National Institute of Standards & Technology

Certificate

Standard Reference Material® 2065

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

This Standard Reference Material (SRM) is a certified transfer standard intended for the verification and calibration of the wavelength/wavenumber scale of ultraviolet (UV)–Visible–Near-Infrared (NIR) spectrometers operating in transmission mode. In this certificate, spectral features are referred to as *bands* if their location is determined by the center-of-gravity (COG) algorithm, whereas those determined by a five point cubic polynomial fit are referred to as *peak* locations. SRM 2065 is certified for the location of the seven absorbance bands (COG) in the spectral region from 10 300 cm^{-1} to 5 130 cm^{-1} at 4 cm^{-1} resolution. In addition, SRM 2065 is certified for the location of seven absorbance bands in the spectral region from 970 nm to 1 946 nm and 13 additional transmittance peaks spanning the spectral region from 334 nm to 805 nm.

SRM 2065 is a glass consisting of a combination of rare earth oxides of mole fractions 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 base glass containing oxides of lanthanum (La_2O_3), boron (B_2O_3), silicon (SiO_2), and zirconium (ZrO_2). The optical filter is 25 mm in diameter and 1.5 mm thick. This combination of the rare earth oxide concentrations and filter thickness yields absorption bands between 0.1 and 0.6 absorbance units in the NIR and 5 % to 60 % transmittance in the UV-Visible.

Certification: The certified absorbance/transmittance band locations for SRM 2065 are given in Tables 1, 3, and 5 of this certificate.

Expiration of Certification: The certification of **SRM 2065** is valid, within the measurement uncertainty specified, until **31 December 2028**, provided the SRM is handled and stored in accordance with instructions given in this certificate (see "Instructions for 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 required for certification of this SRM were performed by S.J. Choquette, of NIST and G.W. Kramer, formerly of NIST.

Production and certification of SRM 2065 were performed by S.J. Choquette, D.L. Duewer of the NIST Chemical Sciences Division, and L.E. O'Neal, formerly of NIST. Assistance was provided by L.M. Hanssen, of the NIST Sensor Science Division, and C. Zhu, and E.A. Early, formerly of NIST.

Statistical consultation was provided by J.J. Filliben of the NIST Statistical Engineering Division and A.I. Aviles, formerly of NIST.

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

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Certificate Issue Date: 07 June 2019
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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 [1]. The certified vacuum wavenumber locations for the seven absorption bands spanning the range from 10 300 cm^{-1} to 5 130 cm^{-1} are listed in Table 1. These values were obtained at 4 cm^{-1} constant wavenumber resolution and are certified for 25 °C ± 1.5 °C. The absorbance spectrum (NIR) of SRM 2065 is illustrated in Figure 1 of this certificate. Atmospheric water vapor is a significant source of variance for band 3, and this band should be used with caution when calibrating commercial spectrometers with SRM 2065. The certified values for the NIR air wavelength band locations for the seven absorption bands from 976 nm to 1946 nm for 3 nm spectral resolution at 22 °C ± 2 °C are listed in Table 3.

The certified air wavelength values for the 12 transmittance peaks (334 nm to 645 nm) of SRM 2065 in the UV-Visible are listed in Table 5 for 1 nm spectral bandwidth. The UV–Visible and NIR transmittance spectra of SRM 2065 are shown in Figure 2.

Reference Values: A NIST reference value is a noncertified value that is the best estimate of the true value based on available data; however, the values do not meet the NIST criteria for certification [1]. The reference values for the vacuum wavenumber locations of the seven absorption bands spanning the range from 10 300 cm^{-1} to 5 130 cm^{-1} for six additional spectral resolutions are listed in Table 2. These values are valid for filter temperatures of 25 °C ± 1.5 °C. When using these optical standards to verify the wavenumber scale of a spectrometer, the certified or reference values that are most representative of the spectral bandwidth of the spectrometer being tested should be used. The reference values of the NIR (976 nm – 1946 nm) air wavelength band locations of SRM 2065 at 5 nm and 10 nm spectral resolution are given in Table 4.

The reference values of the temperature coefficients and 0 °C intercepts of the vacuum wavenumber COG band locations of SRM 2065 at 4 cm^{-1} resolution are listed in Table 7. The filter temperature can be a significant source of variance of the NIR band locations. Band locations of the filter were determined using the COG algorithm with a 10 % band fraction over a temperature range between 6 °C and 59 °C. The location of each absorbance band as a function of temperature was determined by a least-squares fit to obtain the temperature coefficients given in Table 7.

