National Institute of Standards & Technology

Certificate

Standard Reference Material® 2035

Near Infrared Transmission Wavelength Standard from 10 300 cm^{-1} to 5130 cm^{-1}

This Standard Reference Material (SRM) is a certified transfer standard intended for the verification and calibration of the wavenumber/wavelength scale of near infrared spectrometers operating in transmission mode. SRM 2035 is certified for the location of the center of gravity (COG) of seven absorbance bands in the spectral range from 10 300 cm^{-1} (971 nm) to 5130 cm^{-1} (1949 nm) at six spectral bandwidths from 4 cm^{-1} to 128 cm^{-1}.

SRM 2035 is a glass filter consisting of a mole fraction 3.00 % holmium oxide (Ho_2O_3), a mole fraction of 1.30 % samarium oxide (Sm_2O_3), a mole fraction of 0.68 % ytterbium oxide (Yb_2O_3), and a mole fraction of 0.47 % neodymium oxide (Nd_2O_3) in a base glass containing lanthanum oxide (La_2O_3). The filter is 25 mm in diameter and 1.5 mm thick in an optical mount. This combination of the rare earth oxide concentrations and filter thickness yields absorption bands between 0.1 and 0.6 absorbance units.

Certification: The certified band locations for the SRM 2035 absorbance spectrum are given in Tables 1 and 2 of this certificate.

Expiration of Certification: The certification of this SRM is valid, within the measurement uncertainties specified, until **31 December 2003**, provided the SRM is handled and stored in accordance with the instructions given in this certificate. However, the certification is nullified if the SRM is modified or physically damaged.

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. Return of the attached registration card will facilitate notification.

The production and certification of SRM 2035 was performed by S.J. Choquette and J.C. Travis with the assistance of C. Zhu of the NIST Analytical Chemistry Division.

The SRM filters were cut and polished by J. Fuller of the NIST Fabrication Technology Division.

The overall direction and coordination of the technical measurements leading to certification were performed by S.J. Choquette and G.W. Kramer of the NIST Analytical Chemistry Division.

Statistical consultation was provided by J.J. Filliben of the NIST Statistical Engineering Division.

The support aspects involved in the issuance of this SRM were coordinated through the Standard Reference Materials Program by R.J. Gettings.

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Certificate Issue Date: 22 February 1999

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Measurement Conditions: The certification measurements were made using a Bruker IFS 66 Fourier Transform (FT) spectrophotometer[1]. The NIST spectrophotometer was calibrated in vacuum wavenumber units using NIST SRM 2517 Wavelength Reference Absorption Cell-Acetylene and water vapor bands. Details of the measurements and data analysis can be found in Reference [1].

Certified Values: The certified vacuum wavenumber locations for seven bands from 10 300 cm^{-1} to 5130 cm^{-1} and six spectral bandwidths at 24 °C ± 1.5 °C are given below in Table 1. When using these filters to verify the wavenumber scale of a spectrometer, the certified values that are most representative of the spectral bandwidth of the spectrometer being tested should be used. The absorbance spectrum of SRM 2035 is illustrated in Figure 1 of this certificate. Also shown in Figure 1 is the single channel air reference spectrum (arbitrary units). Atmospheric water vapor is a significant source of variance for band 3 and the associated peak should be used with caution when calibrating commercial spectrometers with SRM 2035.

The certified values for wavelength peak locations for seven bands of SRM 2035 from 971 nm to 1949 nm and six spectral bandwidths determined by the COG method at 24 °C ± 1.5 °C are given in Table 2. These wavelength locations were derived from the constant-wavenumber-resolution FT data.

Reference Values: The reference values [2] of the wavelength band locations at constant wavelength resolution are given in Table 3. The band locations were corroborated with measurements from the commercial spectrophotometer used in the certification of NIST SRM 1920 Near Infrared Reflectance Wavelength Standard [3].

Information Values: Information values [2] of the peak wavelength and wavenumber positions of SRM 2035 derived using the Bruker maximum-finding method (four-point polynomial fit to the top of the peak) are listed in Table 4. These values may be useful in comparing SRM 2035 peak locations on a spectrometer that lacks a center-of-gravity peak location algorithm.

