National Institute of Standards & Technology

Certificate of Analysis

Standard Reference Material 1491

Aromatic Hydrocarbons in Hexane/Toluene

This Standard Reference Material (SRM) is a solution of 24 aromatic hydrocarbons (AHs) in a hexane/toluene solvent blend containing 96% hexane by weight. Certified concentrations are provided for 23 of these AHs. A non-certified concentration is provided for 2-methylnaphthalene. This SRM is intended primarily for use in the calibration of chromatographic instrumentation used for the determination of the certified compounds. A unit of SRM 1491 consists of five 2-mL ampoules, each containing approximately 1.2 mL of solution.

Certified Concentrations of Constituent Aromatic Hydrocarbons

The certified concentrations and estimated uncertainties for the 23 aromatic hydrocarbons are given in Table 1. These values are based on results obtained from the gravimetric preparation of this solution and from analytical determinations using gas chromatography (GC).

Table 1. Certified Concentrations of Aromatic Hydrocarbons in SRM 1491

Compound	Concentration	
	µg/g[a]	µg/mL[b]
Naphthalene	10.30 ± 0.10	6.89 ± 0.07
1-Methylnaphthalene	12.4 ± 0.5	8.3 ± 0.3
Biphenyl	10.46 ± 0.04	7.00 ± 0.03
2,6-Dimethylnaphthalene	10.8 ± 0.4	7.2 ± 0.3
Acenaphthylene	10.40 ± 0.07	6.96 ± 0.05
Acenaphthene	10.89 ± 0.15	7.28 ± 0.10
2,3,5-Trimethylnaphthalene	9.9 ± 0.4	6.6 ± 0.2
Fluorene	10.87 ± 0.08	7.27 ± 0.05
Phenanthrene	10.48 ± 0.07	7.01 ± 0.05
Anthracene	11.69 ± 0.06	7.82 ± 0.04
1-Methylphenanthrene	10.4 ± 0.3	7.0 ± 0.2
Fluoranthene	8.84 ± 0.06	5.91 ± 0.04
Pyrene	8.81 ± 0.08	5.89 ± 0.06
Benz[*a*]anthracene	5.37 ± 0.04	3.59 ± 0.03
Chrysene	10.50 ± 0.06	7.03 ± 0.04
Benzo[*b*]fluoranthene	7.85 ± 0.05	5.25 ± 0.04
Benzo[*k*]fluoranthene	8.33 ± 0.12	5.57 ± 0.08
Benzo[*e*]pyrene	8.40 ± 0.04	5.62 ± 0.03
Benzo[*a*]pyrene	10.14 ± 0.09	6.79 ± 0.06
Perylene	10.65 ± 0.06	7.12 ± 0.04
Indeno[*1,2,3-cd*]pyrene	9.40 ± 0.07	6.29 ± 0.05
Dibenz[*a,h*]anthracene	7.74 ± 0.18	5.18 ± 0.12
Benzo[*ghi*]perylene	7.90 ± 0.13	5.29 ± 0.09

[a]The certified value is the weighted average of the gravimetric and chromatographic concentrations. The uncertainty of the certified value is the half-width of an approximate 95% confidence interval, plus an allowance for bias between the concentration based on the gravimetric preparation and the chromatographically determined concentration.

[b]These values listed in µg/mL units were obtained by multiplying the certified value by the measured density of the SRM solution at 22 °C (0.669 g/mL). These concentrations are for use over the temperature range of 20 to 25 °C.

August 31, 1989
Gaithersburg, MD 20899

Stanley D. Rasberry, Chief
Office of Standard Reference Materials

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Notice and Warning to Users

Handling: This material contains polycyclic aromatic compounds, many of which have been reported to have mutagenic and/or carcinogenic properties, and should be handled with care. Use proper disposal methods.

Expiration of Certification: The certified values are valid, within the limits specified, for three years from the date of purchase. In the event that the certification should become invalid before then, users will be notified by NIST. Please return the attached card to facilitate notification.

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 to 25 °C **immediately** after opening the ampoules and should be processed without delay for the certified concentrations in Table 1 to be valid within the stated uncertainty. Because of the volatility of hexane and toluene, certified values are not applicable to material stored in ampoules that have been opened for more than 2 minutes, even if they are resealed.