Information Values: An information value is a value that may be of interest to the SRM user, but insufficient information is available to assess the uncertainty associated with the value [1]. Information values cannot be used to establish metrological traceability. Information values for the UV–Visible transmittance peak locations of SRM 2065 as a function of spectral resolution are given in Table 6. Information values for the NIR vacuum wavelength temperature coefficients and 0 °C degree intercepts are given in Table 8 for 64 cm^{-1} and Table 9 for 128 cm^{-1} constant wavenumber resolution.

Uncertainties for Certified and Reference Values: The expanded uncertainty (U_{95}) for the wavenumber and wavelength band locations given in Tables 1 through 5 and 7 are determined from the appropriate combination of component standard uncertainties (i.e., estimated standard deviations), with a coverage factor based on the Student's *t*-distribution, 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 % [2]. Components of the uncertainty for the NIR include: calibration of the Fourier transform (FT) spectrometers, COG location estimate, location shift due to temperature, and water vapor interference. Components of the uncertainty for the UV–Visible wavelength values include instrumental line shape anomalies, instrument calibration bias, and a component to account for bias between the COG and cubic fit peak location methods.

Measurement Conditions: The certification measurements for the NIR spectral region (10 300 cm^{-1} to 5 130 cm^{-1}) were made using Bruker IFS66 and Bomem DA FT spectrometers(1). The Bruker FT spectrometer was calibrated in vacuum wavenumber units using NIST SRM 2517 *Wavelength Reference Absorption Cell-Acetylene* [3]. The IFS66 spectrometer calibration was validated with ambient water vapor bands. The Bomem spectrometer was calibrated using ambient water vapor and carbon dioxide bands. The dispersive, air wavelength, NIR measurements were performed on a Perkin Elmer Lambda 900 (PE900) spectrometer, a Varian Cary 5E spectrometer, and the NIST OTD Reference Spectrophotometer for Regular Spectral Transmittance. The air wavelength axis of the PE900 spectrometer was calibrated in the NIR using the emission lines of a Kr atomic emission pen lamp and validated using the values for the second order positions of the emission lines of the internal D_2 source. The Varian Cary 5E was calibrated using the internal D_2 source and an external Hg emission lamp.

(1)Certain commercial equipment, instruments, or materials are identified in this certificate in order 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.

The certification measurements for the UV–Visible (334 nm to 804 nm) air wavelength band locations were obtained using the PE900 and the NIST ACD National Reference UV–Visible Spectrometer (HAS II) [4]. The HAS II instrument is qualified quarterly for photometric and wavelength calibration. It is wavelength calibrated using Hg and Ne atomic emission pen lamps and validated with SRM 2034 *Holmium Oxide Wavelength Solution Standard* from 240 nm to 650 nm. The PE900 was wavelength calibrated in the UV–Visible using a Hg emission pen lamp and validated with SRM 2034 and the emission lines of the internal D_2 source.

Details of the measurements and data analysis for both the NIR and UV–Visible Measurements can be found in reference 5.

Wavenumber and Wavelength Band Location Methodology: The method used to determine the certified NIR wavenumber (υ) and wavelength (λ) band locations of SRM 2065 is the COG technique [6-8]. 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 a five-point cubic polynomial fit to the transmittance minimum, are referred to as *peak* locations. Only those values listed in Tables 5 and 6 (1 nm, 3 nm and 5 nm resolution UV–Visible peak transmittance locations) are peak locations. For COG calculations, a 10 % fraction of the band was used for both wavenumber and wavelength absorption data. Further information on the use of this algorithm with other NIST SRMs can be found in Reference [8].

INSTRUCTIONS FOR HANDLING, STORAGE, AND USE

Handling and Storage: To maintain the integrity of SRM 2065, 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.

Use: Carefully insert SRM 2065 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 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 of 25 °C ± 1.5 °C. Compare each measured band location to its certified value listed in the appropriate table (Tables 1, 3, or 5) for the spectral bandwidth most representative of the spectrometer being used. Band locations in Tables 1 and 2 are vacuum wavenumber values, while those in Tables 3 and 5 are air wavelength values. To convert the values in Tables 1 and 2 to air wavenumber, the appropriate correction for the index of refraction of air must be applied [9]. Taking into account the certification uncertainty of each band of SRM 2065, any statistically significant differences between the measured and certified band locations may then be used to recalibrate the spectrometer wavenumber/wavelength scale.