Wavenumber and Wavelength Band Location Methodology: The method used to determine the certified wavenumber (ν) and reference wavelength (λ) band locations of SRM 2035 is the COG technique [4,5]. If another technique is used, a comparison with the certified values may not be valid. In this certificate, positions determined with the COG algorithm are referred to as *band* locations, whereas those determined by other techniques are referred to as *peak* locations. Only those values listed in Table 4 are peak locations. For COG calculations, a 10 % fraction was used for both wavenumber and wavelength absorption data. Table 2 lists the certified values for the wavelength locations of SRM 2035 determined by the COG method. These values were derived from the certified FT spectrometer measurements by converting wavenumber scale to air wavelength. Because resolution varies nonlinearly when converting from the wavenumber to the wavelength scale, the appropriate wavelength bandwidth is listed for each band. Table 3 lists the calculated wavelength band locations at constant wavelength bandwidth. These values were determined by interpolating the appropriate data from Table 2. Because all sources of error and bias have not been fully investigated in this procedure, the locations in Table 3 are reference values.

NIST will provide, upon request, a copy of the COG algorithm used for band certification by contacting S.J. Choquette at <steven.choquette@nist.gov> or fax 301-977-0587.

Certification Uncertainty: The expanded uncertainty (U) for the peak wavenumber and wavelength values is given in Tables 1 to 3. U is determined from the root-mean-square combination of component standard uncertainties (i.e. estimated standard deviations) and a coverage factor $k = 2$ computed according to reference [6]. The coverage factor defines the interval within which the unknown value of the band wavenumber location can be asserted to lie with a level of confidence of approximately 95 %. Components of the uncertainty include: calibration of the NIST FT spectrometer with SRM 2517 [7], COG location estimate, location shift due to temperature, and water vapor interference. Expanded uncertainties for the reference wavelength values include propagation of errors in the interpolation technique.

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[1]Certain commercial equipment is identified to specify adequately the experimental procedure. Such identification does not imply a recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the equipment is the best available for the purpose.

Temperature Coefficients: The filter temperature can be a significant source of variance of the band location. Band locations of the filter were determined using the COG algorithm with a 10 % fraction over a temperature range between 6 °C and 50 °C. The location of each absorbance band as a function of temperature was determined by least squares fit to obtain the fit temperature coefficients given in Table 5. The uncertainties of the values listed in Tables 1 to 3 include a temperature variation of 3 °C uniformly distributed around a nominal measurement temperature of 24 °C.

Handling and Storage: To maintain the integrity of SRM 2035, the filter should only be handled in its optical mount. While not in use, the SRM should be stored in the container provided or one with similar or better mechanical protection.

Instructions for Use: Carefully insert SRM 2035 into the sample beam of the spectrometer being tested. Measurements under a dry nitrogen purge are highly recommended. If a nitrogen purge is not available, the location of band 3 may significantly differ from the certified values. Acquire the absorbance spectrum, referenced to air, at a nominal temperature of 24 °C ± 1.5 °C. Compare each measured band location to its certified value listed in Table 1 or 3 for the spectral bandwidth most representative of the spectrophotometer being used. Band locations in Table 1 are vacuum wavenumber values, while those in Tables 2 and 3 are air wavelength values. To convert between the values in Tables 1 and 2, the appropriate correction for the index of refraction of air must be applied [8]. Taking into account the certification uncertainty of each band of SRM 2035, any significant differences between the measured and certified band locations may then be used to recalibrate the spectrometer wavenumber scale.

REFERENCES

[1] Choquette, S.J., Travis, J.C., and Zhu, C., "Production and Certification of SRM 2035, Near Infrared Transmission Wavelength Standard," NIST Special Publication 260-xxx, (1999). (In preparation)

[2] May, W.E. and Parris, R.E., "Definitions of Terms and Modes Used at NIST for Value-Assignment of Reference Materials for Chemical Measurements," NIST Special Publication 260-136. (In preparation)

[3] Weidner, V.R., Barnes, P.Y., and Eckerle, K.L., " A Wavelength Standard for the Near Infrared Based on the Reflectance of Rare-Earth Oxides," NBS Journal of Research, **Vol. 91**, No.5, pp. 243-253, (September-October 1986).

[4] Cameron, D.G., Kauppinen, J.K, Moffat, J.K., and Mantsch, H.H., "Precision in Condensed Phase Vibrational Spectroscopy," *Appl., Spectrosc.* **36**, pp. 245-250, (1982).

[5] Zhu, C. and Hanssen, L.M., "Studies of a Polystyrene Wavenumber Standard for Infrared Spectrometry," *11th International Conference of Fourier Transform Spectrometry, AIP proceedings **430***, Ed. J.A. de Haseth, pp. 491-494, American Institute of Physics, NY, (1998).

