National Institute of Standards & Technology

Certificate of Analysis

Standard Reference Material 2260

Aromatic Hydrocarbons in Toluene (Nominal Concentration 60 μg/mL)

This Standard Reference Material (SRM) is a solution of 24 aromatic hydrocarbons (AHs) in toluene. Certified concentrations are provided for 23 of these AHs. A noncertified concentration is provided for 2-methylnaphthalene. This SRM is intended primarily for use in the calibration of chromatographic instruments used for the determination of the certified compounds. A unit of SRM 2260 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 the analytical results determined by using gas chromatography.

Notice and Warning to Users

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

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, purchasers will be notified by NIST. Please return the attached registration card to facilitate notification.

Storage: Sealed ampoules, as received, should be stored in the dark at temperatures between 10 and 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Use: Sample aliquots for analysis should be withdrawn at 20 to 25 °C immediately after opening the ampoules and should be processed without delay for the certified concentrations in Table 1 to be valid within the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 toluene, 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 analytical determinations were performed at the NIST Center for Analytical Chemistry, Organic Analytical Research Division, by R. M. Parris and R. E. Rebbert.

The coordination of the technical measurements leading to certification was under the direction of R. M. Parris and R. E. Rebbert.

Statistical analysis was provided by S. B. Schiller of the NIST Center for Computing and Applied Mathematics, Statistical Engineering Division.

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The technical and support aspects involved in the preparation, certification, and issuance of this Standard Reference Material were coordinated through the Standard Reference Materials Program by T. E. Gills.

Gaithersburg, MD 20899
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Standard Reference Materials Program

Table 1. Certified Concentrations of Aromatic Hydrocarbons in SRM 2260

Compound[a]	Concentration	
	$\mu g/g^b$	$\mu g/mL^c$
Naphthalene	76.3 ± 1.1	66.0 ± 1.1
1-Methylnaphthalene	75.7 ± 4.0	65.5 ± 3.6
Biphenyl	76.14 ± 0.46	65.84 ± 0.58
2,6-Dimethylnaphthalene	75.9 ± 3.5	65.6 ± 3.2
Acenaphthylene	73.09 ± 0.48	63.20 ± 0.59
Acenaphthene	78.9 ± 1.6	68.2 ± 1.6
2,3,5-Trimethylnaphthalene[d]	67.5 ± 3.5	58.4 ± 3.2
Fluorene	75.62 ± 0.61	65.38 ± 0.70
Phenanthrene	76.01 ± 0.75	65.72 ± 0.82
Anthracene	57.54 ± 0.44	49.75 ± 0.52
1-Methylphenanthrene	75.2 ± 2.2	65.0 ± 2.1
Fluoranthene	76.31 ± 0.75	65.98 ± 0.83
Pyrene	76.20 ± 0.79	65.89 ± 0.86
Benz[*a*]anthracene	66.0 ± 1.7	57.1 ± 1.6
Chrysene	76.6 ± 1.9	66.2 ± 1.9
Benzo[*b*]fluoranthene	75.97 ± 0.46	65.68 ± 0.57
Benzo[*k*]fluoranthene	75.67 ± 0.87	65.42 ± 0.93
Benzo[*e*]pyrene	75.98 ± 0.89	65.69 ± 0.95
Benzo[*a*]pyrene	68.61 ± 0.52	59.32 ± 0.61
Perylene	57.48 ± 0.26	49.69 ± 0.36
Indeno[1,2,3-*cd*]pyrene	67.4 ± 1.1	58.3 ± 1.1
Dibenz[*a,h*]anthracene	57.1 ± 1.6	49.3 ± 1.5
Benzo[*ghi*]perylene	67.9 ± 1.6	58.7 ± 1.5

[a]The compounds are listed in the order of their elution from a nonpolar gas chromatographic column.