REFERENCES

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Certificate Revision History: 07 June 2019 (Change of expiration date; editorial changes); 29 September 2008 (Extension of certification period); 05 December 2007 (Update of expiration date and editorial changes); 28 March 2002 (Original certificate date).

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 https://www.nist.gov/srm.

Table 1. Certified[a] Vacuum Wavenumber Band Locations[c] of SRM 2065 and Uncertainties[d] at 4 cm^{-1} Resolution

Resolution (cm^{-1})	B_1 (cm^{-1})	B_2 (cm^{-1})	B_3 (cm^{-1})	B_4 (cm^{-1})	B_5 (cm^{-1})	B_6 (cm^{-1})	B_7 (cm^{-1})
4	5139.3 ± 0.5	6806.3 ± 0.9	7314.9 ± 0.7	8180.1 ± 0.9	8682.6 ± 1.3	9294.4 ± 0.8	10245.6 ± 0.6

Table 2. Reference[b] Vacuum Wavenumber Band Locations[c] of SRM 2065 and Uncertainties[d] for Given Resolutions

Resolution (cm^{-1})	B_1 (cm^{-1})	B_2 (cm^{-1})	B_3 (cm^{-1})	B_4 (cm^{-1})	B_5 (cm^{-1})	B_6 (cm^{-1})	B_7 (cm^{-1})
2	5139.3 ± 0.5	6806.3 ± 0.9	7314.9 ± 0.7	8180.1 ± 0.9	8682.6 ± 1.3	9294.4 ± 0.8	10245.6 ± 0.6
8	5139.3 ± 0.5	6806.3 ± 0.9	7314.9 ± 0.7	8180.1 ± 0.9	8682.7 ± 1.3	9294.4 ± 0.8	10245.6 ± 0.6
16	5139.5 ± 0.5	6806.4 ± 0.9	7315.0 ± 0.7	8180.1 ± 0.9	8683.0 ± 1.3	9294.4 ± 0.8	10245.3 ± 0.6
32	5139.8 ± 0.5	6806.7 ± 0.9	7315.0 ± 0.7	8180.4 ± 0.9	8684.2 ± 1.3	9294.6 ± 0.8	10244.5 ± 0.6
64	5140.2 ± 0.5	6807.8 ± 0.9	7315.3 ± 0.7	8181.7 ± 0.9	8687.3 ± 1.4	9294.9 ± 0.8	10243.2 ± 0.6
128	5136.2 ± 1.0	6810.0 ± 0.9	7314.3 ± 2.0	8185.8 ± 1.1	8690.4 ± 1.4	9297.1 ± 0.8	10246.4 ± 2.0

[a] 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 taken into account [1]. The 4 cm^{-1} constant wavenumber band locations are certified. All other band locations as a function of spectral resolution should be considered reference values only. The measurands are the band locations. The certified values are metrologically traceable to the derived SI unit of reciprocal meters (m^{-1}), expressed as reciprocal centimeters (cm^{-1}).

[b] A NIST reference value is a noncertified value that is the best estimate of the true value based on available data; however, the values do not meet the NIST criteria for certification [1]. The measurands are the band locations as determined by the methods as described above. The values are metrologically traceable to the derived SI unit of reciprocal meters (m^{-1}), expressed as reciprocal centimeters (cm^{-1}).

[c] Band location determined using a Center-of-Gravity method with a band fraction of 0.1; see Figure 1 for band identification.

[d] Uncertainties represent U_{95}, the expanded uncertainty calculated in accordance with reference 2.

Table 3. Certified Air Wavelength Band Locations[a] for SRM 2065 and Uncertainties at 3 nm Spectral Bandwidth

Band	3 nm Spectral Bandwidth Band Location[b] (nm)
7	975.9 ± 0.3
6	1075.7 ± 0.2
5	1151.4 ± 0.1
4	1222.2 ± 0.4
3	1366.7 ± 0.4
2	1469.0 ± 0.4
1	1945.5 ± 0.3

Table 4. Reference Air Wavelength Band Locations[c] for SRM 2065and Uncertainties for Given Spectral Bandwidths

Band	5 nm Spectral Bandwidth Band Location (nm)	10 nm Spectral Bandwidth Band Location (nm)
7	976.0 ± 0.2	976.0 ± 0.6
6	1075.8 ± 0.9	1075.9 ± 2.2
5	1151.3 ± 1.0	1151.1 ± 3.4
4	1222.2 ± 0.3	1222.2 ± 0.9
3	1366.8 ± 0.5	1367.1 ± 0.2
2	1469.1 ± 1.7	1469.2 ± 3.7
1	1945.5 ± 0.7	1945.6 ± 1.5

[a] 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 taken into account [1]. The measurands are the band locations. The certified values are metrologically traceable to the derived SI unit of meters (m), expressed as nanometers (nm).

