National Institute of Standards & Technology

Certificate

Standard Reference Material® 2035b

Ultraviolet-Visible-Near-Infrared Wavelength/Wavenumber Transmission Standard

This Standard Reference Material (SRM) is a certified transfer standard intended for the verification and calibration of the wavenumber/wavelength scale of ultraviolet-visible (UV-Vis) and near infrared (NIR) spectrometers operating in transmission mode. A unit of SRM 2035b consists of an optical filter, 25 mm in diameter and 1.5 mm thick, that should be handled in its original optical mount and stored in the wooden container provided.

SRM 2035b is a glass filter consisting of mole fractions of 3.00 % holmium oxide (Ho_2O_3), 1.30 % samarium oxide (Sm_2O_3), 0.68 % ytterbium oxide (Yb_2O_3), and 0.47 % neodymium oxide (Nd_2O_3) in a matrix containing lanthanum oxide (La_2O_3), boron oxide (B_2O_3), silicon dioxide (SiO_2), and zirconium dioxide (ZrO_2).

Certification: 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. In this certificate, spectral features are referred to as *bands* if their location is determined by the center-of-gravity (COG) or centroid algorithm, whereas those determined by a five point cubic polynomial fit are referred to as *peak* locations. SRM 2035b is certified for the 10 % band fraction centroid of seven bands spanning the spectral region from 10 300 cm^{-1} to 5 100 cm^{-1} at 8 cm^{-1} resolution (vacuum wavenumber). The same seven bands are certified for the 10 % band fraction centroid location in the spectral region from 971 nm to 1960 nm at 1 nm and 3 nm spectral bandwidths (air wavelength). The certified absorption band locations for these seven bands are given in Table 1 for vacuum wavenumber and Table 2 for air wavelength. SRM 2035b is certified for thirteen additional peak locations in the spectral region from 334 nm to 805 nm at 1 nm and 3 nm spectral bandwidths. The certified transmittance peak locations for these thirteen peaks are given in Table 3 for air wavelength.

Expiration of Certification: The certification of **SRM 2035b** is valid, within the measurement uncertainty specified, until **01 January 2027**, 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 or register online) will facilitate notification.

Overall direction and coordination of the technical measurements leading to the certification of this SRM were provided by S.J. Choquette of NIST.

Production and certification of SRM 2035b was conducted by A.A. Urbas of the NIST Chemical Sciences Division.

Statistical consultation was provided by H. Iyer of the NIST Statistical Engineering Division.

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

Carlos A. Gonzalez, Chief
Chemical Sciences Division

Gaithersburg, MD 20899
Certificate Issue Date: 12 January 2018

Steven J. Choquette, Director
Office of Reference Materials

INSTRUCTIONS FOR HANDLING, STORAGE, AND USE

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

Use: Carefully insert SRM 2035b into the sample beam of the spectrometer being tested. Measurements under a dry (air or nitrogen) purge are highly recommended for NIR measurements. If a dry purge is not available, the locations of band 1 and band 3 may differ significantly from the certified values. Acquire the absorbance/transmittance spectrum, referenced to air at a nominal temperature between 20 ºC and 25 ºC. Compare measured band or peak locations to its certified value listed in the appropriate table (Tables 1, 2 and 3). Band locations in Table 1 (NIR) are vacuum wavenumber values at constant 8 cm^{-1} resolution. Investigations have shown that these band locations remain within the stated uncertainties for resolutions higher than 8 cm^{-1} (e.g., 4 cm^{-1}, 2 cm^{-1}, etc.); however, they are not certified for use with resolutions lower than 8 cm^{-1}. Band locations in Table 2 (NIR) are air wavelength values at spectral bandwidths of 1 nm and 3 nm. Peak locations in Table 3 (UV-Vis) are air wavelength values at spectral bandwidths of 1 nm and 3 nm. Comparison should be made to the spectral bandwidth more representative of the spectrometer being used. Taking into account the certification uncertainty of each band of SRM 2035b, any statistically significant differences between the measured and certified band locations may be used to recalibrate the spectrometer wavenumber/wavelength scale. For air wavelength measurements, a data point spacing equal to or less than 0.5 nm is recommended. For vacuum wavenumber measurements, a data point spacing equal to or less than 1.0 cm^{-1} is recommended.

PREPARATION AND ANALYSIS[(1)]

Preparation: The SRM glass composition was melted at Schott Glass (Duryea, PA). The finished SRM filters were supplied to NIST by Avian Technologies (Sunapee, NH).