[6] *Guide to the Expression of Uncertainty in Measurement*, ISBN 92-67-10188-9, lst Ed. ISO, Geneva, Switzerland, (1993): 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).

[7] Gilbert, S.L. and Swann, W.C., "Standard Reference Materials: Acetylene C_2H_2 Absorption Reference for 1510 nm-1540 nm Wavelength Calibration- SRM 2517," NIST Special Publication 260-133, (1997).

[8] Eden, B., "The Refractive Index of Air," Metrologia, **2**, p. 12, (1966).

Users of this SRM should ensure that the certificate in their possession is current. This can be accomplished by contacting the SRM Program at: Telephone (301) 975-6776 (select "Certificates"), Fax (301) 926-4751, e-mail srminfo@nist.gov, or via the Internet http://ts.nist.gov/srm.

Table 1. Certified[1] Band Locations[2] of SRM 2035 and Uncertainties[3] at Constant Wavenumber Resolution

Resolution cm^{-1}	Band 1 cm^{-1}	Band 2 cm^{-1}	Band 3 cm^{-1}	Band 4 cm^{-1}	Band 5 cm^{-1}	Band 6 cm^{-1}	Band 7 cm^{-1}
4	5138.45 ± 0.2	6804.65 ± .05	7313.46 ± 0.66	8178.58 ± 0.24	8681.56 ± 0.27	9293.38 ± 0.29	10 245.43 ± 0.15
8	5138.52 ± 0.2	6804.55 ± 0.33	7313.32 ± .032	8178.67 ± 0.24	8682.08 ± 0.18	9294.00 ± 0.28	10 245.21 ± 0.12
16	5138.64 ± 0.2	6804.72 ± 0.33	7313.48 ± 0.16	8178.83 ± 0.24	8682.61 ± 0.18	9293.96 ± 0.28	10 244.82 ± 0.12
32	5139.01 ± 0.2	6805.22 ± 0.33	7313.63 ± 0.15	8179.37 ± 0.24	8684.34 ± 0.18	9294.05 ± 0.28	10 243.73 ± 0.12
64	5139.44 ± 0.2	6806.66 ± 0.33	7313.82 ± 0.15	8181.22 ± .024	8687.91 ± .018	9294.67 ± 0.28	10 242.74 ± 0.12
128	5135.5 ± 0.2	6807.11 ± 0.33	7309.10 ± 0.22	8185.68 ± 0.24	8685.89 ± 0.18	9296.67 ± 0.28	10 248.77 ± 0.12

1. A NIST Certified Value represents data reported on an SRM Certificate for which NIST has the highest confidence in its accuracy in that all known or suspected sources of bias have been fully investigated or accounted for by NIST.
2. Band location determined using a center-of-gravity method with $f = 0.1$
3. Uncertainties represent U, the expanded uncertainty with coverage factor $k = 2$

Table 2. Summary of Certified[1] Center-of-Gravity Band Locations of SRM 2035 Air Wavelengths[2]
Constant Wavenumber Resolution

	4 cm^{-1}		8 cm^{-1}		16 cm^{-1}		32 cm^{-1}		64 cm^{-1}		128 cm^{-1}	
Band	Position nm	Resolution[3] nm	nm	Resolution nm	Nm	Resolution nm	Nm	Resolution nm	Nm	Resolution nm	Nm	Resolution nm
1	1945.61 (0.079)[4]	1.52	1945.59 (0.078)	3.03	1945.55 (0.078)	6.06	1945.41 (0.078)	12.12	1945.27 (0.079)	24.24	1946.87 (0.087)	48.49
2	1469.24 (0.074)	0.86	1469.23 (0.076)	1.73	1469.19 (0.075)	3.46	1469.09 (0.074)	6.91	1468.77 (0.073)	13.82	1468.69 (0.074)	27.65
3	1367.04 (0.51)	0.75	1367.01 (0.50)	1.50	1366.99 (0.050)	2.99	1366.96 (0.050)	5.98	1366.93 (0.50)	11.97	1367.81 (0.50)	23.93
4	1222.39 (0.039)	0.60	1222.38 (0.037)	1.20	1222.36 (0.037)	2.39	1222.28 (0.037)	4.78	1222.00 (0.038)	9.57	1221.35 (0.039)	19.14
5	1151.51 (0.029)	0.53	1151.49 (0.030)	1.06	1151.43 (0.030)	2.12	1151.20 (0.027)	4.25	1150.72 (0.028)	8.49	1151.00 (0.046)	16.99
6	1075.69 (0.037)	0.46	1075.70 (0.037)	0.93	1075.70 (0.037)	1.85	1075.69 (0.036)	3.71	1075.62 (0.034)	7.41	1075.38 (0.035)	14.82
7	975.79 (0.013)	0.38	975.798 (0.013)	0.76	975.84 (0.012)	1.52	975.95 (0.012)	3.05	976.041 (0.012)	6.10	975.48 (0.014)	12.20

