the user registration form that is supplied with the RM. Registration will facilitate notification. Before making use of any of the values delivered by this material, users should verify they have the most recent version of this documentation, available through the NIST SRM website (https://www.nist.gov/srm).

Safety: This material contains per- and polyfluoroalkyl substances, many of which have been reported to have toxic and/or carcinogenic properties and should be handled with care. Use proper disposal methods. Please consult the Safety Data Sheet provided with this material.

Storage: The original unopened ampoules of RM 8690 should be stored at room temperature (20 °C ± 5 °C). The value assignment does not apply to contents of previously opened ampoules as the stability of the measurands in opened ampoules has not been investigated.

Use: Open ampoules carefully to prevent contamination or injury. The ampoules are pre-scored and should **NOT** be opened using a file. Sample aliquots for analysis should be withdrawn at 20 °C to 25 °C **immediately** after opening and should be processed without delay for the values in Table 1 to be valid within the stated uncertainties.

Additional Information: The non-certified value is a weighted mean of average mass fractions, with one average from gravimetric preparation and two averages from chromatographic measures [2,3]. The expanded uncertainty was determined using the Horn-Horn-Duncan (HHD) method [4] for variances and with the bootstrap method [5], which is consistent with the ISO/JCGM Guides [6,7]. The effective coverage factor, k, is 2.

Full details on the production and evaluation of RM 8690 are provided free of charge in reference 8.

REFERENCES

[1] Beauchamp, C.R.; Camara, J.E.; Carney, J.; Choquette, S.J.; Cole, K.D.; DeRose, P.C.; Duewer, D.L.; Epstein, M.S.; Kline, M.C.; Lippa, K.A.; Lucon, E.; Phinney, K.W.; Polakoski, M.; Possolo, A.; Sharpless, K.E.; Sieber, J.R.; Toman, B.; Winchester, M.R.; Windover, D.; *Metrological Tools for the Reference Materials and Reference Instruments of the NIST Material Measurement Laboratory*; NIST Special Publication 260-136; U.S. Government Printing Office: Washington, DC (2020); available at https://nvlpubs.nist.gov/nistpubs/SpecialPublications/NIST.SP.260-136-2020.pdf (accessed Mar 2023).

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[4] Horn, R.A.; Horn, S.A.; Duncan, D.B.; *Estimating Heteroscedastic Variance in Linear Models*; J. American Statistical Association, Vol. 70, pp. 380-385 (1975).

[5] Efron, B.; Tibshirani, R.J.; An Introduction to the Bootstrap; Chapman & Hall (1993).

[6] JCGM 100:2008; Evaluation of Measurement Data — Guide to the Expression of Uncertainty in Measurement (GUM 1995 with Minor Corrections); Joint Committee for Guides in Metrology (2008); available at https://www.bipm.org/en/committees/jc/jcgm/publications (accessed Mar 2023); see also Taylor, B.N.; Kuyatt, C.E.; Guidelines for Evaluating and Expressing the Uncertainty of NIST Measurement Results; NIST Technical Note 1297; U.S. Government Printing Office: Washington, DC (1994); available at https://www.nist.gov/pml/nist-technical-note-1297 (accessed Mar 2023).

[7] JCGM 101:2008; Evaluation of Measurement Data – Supplement 1 to the Guide to Expression of Uncertainty in Measurement; Propagation of Distributions Using a Monte Carlo Method; Joint Committee for Guides in Metrology (BIPM, IEC, IFCC, ILAC, ISO, IUPAC, IUPAP and OIML), International Bureau of Weights and Measures (BIPM), Sèvres, France (2008); available at https://www.bipm.org/en/committees/jc/jcgm/publications (accessed Mar 2023).

[8] Reiner J.L.; Place B.J.; Heckert N.A.; Peter K.T.; Rodowa A.E.; *Characterization of Reference Materials® 8690 to 8693 Per- and Polyfluoroalkyl Substances (PFAS) in Four Formulations of Aqueous Film-Forming Foams (AFFF)*. (National Institute of Standards and Technology, Gaithersburg, MD), NIST Special Publication (SP) 260-234. (2023); available at https://doi.org/10.6028/NIST.SP.260-234 (accessed Mar 2023).

If you use this RM in published work, please reference:

Reiner JL, Place BJ, Heckert NA, Peter KT, Rodowa AE (2023) Characterization of Reference Materials 8690 to 8693 Per- and Polyfluoroalkyl Substances (PFAS) in Four Formulations of Aqueous Film-Forming Foams (AFFF). (National Institute of Standards and Technology, Gaithersburg, MD), NIST Special Publication (SP) 260-234. https://doi.org/10.6028/NIST.SP.260-234

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