Measurement Conditions: Certification of SRM 2035b was accomplished by careful comparative measurements to SRM 2035a on several spectrometer systems. This represents a departure from the certification procedures used in prior related SRMs (2035, 2035a and 2065) based on the same nominal glass composition and format. Certification measurements were conducted by analyzing multiple SRM 2035a and SRM 2035b units under identical measurements conditions on each instrument. For NIR vacuum wavenumber band locations, measurements were performed on a Bruker Vertex-70 Fourier-transform (FT) spectrometer. For NIR air wavelength band locations, measurements were performed on Perkin Elmer Lambda 900 and Cary 6000i dispersive spectrometers, and the Bruker Vertex-70 FT spectrometer. The Bruker Vertex-70 FT was calibrated in air wavelength by applying the appropriate correction for the refractive index of air [1] to the calibrated vacuum wavenumber axis. For UV-Vis air wavelength peak locations, measurements were performed on Perkin Elmer Lambda 900 and Cary 6000i spectrometers. These spectrometers and several others were used in the certification of SRM 2035a, which was based on a multi-instrument consensus. The certified values are metrologically traceable to the SI unit of meters (m). SRM 2035b is traceable to the SI through SRM 2035a.

Wavenumber and Wavelength Band/Peak Location Methodology: The method used to determine the certified NIR wavenumber (υ) and wavelength (λ) band locations of SRM 2035b is the center-of-gravity (COG) technique [2-5]. *If another technique is used, a comparison with the certified values will not be valid*. In this certificate, positions determined with the centroid algorithm are referred to as *band* locations. Values listed in Tables 1 and 2 are band locations. For SRM 2035b COG calculations, 10 % fractions of the bands were used for both wavenumber and wavelength data. Further information on the use of this algorithm with other NIST SRMs can be found in References [6–8]. The method used to determine the certified UV-Vis wavelength (λ) peak locations of SRM 2035b was a cubic polynomial fit to five points spanning the transmittance peak minimum. Values listed in Table 3 are peak locations.

Certified Values: 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 [9]. The certified vacuum wavenumber locations for the seven absorption bands spanning the range from 10 300 cm^{-1} to 5 100 cm^{-1} are listed in Table 1. These values were obtained at 8 cm^{-1} constant wavenumber resolution and are certified for operation between 20 °C and 25 °C. The certified values represent a bias adjusted band location relative to the certified values of SRM 2035a. The NIR absorbance spectrum of SRM 2035b in vacuum wavenumber is shown in Figure 1.

[(1)]Certain commercial instruments, materials, or processes 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 instruments, materials, or processes identified are necessarily the best available for the purpose.

Atmospheric water vapor is a significant source of variation for band 3, and this band should be used with caution when calibrating commercial spectrometers with SRM 2035b.

The certified values for the NIR air wavelength band locations for the seven absorption bands from 971 nm to 1960 nm for 1 nm and 3 nm spectral slit width (SSW) resolutions are listed in Table 2 and are certified for operation between 20 °C and 25 °C. The certified values represent a bias adjusted band location relative to the certified values of SRM 2035a. The NIR absorbance spectrum of SRM 2035b in air wavelength is illustrated in Figure 2.

The certified values for the UV-Vis air wavelength peak locations for the thirteen peaks from 334 nm to 805 nm for 1 nm and 3 nm spectral slit width (SSW) resolutions are listed in Table 3 and are certified for operation between 20 °C and 25 °C. The certified values represent a bias adjusted peak location relative to the certified values of SRM 2035a. The UV-Vis transmittance spectrum of SRM 2035b in air wavelength is illustrated in Figure 3.

Certification Uncertainty: The expanded uncertainties ($U_{95\,\%}$) for the wavenumber and wavelength band and peak locations given in Tables 1, 2 and 3 are determined from the appropriate combination of instrument-specific standard uncertainties to define the interval within which the unknown value of the band/peak can be asserted to lie with a level of confidence of approximately 95 % [10–13] when measured between 20 °C and 25 °C. Components of the uncertainty for the wavenumber and wavelength band and peak locations include: within-instrument variation, between-instrument bias, calibration of the NIST FT and scanning dispersive spectrometer systems, location shifts due to temperature, water vapor interference, and short-term precision variance (i.e., estimated standard deviations). For the NIR wavenumber band locations the Type A uncertainty components were determined independently for each band and the combined, band specific uncertainties were expanded by a coverage factor ($k = 3$). For the NIR wavelength band locations the Type A uncertainty components were determined using pooled uncertainties across both spectral bandwidths in three band groupings that were selected based on the general correspondence of band specific uncertainties. These band group specific uncertainties were expanded by a coverage factor ($k = 3$). For the UV-Vis peak locations, a pooled uncertainty across all peaks and spectral bandwidths was estimated and the combined overall uncertainty was expanded by a coverage factor ($k = 3$). The use of a $k = 3$ coverage factor in these cases was based on the assumption that error distributions for the peak and band location estimates are unimodal and symmetric but not necessarily Gaussian [14].