Preparation of the SRM and analytical determinations were performed in the Organic Analytical Research Division, Center for Analytical Chemistry, by R. M. Parris and R. E. Rebbert.

The coordination of the technical measurements leading to certification was under the direction of S. N. Chesler, and R. M. Parris.

Statistical consultations were provided by S. B. Schiller of the Statistical Engineering Division.

Partial support for the preparation and certification of this Standard Reference Material was provided by the National Oceanographic and Atmospheric Administration, National Ocean Service, Office of Oceanography and Marine Assessment.

The technical and support aspects involved in the preparation, certification, and issuance of this Standard Reference Material were coordinated through the Office of Standard Reference Materials by R. Alvarez.

Preparation and Analysis

All chemicals used in the preparation of this SRM were obtained from the Community Bureau of Reference (BCR), Brussels, Belgium or commercial sources. The AH solution was prepared at the National Institute of Standards and Technology (NIST) by weighing the individual AH components and toluene and mixing until completely dissolved. Hexane was added to this solution which was then thoroughly mixed. The total mass of this solution was measured and the concentrations calculated from this gravimetric procedure are given in Table 2. These gravimetric concentrations were adjusted for the consensus purity estimation of each component. For each BCR component, the certified mass fraction of the certified reference material was used as the consensus purity estimation after confirmation with flame ionization gas chromatography. The consensus purity estimations for the other aromatic hydrocarbon components were based on analyses using flame ionization gas chromatography and, where appropriate, liquid chromatography with absorbance detection and/or differential scanning calorimetry. This bulk solution was then chilled to approximately -5 °C and 1.2-mL aliquots were dispensed into 2-mL amber ampoules which were then flame sealed.

Aliquots from twelve randomly selected ampoules were analyzed in duplicate by using flame ionization capillary gas chromatography employing an immobilized non-polar stationary phase column. The three internal standards (ISs) added to each sample for quantification purposes were 1,2-dimethylnaphthalene, 1-ethylpyrene and m-tetraphenyl. Calibration solutions consisting of weighed amounts (adjusted for the consensus purity estimations) of the AH and IS compounds in a hexane-toluene solvent blend were chromatographically analyzed to determine analyte response factors. The chromatographically determined concentrations are also given in Table 2.

Non-certified concentrations of 2-methylnaphthalene and toluene, a representative chromatogram from the GC analysis, CAS Registry Numbers, and retention index data are shown in the Appendix.

Table 2. Summary of Results[a]

Compound	Concentration, μg/g	
	Calculated[b]	GC/FID[c]
Naphthalene	10.30	10.31 ± 0.05
1-Methylnaphthalene	12.48	12.23 ± 0.05
Biphenyl	10.45	10.46 ± 0.04
2,6-Dimethylnaphthalene	10.80	10.79 ± 0.03
Acenaphthylene	10.39	10.40 ± 0.04
Acenaphthene	10.88	10.89 ± 0.06
2,3,5-Trimethylnaphthalene	9.85	9.98 ± 0.03
Fluorene	10.87	10.88 ± 0.04
Phenanthrene	10.48	10.48 ± 0.07
Anthracene	11.69	11.70 ± 0.11
1-Methylphenanthrene	10.42	10.49 ± 0.12
Fluoranthene[d]	8.84	8.81 ± 0.07
Pyrene[d]	8.86	8.76 ± 0.06
Benz[*a*]anthracene[d]	5.36	5.39 ± 0.05
Chrysene	10.49	10.53 ± 0.08
Benzo[*b*]fluoranthene[d]	7.82	7.87 ± 0.05
Benzo[*k*]fluoranthene[d]	8.39	8.3 ± 0.2
Benzo[*e*]pyrene	8.41	8.38 ± 0.05
Benzo[*a*]pyrene	10.17	10.12 ± 0.05
Perylene	10.64	10.68 ± 0.10
Indeno[*1,2,3-cd*]pyrene[d]	9.40	9.41 ± 0.10
Dibenz[*a,h*]anthracene[d]	7.83	7.6 ± 0.2
Benzo[*ghi*]perylene[d]	7.83	7.98 ± 0.11

[a]The summary of results given above is presented for use only as background information. These values are not certified.

[b]Calculated concentration based on the mass of the AH compound in the total mass of the solution.

