National Institute of Standards & Technology

Certificate of Analysis

Standard Reference Material® 1494

Aliphatic Hydrocarbons in 2,2,4-Trimethylpentane

This Standard Reference Material (SRM) is a solution of 20 compounds, including even and odd carbon number aliphatic hydrocarbons from *n*-decane to *n*-eicosane, even carbon number aliphatic hydrocarbons from *n*-eicosane to *n*-etratriacontane, and pristine and phytane in 2,2,4-trimethylpentane (*iso*-octane). This SRM is intended primarily for use in the calibration of chromatographic instrumentation used for the determination of aliphatic hydrocarbons. A unit of SRM 1494 consists of five 2 mL ampoules, each containing approximately 1.2 mL of solution.

Certified Concentrations of Constituents: The certified values and estimated uncertainties for the 20 constituents, expressed as mass fractions and concentrations, are given in Table 1 along with the Chemical Abstract Service (CAS) Registry Numbers. The certified values are based on results obtained from the gravimetric preparation of this solution and from the analytical results determined by using gas chromatography. 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].

Expiration of Certification: The certification of **SRM 1494** is valid, within the measurement uncertainty specified, until **30 April 2023**, provided the SRM is handled and stored in accordance with the instructions given in this certificate (see "Instructions for Handling, Storage, and Use"). The certification is nullified if the SRM is damaged, contaminated, or otherwise 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) will facilitate notification.

Coordination of the technical measurements leading to the certification of this SRM was under the direction of M.M. Schantz and S.A. Wise of the NIST Chemical Sciences Division.

Preparation and analytical measurements of the SRM were performed by R.M. Parris, R.E. Rebbert, and M.M. Schantz of the NIST Chemical Sciences Division. Ampoules of this SRM were prepared by R. Parris of the NIST Chemical Sciences Division, M.P. Cronise and C.N. Fales of the NIST Office of Reference Materials.

Consultation on the statistical design of the experimental work and evaluation of the data were provided by S.D. Leigh of the NIST Statistical Engineering Division.

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

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Chemical Sciences Division

Gaithersburg, MD 20899
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Certificate Revision History on Last Page

Robert L. Watters, Jr., Director
Office of Reference Materials

INSTRUCTIONS FOR HANDLING, STORAGE AND USE

Handling: This material contains aliphatic compounds and should be handled with care. Use proper disposal methods.

Storage: Sealed ampoules, as received, should be stored in the dark at temperatures lower than 30 °C.

Use: Sample aliquots for analysis should be withdrawn at 20 °C to 25 °C immediately after opening the ampoules and should be processed without delay for the certified values in Table 1 to be valid within the stated uncertainty. Because of the volatility of 2,2,4-trimethylpentane, certified values are not applicable to material stored in ampoules that have been opened for more than 5 minutes, even if they are resealed.

PREPARATION AND ANALYSIS[(1)]

The compounds used in the preparation of this SRM were obtained from Fluka (Milwaukee, WI), Alltech Associates (Deerfield, IL), Ultra Scientific (North Kingston, RI), and JT Baker (Phillipsburg, NJ). The solution was prepared at NIST by weighing and mixing the individual compounds and 2,2,4-trimethylpentane. The weighed components were added to the 2,2,4-trimethylpentane and mixed overnight. The total mass of this solution was measured, and the concentrations were calculated from this gravimetric procedure. These gravimetric concentrations were adjusted for the purity estimation of each component, which was determined using gas chromatography with flame ionization detection (GC-FID) with two stationary phases of different polarities and differential scanning calorimetry. This bulk solution was then chilled to approximately –5 °C and 1.2 mL aliquots were dispensed into 2 mL amber glass ampoules, which were then flame sealed.

Aliquots from six ampoules selected using a random stratified sampling scheme were analyzed in duplicate by using GC-FID with a non-polar 5 % phenyl methylpolysiloxane phase. The internal standards added to each sample for quantification purposes were 2-methyltetradecane (*iso*-pentadecane) and 3-methyltricosane. Calibration solutions consisting of weighed amounts of the compounds (adjusted for the purity estimation) and the internal standard compounds in 2,2,4-trimethylpentane were chromatographically analyzed to determine analyte response factors.

[(1)] Certain commercial equipment, instrumentation, or materials are identified in this certificate to adequately specify the experimental procedure. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the materials or equipment identified are necessarily the best available for the purpose.

Table 1. Certified Concentrations of Components in SRM 1494

Compound	CAS Registry No.[a]	Mass Fraction[b] (µg/g)	Concentration[c] (µg/mL)
n-decane	124-18-5	178.2 ± 4.5	122.9 ± 3.1
n-undecane	1120-21-4	203.2 ± 5.3	140.2 ± 3.7
n-dodecane	112-40-3	178.9 ± 4.4	123.4 ± 3.0
n-tridecane	629-50-5	167.7 ± 3.8	115.7 ± 2.6
n-tetradecane	629-59-4	166.1 ± 3.8	114.6 ± 2.6
n-pentadecane	629-62-9	161.9 ± 3.7	111.7 ± 2.6
n-hexadecane	544-76-3	141.1 ± 3.0	97.3 ± 2.1
n-heptadecane	629-78-7	131.7 ± 2.9	90.9 ± 2.0
pristane	1921-70-6	80.5 ± 2.1	55.5 ± 1.4
n-octadecane	593-45-3	121.9 ± 2.8	84.1 ± 1.9
phytane	638-36-8	9.31 ± 0.29	6.42 ± 0.20
n-nonadecane	629-92-5	105.2 ± 2.5	72.6 ± 1.7
n-eicosane	112-95-8	102.7 ± 4.4	70.9 ± 3.0
n-docosane	629-97-0	81.8 ± 1.8	56.4 ± 1.2
n-tetracosane	646-31-1	61.3 ± 1.8	42.3 ± 1.2
n-hexacosane	630.02-4	44.8 ± 1.2	30.9 ± 0.8
n-octacosane	646-31-1	30.71 ± 0.95	21.19 ± 0.66
n-triacontane	638-68-6	21.85 ± 0.65	15.07 ± 0.45
n-dotriacontane	544-85-4	17.58 ± 0.60	12.13 ± 0.41
n-tetratriacontane	14167-59-0	15.18 ± 0.43	10.47 ± 0.30

[a] Chemical Abstracts, Fourteenth Collective Index. Index Guide, American Chemical Society, Columbus, OH, 2001.

[b] The mass fraction results are expressed as the certified value ± the expanded uncertainty. The certified value is the average of the concentrations determined by gravimetric and chromatographic measurements. The expanded 95 % uncertainty uses a coverage factor of 2 and includes both correction for estimated purity and allowance for differences between the concentration determined by gravimetric preparation and chromatographic measurements [2].

[c] The concentrations listed in microgram per milliliter units were obtained by multiplying the certified values in micrograms per gram by the density of the solution at 22 °C (0.6899 g/mL). These concentrations are for use in the temperature range of 20 °C to 25 °C and an allowance for the change in density over this temperature range is included in the uncertainties.

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.; *Definitions of Terms and Modes Used at NIST for Value-Assignment 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 Apr 2013)

[2] 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 http://www.bipm.org/utils/common/documents/jcgm/JCGM_100_2008_E.pdf (accessed Apr 2013); 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 http://www.nist.gov/pml/pubs/tn1297/index.cfm (accessed Apr 2013).

Certificate Revision History: 17 April 2013 (Extended certification period; editorial changes); 04 July 2004 (Original certificate date).

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.