Table 1. Certified Values for NIR Band Locations[a] and Uncertainties[b] for Vacuum Wavenumber at 8 cm^{-1} Resolution

Band	Band Location (cm^{-1})		
1	5139.01	±	0.46
2	6805.66	±	0.99
3	7314.09	±	0.35
4	8179.56	±	0.84
5	8682.50	±	0.23
6	9294.41	±	0.48
7	10245.58	±	0.19

[a] Band locations determined using a centroid method with a band fraction of 0.1; see Figure 1 for band identification.

[b] The listed uncertainties represent the expanded uncertainty ($U_{95\,\%}$) calculation ($k = 3$) in accordance with reference 10. The certified values were derived relative to measurements against SRM 2035a that represent the consensus mean band locations from measurements on four Fourier transform (FT) spectrometer systems. The measurand is the band location at 8 cm^{-1} resolution. The certified values are metrologically traceable to the derived SI unit of reciprocal meters (m^{-1}), expressed as reciprocal centimeters (cm^{-1}).

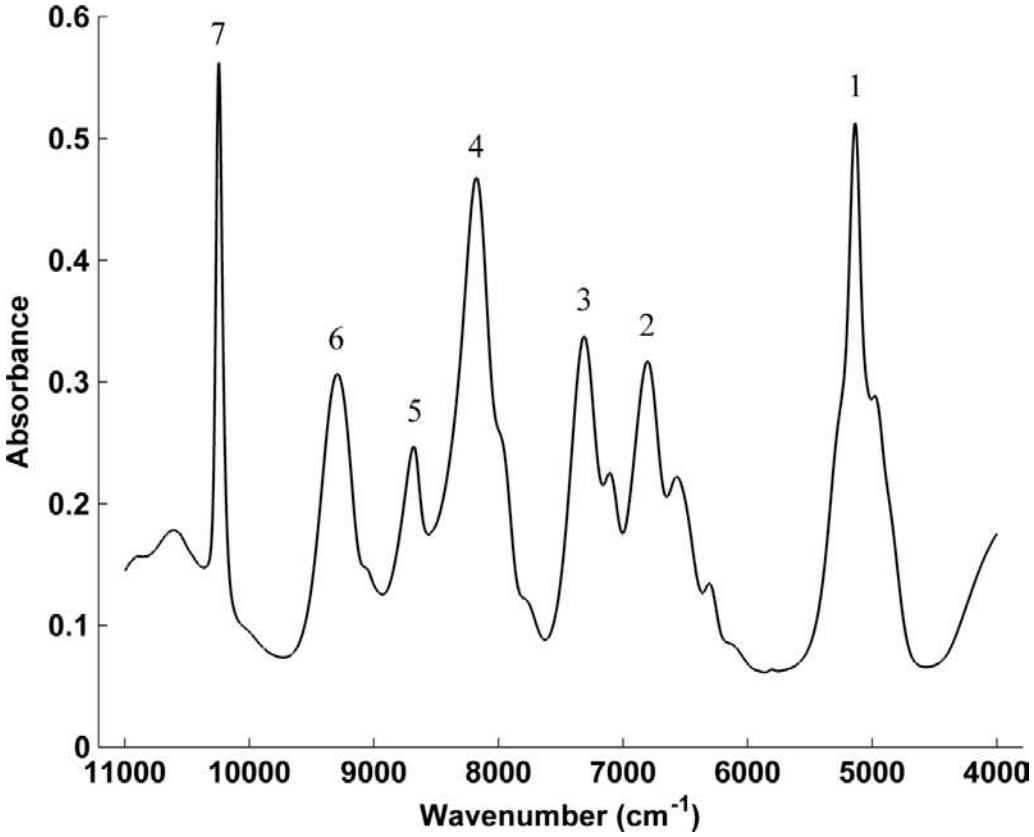

Figure 1. NIR Absorbance Spectrum of SRM 2035b in Vacuum Wavenumber with Band Locations Indicated