[c]Concentrations determined by using gas chromatography with flame ionization detection. The listed uncertainties represent one standard deviation of a single measurement and recognize only the within-method variability.

[d]These AH components used in the preparation of SRM 1491 were Certified Reference Materials from the Community Bureau of Reference (BCR), Commission of the European Communities, Brussels, Belgium.

Appendix to SRM Certificate

Standard Reference Material 1491

The following information is supplied for the convenience of the user of this Standard Reference Material. The information provided does not meet the requirements for certification by the National Institute of Standards and Technology.

Non-certified Quantitative Values

The following table contains supplementary analytical results obtained during the course of certification of this SRM. NIST does not recommend that this information be used for calibration, bias evaluation, or similar purposes for which certified values are used.

Because of the possibility of bias associated with the low purity of the 2-methylnaphthalene compound, a certified concentration was not determined. The concentration of toluene was calculated based only on gravimetric measurements made during the preparation of SRM 1491.

Table A-1. Non-certified concentrations

	Non-certified Concentration	
	Calculated[a]	GC/FID[b]
2-Methylnaphthalene	11.3 μg/g	11.8 ± 0.04 μg/g
Toluene	35.6 mg/g	

[a]Calculated concentration based on the mass of the component in the total mass of the solution.

[b]Concentration determined by using gas chromatography with flame ionization detection. The listed uncertainty represents one standard deviation of a single measurement and represents only the precision of the measurement process.

Descriptive Information

The following supplementary information may be of interest in connection with the use of this SRM.

A representative chromatogram from the GC analysis is shown in Figure A-1. The numbered peaks are identified in Table A-2. In addition, retention index data are provided in Table A-2 to assist the user in identifying the individual compounds in the SRM. These retention indices (which are not certified and are provided for information only) were determined at NIST using the method described by Lee et al. in Anal. Chem. 51, 768 (1979). Chemical Abstracts Service (CAS) Registry Numbers are also listed in Table A-2.

Table A-2. Retention Indices and Chemical Abstracts Service (CAS) Registry Numbers of Components of SRM 1491

Peak No.[a]	Compound	Retention Indices NIST	Retention Indices Literature Values[b]	CAS Registry No.[c]
1	Naphthalene	200.0	200.0	91-20-3
2	2-Methylnaphthalene	220.5	220.2	91-57-6
3	1-Methylnaphthalene	223.4	223.0	90-12-0
4	Biphenyl	236.4	236.4	92-52-4
5	2,6-Dimethylnaphthalene	240.4	240.3	581-42-0
6	Acenaphthylene	247.7	246.9	208-96-8
7	Acenaphthene	253.7	253.1	83-32-9
8	2,3,5-Trimethylnaphthalene	267.2	267.5	2245-38-7
9	Fluorene	269.9	269.7	86-73-7
10	Phenanthrene	300.0	300.0	85-01-8
11	Anthracene	301.4	301.1	120-12-7
12	1-Methylphenanthrene	323.5	323.6	832-69-9
13	Fluoranthene	344.5	344.5	206-44-0
14	Pyrene	351.9	351.5	129-00-0
15	Benz[*a*]anthracene	398.7	398.8	56-55-3
16	Chrysene	400.0	400.0	218-01-9
17	Benzo[*b*]fluoranthene	443.1	443.1	205-99-2
18	Benzo[*k*]fluoranthene	444.1	444.0	207-08-9
19	Benzo[*e*]pyrene	452.7	452.3	192-97-2
20	Benzo[*a*]pyrene	454.6	454.0	50-32-8
21	Perylene	457.6	457.2	198-55-0
22	Indeno[*1,2,3-cd*]pyrene	493.9	493.2	193-39-5
23	Dibenz[*a,h*]anthracene	495.9	496.2	53-70-3
24	Benzo[*ghi*]perylene	501.4	500.3	191-24-2

[a]See Figure A-1.

[b]D. L. Vassilaros, R. C. Kong, P. W. Later and M. L. Lee, J. Chromatogr. **252**, 1 (1982).

[c]Chemical Abstracts, Eleventh Collective Index, Index Guide, American Chemical Society, Columbus, Ohio 1986.

Figure A -1. **Capillary Gas Chromatogram of SRM 1491, Aromatic Hydrocarbons in Hexane/Toluene (Numbered peaks are identified in Table A-2.)**