[b]The certified value is an equally weighted mean of the gravimetric and average chromatographic concentrations. The uncertainty of the certified value is the half-width of a 95% confidence interval for the mean, with an allowance for systematic error between the methods. A significant portion of the total uncertainty is due to the uncertainty in the purity determinations of the AH materials.

[c]The values listed in $\mu g/mL$ units were obtained by multiplying the certified value (prior to rounding) by the density of toluene at 22.5 °C (0.8646 g/mL). These concentrations are for use in the temperature range of 20 to 25 °C and an allowance for the change in the density over this temperature range is included in the uncertainties.

[d]The CAS nomenclature for this compound is 1,6,7-trimethylnaphthalene.

Preparation and Analysis

All chemicals used in the preparation of this SRM were obtained from commercial sources or the Community Bureau of Reference (BCR), Brussels, Belgium. 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 and homogenized. The total mass of this solution was then measured. The calculated concentration based on the mass of the AH compound (adjusted for its consensus purity estimate) in the total mass of the solution is given in Table 2 for each component. For each component obtained from the BCR, the certified mass fraction of the certified reference material was used as the consensus purity estimation after NIST confirmation of this purity with capillary gas chromatography with flame ionization detection (GC-FID). The consensus purity estimations for the aromatic hydrocarbon components obtained from commercial sources were based on NIST analyses using GC-FID 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 that were then flame sealed.

Aliquots from 12 randomly selected ampoules were analyzed by using GC-FID with an immobilized nonpolar stationary phase capillary column. The three internal standards added to each sample for quantification purposes were 1,2-dimethylnaphthalene, 1-ethylpyrene and m-tetraphenyl. Calibration solutions consisting of weighed amounts of NIST SRM 1491 (Aromatic Hydrocarbons in Hexane/Toluene) and the internal standard solution were chromatographically analyzed to determine analyte response factors. The chromatographically determined concentrations are also given in Table 2.

The noncertified concentration of 2-methylnaphthalene, a representative chromatogram from the GC analysis, CAS Registry Numbers, and retention index data are shown in the Appendix.

Table 2. Summary of Calculated and Chromatographic Results[a]

Compound	Concentration, μg/g	
	Calculated[b]	GC/FID[c]
Naphthalene	76.5	76.1 (0.8)
1-Methylnaphthalene	75.9	75.5 (0.3)
Biphenyl	76.4	75.9 (0.1)
2,6-Dimethylnaphthalene	76.1	75.7 (0.1)
Acenaphthylene	73.2	73.0 (0.2)
Acenaphthene	79.1	78.8 (0.1)
2,3,5-Trimethylnaphthalene	68.2	66.8 (0.2)
Fluorene	75.7	75.5 (0.1)
Phenanthrene	76.3	75.7 (0.4)
Anthracene	57.7	57.4 (0.3)
1-Methylphenanthrene	75.8	74.6 (0.5)
Fluoranthene[d]	76.1	76.5 (0.5)
Pyrene[d]	76.2	76.2 (0.6)
Benz[*a*]anthracene[d]	65.6	66.4 (1.1)
Chrysene	76.3	76.9 (1.4)
Benzo[*b*]fluoranthene[d]	76.0	75.9 (0.6)
Benzo[*k*]fluoranthene[d]	76.0	75.3 (0.6)
Benzo[*e*]pyrene	76.3	75.7 (0.6)
Benzo[*a*]pyrene	68.7	68.5 (0.3)
Perylene	57.5	57.5 (0.2)
Indeno[1,2,3-*cd*]pyrene[d]	67.5	67.3 (1.1)
Dibenz[*a,h*]anthracene[d]	57.6	56.6 (1.1)
Benzo[*ghi*]perylene[d]	67.5	68.2 (1.4)

[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 (adjusted for consensus purity estimate, see text) in the total mass of the solution.

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

[d]These AH components used in the preparation of SRM 2260 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 2260

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.

Noncertified 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 value was not determined.