Table 2. Certified Values for NIR Band Locations[a] and Uncertainties[b] for Air Wavelength

Band	1 nm SSW Band Location (nm)	3 nm SSW Band Location (nm)
1	1945.70 ± 0.39	1945.65 ± 0.39
2	1469.06 ± 0.19	1469.04 ± 0.19
3	1366.82 ± 0.09	1366.82 ± 0.09
4	1222.23 ± 0.19	1222.21 ± 0.19
5	1151.45 ± 0.09	1151.36 ± 0.09
6	1075.65 ± 0.09	1075.65 ± 0.09
7	975.75 ± 0.09	975.86 ± 0.09

[a] Band locations determined using a centroid method with a band fraction of 0.1; see Figure 2 for band identification.

[b] The listed uncertainties represent the expanded uncertainty ($U_{95\,\%}$) calculation ($k = 3$) in accordance with reference 10. The certified values were derived relative to measurements against SRM 2035a that represent the mean band locations from three scanning dispersive spectrometer systems and one FT spectrometer system. The measurand is the band location at 1 nm and 3 nm SSW. The certified values are metrologically traceable to the SI unit of meters, expressed as nanometers.

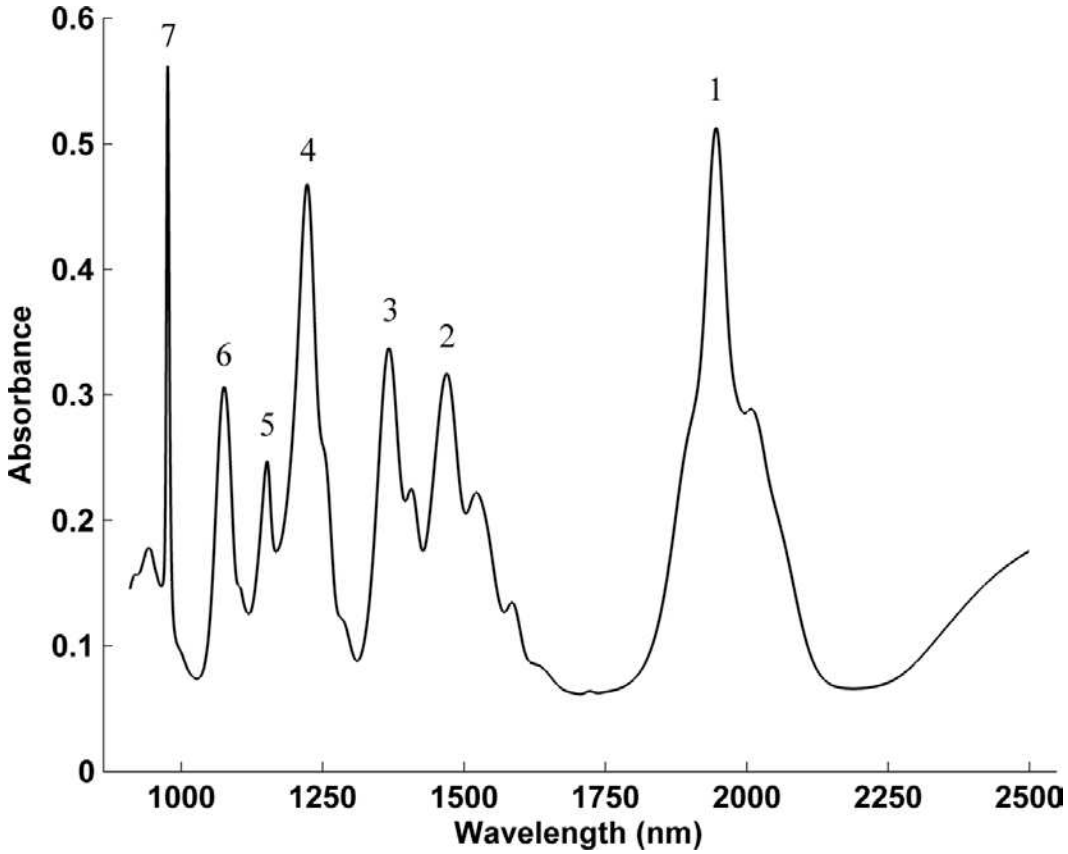

Figure 2. NIR Absorbance Spectrum of SRM 2035b in Air Wavelength with Band Locations Indicated.