1. A NIST Certified Value represents data reported on an SRM Certificate for which NIST has the highest confidence in its accuracy in that all known or suspected sources of bias have been fully investigated or accounted for by NIST.
2. Data acquired on an FT spectrometer and converted to air wavelength at constant wavenumber resolution
3. Resolution in wavelengths (λ) is related to wavenumbers (ν) by: $d\lambda = -\frac{1}{\nu^2} d\nu$
4. Data in parenthesis is the expanded uncertainty U with a coverage factor of $k = 2$ for the indicated peak

Table 3. Reference Values[1] of COG Wavelength Band Locations for SRM 2035 Interpolated from FT Data. Constant Wavelength Resolution

Band	1 nm	3 nm	5 nm	10 nm	U^2
1	1945.6	1945.6	1945.6	1945.6	1
2	1469.2	1469.2	1469.1	1469.3	1
3	1367.0	1367.0	1367.0	1367.2	2
4	1222.4	1222.3	1222.3	1222.3	1
5	1151.5	1151.3	1151.1	1150.9	1
6	1075.7	1075.7	1075.7	1075.8	1
7	975.8	975.9	976	975.9	1

1. A NIST Reference Value is a best estimate of the true value provided on a NIST Certificate/Certificate of Analysis/Report of Investigation where all known or suspected sources of bias have not been fully investigated by NIST.
2. U is the expanded uncertainty with a coverage factor of $k = 2$ for the indicated band

Table 4. Summary of Maximum Peak Location[1] for SRM 2035: Information Values[2]

4 cm^{-1} bandwidth		8 cm^{-1} bandwidth		16 cm^{-1} bandwidth		32 cm^{-1} bandwidth		64 cm^{-1} bandwidth		128 cm^{-1} bandwidth	
Nm	cm^{-1}	Nm	cm^{-1}	Nm	cm^{-1}	Nm	cm^{-1}	nm	cm^{-1}	nm	cm^{-1}
1945.8	5137.9	1945.7	5138.0	1945.7	5138.2	1945.47	5138.8	1945.2	5139.5	1946.2	5136.9
1469.6	6803.9	1469.4	6803.4	1469.3	6804.0	1469.20	6804.6	1468.8	6806.3	1468.6	6807.4
1366.4	7316.5	1366.8	7315.2	1366.9	7314.0	1366.95	7313.6	1366.9	7313.9	1367.6	7310.0
1222.5	8178.0	1222.5	8177.3	1222.5	8178.0	1222.39	8178.5	1222.1	8180.5	1221.4	8185.5
1151.7	8680.6	1151.7	8680.9	1151.6	8681.6	1151.29	8683.6	1150.7	8687.7	1150.9	8686.3
1075.7	9294.0	1075.7	9294.1	1075.7	9293.9	1075.67	9294.0	1075.6	9294.5	1075.4	9296.9
975.8	10245.6	975.8	10245.4	975.8	10245.0	975.93	10243.8	976.0	10242.7	975.5	10248.5

1. Peak locations are determined using a four-point polynomial fit to the top of the band, wavelength (λ) in air, wavenumbers (υ) are corrected to vacuum.
2. A NIST information value is considered to be a value that will be of interest and use to the user, but insufficient information is available to access the uncertainty associated with the value.

Table 5. Temperature Coefficients for Band Locations of SRM 2035: Information Values[1].

Band	Nominal Band Location	Coefficient (cm^{-1}/ °C)	Coefficient (nm/°C)
1	5138.45	-0.051	0.019
2	6804.65	0.091	-0.02
3	7313.46	0.017	-0.0032
4	8178.58	0.062	-0.0093
5	8681.56	-0.042	0.0056
6	9293.38	-0.076	0.0088
7	10245.43	0.019	-0.0018

1. A NIST information value is considered to be a value that will be of interest and use to the user, but insufficient information is available to access the uncertainty associated with the value.

Figure 1.
Near Infrared Spectrum of SRM 2035 and Single Beam Air Reference