Table A-1. Noncertified concentration

	Noncertified Concentration, $\mu g/g$	
Compound	Calculated[a]	GC/FID[b]
2-Methylnaphthalene	75.3	73.2 (0.5)

[a]Calculated concentration based on the mass of the component (adjusted for consensus purity estimate) 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, gas chromatographic 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. Gas Chromatographic Retention Indices and Chemical Abstracts Service (CAS) Registry Numbers of Components of SRM 2260

Peak No.[a]	Compound	Retention Indices NIST Values[b]	Literature Values[c]	CAS Registry No.[d]
1	Naphthalene[e]	200.00	200.00	91-20-3
2	2-Methylnaphthalene	220.69 (0.02)	220.22 (0.23)	91-57-6
3	1-Methylnaphthalene	223.72 (0.02)	223.01 (0.28)	90-12-0
4	Biphenyl	236.20 (0.03)	236.44 (0.19)	92-52-4
5	2,6-Dimethylnaphthalene	240.39 (0.03)	240.28 (0.22)	581-42-0
6	Acenaphthylene	247.89 (0.02)	246.92 (0.31)	208-96-8
7	Acenaphthene	254.01 (0.12)	253.14 (0.28)	83-32-9
8	2,3,5-Trimethylnaphthalene[f]	267.23 (0.03)	267.54 (0.17)	2245-38-7
9	Fluorene	270.08 (0.02)	269.73 (0.30)	86-73-7
10	Phenanthrene[e]	300.00	300.00	85-01-8
11	Anthracene	301.68 (0.14)	301.08 (0.11)	120-12-7
12	1-Methylphenanthrene	323.77 (0.01)	323.64 (0.42)	832-69-9
13	Fluoranthene	344.48 (0.02)	344.51 (0.06)	206-44-0
14	Pyrene	352.16 (0.02)	351.51 (0.15)	129-00-0
15	Benz[*a*]anthracene	398.59 (0.03)	398.76 (0.04)	56-55-3
16	Chrysene[e]	400.00	400.00	218-01-9
17	Benzo[*b*]fluoranthene	443.22 (0.03)	443.13 (0.11)	205-99-2
18	Benzo[*k*]fluoranthene	444.20 (0.02)	444.02 (0.07)	207-08-9
19	Benzo[*e*]pyrene	453.20 (0.05)	452.29[g]	192-97-2
20	Benzo[*a*]pyrene	454.91 (0.03)	454.02 (0.07)	50-32-8
21	Perylene	458.17 (0.03)	457.17 (0.06)	198-55-0
22	Indeno[1,2,3-*cd*]pyrene	494.33 (0.04)	493.24 (0.09)	193-39-5
23	Dibenz[*a*,*h*]anthracene (Picene[e])	495.87 (0.04) 500.00	496.20 (0.30)	53-70-3
24	Benzo[*ghi*]perylene	502.02 (0.04)	500.29 (0.05)	191-24-2

[a]See Figure A-1.

[b]Retention index value is the mean of eight determinations and the uncertainty, listed in parentheses, is one standard deviation of the mean.

[c]D. L. Vassilaros, R. C. Kong, P. W. Later and M. L. Lee, Linear Retention Index System for Polycyclic Aromatic Compounds: Critical Evaluation and Additional Indices, J. Chromatogr. 252, 1-20 (1982).

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

[e]In this linear retention index system for temperature-programmed capillary gas chromatography of PAH, naphthalene, phenanthrene, chrysene and picene (with defined retention indices of 200, 300, 400, and 500, respectively) are used as the internal standards for calculating the retention indices of the other compounds.

[f]The CAS nomenclature for this compound is 1,6,7-trimethylnaphthalene.

[g]The retention times of chrysene and benzo[e]pyrene were used to calculate this retention time of picene (see footnote e).