Table 3. Certified Values for UV-Vis Peak Locations[a] and Uncertainties[b] for Air Wavelength

Peak	1 nm SSW Peak Location (nm)	3 nm SSW Peak Location (nm)
8	804.13 ± 0.10	804.08 ± 0.10
9	747.69 ± 0.10	747.66 ± 0.10
10	642.47 ± 0.10	642.53 ± 0.10
11	583.43 ± 0.10	583.38 ± 0.10
12	537.68 ± 0.10	537.91 ± 0.10
13	485.54 ± 0.10	485.44 ± 0.10
14	417.91 ± 0.10	418.00 ± 0.10
15	402.57 ± 0.10	402.40 ± 0.10
16	386.19 ± 0.10	386.10 ± 0.10
17	374.69 ± 0.10	374.50 ± 0.10
18	360.84 ± 0.10	361.27 ± 0.10
19	345.29 ± 0.10	345.59 ± 0.10
20	334.58 ± 0.10	334.26 ± 0.10

[a] Peak locations determined using a five-point cubic polynomial fit; see Figure 3 for band identification.

[b] The listed uncertainties represent the expanded uncertainty ($U_{95\,\%}$) calculation ($k = 3$) in accordance with reference 10. For the Type A component, a pooled uncertainty was estimated across all peaks. The certified values were derived relative to measurements against SRM 2035a that represent the mean band locations from four scanning dispersive spectrometer systems. The measurand is the band location at 1 nm and 3 nm SSW. The certified values are metrologically traceable to the SI unit of meters, expressed as nanometers.

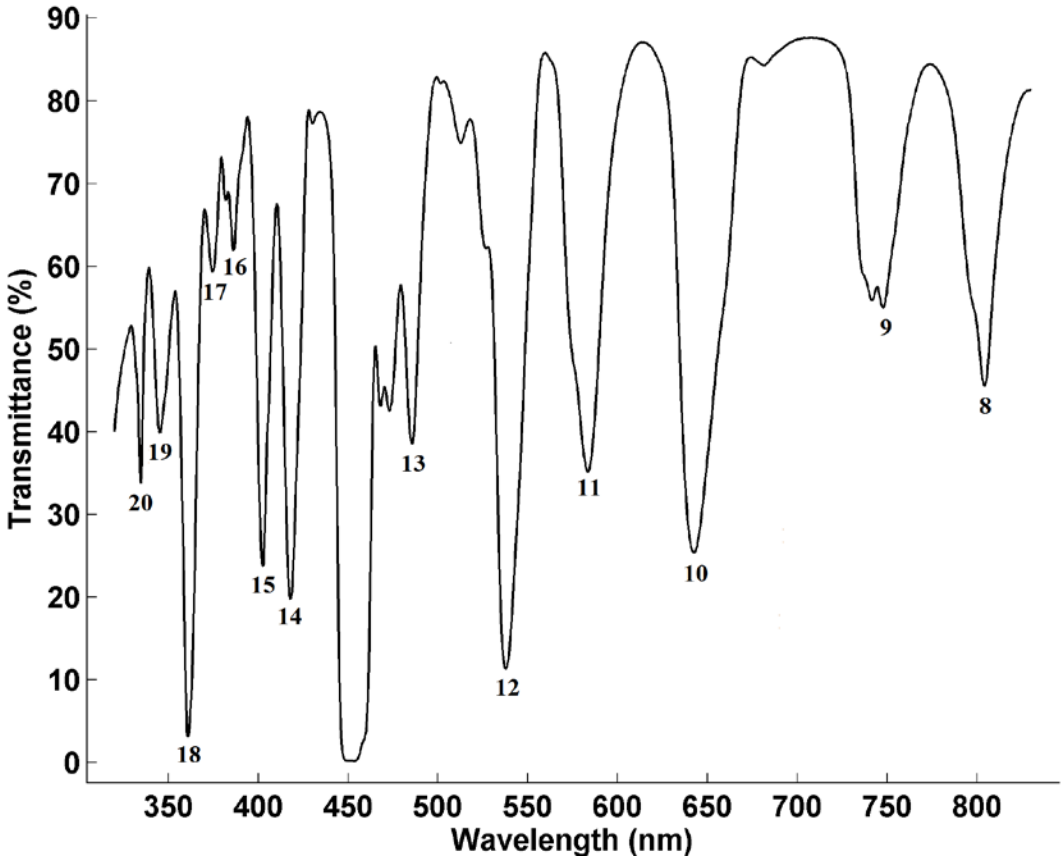

Figure 3. UV-Vis Absorbance Spectrum of SRM 2035b in Air Wavelength with Peak Locations Indicated.

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Users of this SRM should ensure that the Certificate 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.