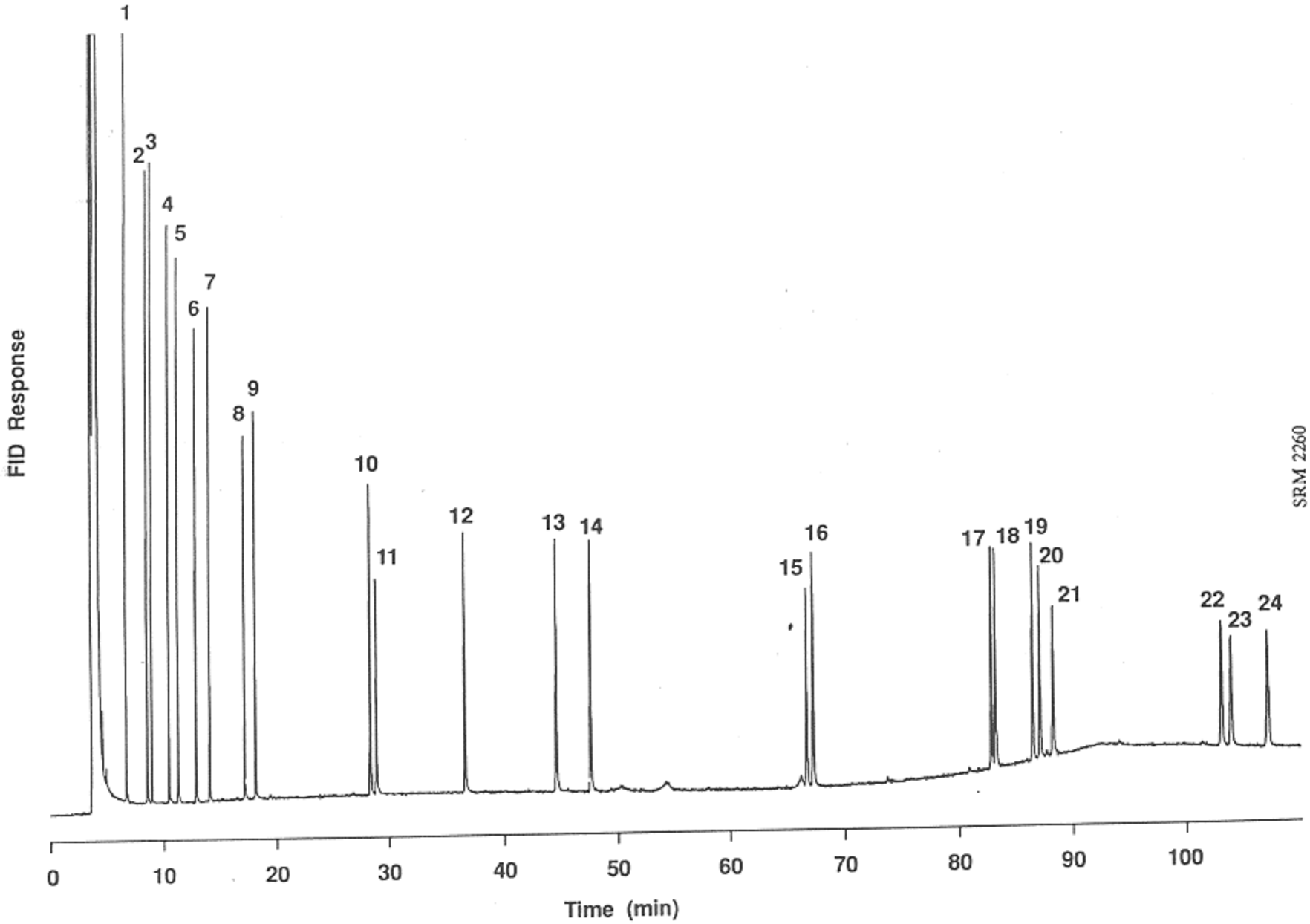

Figure A-1. Capillary Gas Chromatogram of SRM 2260 (numbered peaks are identified in Table A-2)