[b] Uncertainties represent U_{95}, the expanded uncertainty calculated in accordance with reference 2.

[c] A NIST reference value is a noncertified value that is the best estimate of the true value based on available data; however, the values do not meet the NIST criteria for certification [1]. The measurands are the band locations as determined by the methods as described above. The values are metrologically traceable to the derived SI unit of meters (m), expressed as nanometers (nm).

Table 5. Certified Air Wavelength Peak Locations[a] of SRM 2065 and Uncertainties at 1 nm Spectral Bandwidth

Peak	Average Peak Position[b] (nm)
20	334.6 ± 0.1
19	345.4 ± 0.2
18	360.8 ± 0.2
17	374.5 ± 0.1
16	386.1 ± 0.1
15	402.5 ± 0.2
14	417.9 ± 0.1
13	485.4 ± 0.1
12	537.7 ± 0.5
11	583.4 ± 0.3
10	642.4 ± 0.6
9	747.7 ± 0.4
8	804.3 ± 0.5

Table 6. Information Air Wavelength Peak Locations[c] of SRM 2065 at 3 nm and 5 nm Resolution

Peak	Spectral Bandwidth		
	1 nm	3 nm	5 nm
20	334.6	334.3	334.3
19	345.4	345.6	346.3
18	360.8	361.2	361.6
17	374.5	N/D	N/D
16	386.1	N/D	N/D
15	402.5	402.4	402.7
14	417.9	418.0	418.3
13	485.4	485.3	485.5
12	537.7	537.9	538.3
11	583.4	583.4	583.4
10	642.4	642.5	642.9
9	747.7	747.7	N/D
8	804.3	804.3	804.3

[a] 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 taken into account [1]. The measurands are the band locations. The certified values are metrologically traceable to the derived SI unit of meters (m), expressed as nanometers (nm).

[b] Uncertainties represent U_{95}, the expanded uncertainty calculated in accordance with reference 2.

[c] An information value is a value that may be of interest to the SRM user, but insufficient information is available to assess the uncertainty associated with the value. Information values cannot be used to establish metrological traceability.

Table 7. Reference Values[a] for Temperature Coefficients and Intercepts for Vacuum Wavenumber Band Locations at 4 cm^{-1} Resolution

Band	Temperature Coefficient[b] (cm^{-1}/°C)	0 °C Intercept (cm^{-1})
1	-0.0517 ± 0.0010	5140.64 ± 0.04
2	0.0912 ± 0.0004	6804.01 ± 0.03
3	0.006 ± 0.014	7314.84 ± 0.48
4	0.0619 ± 0.0011	8178.45 ± 0.04
5	-0.0419 ± 0.0011	8683.61 ± 0.07
6	-0.0783 ± 0.0009	9296.41 ± 0.08
7	0.0191 ± 0.0006	10245.15 ± 0.03

Table 8. Information Values[c] for Temperature Coefficients and Intercepts for Vacuum Wavenumber Locations at 64 cm^{-1} Resolution

Band	Coefficient (cm^{-1}/°C)	0 °C Intercept (cm^{-1})
1	-0.085	5142.53
2	0.085	6806.35
3	0.003	7315.64
4	0.069	8181.11
5	-0.073	8690.86
6	-0.075	9297.66
7	0.022	10242.63

Table 9. Information Values for Temperature Coefficients and Intercepts for Vacuum Wavenumber Band Locations at 128 cm^{-1} Resolution

Band	Coefficient (cm^{-1}/°C)	0 °C Intercept (cm^{-1})
1	-0.22	5141.59
2	0.073	6807.15
3	-0.055	7312.24
4	0.084	8185.24
5	N/D	N/D
6	-0.082	9300.25
7	0.025	10248.71

[a] A NIST reference value is a noncertified value that is the best estimate of the true value based on available data; however, the values do not meet the NIST criteria for certification [1]. The measurands are the band locations as determined by the methods as described above. The values are metrologically traceable to the derived SI unit of reciprocal meters (m^{-1}), expressed as reciprocal centimeters (cm^{-1}).

[b] Uncertainties represent U_{95}, the expanded uncertainty calculated in accordance with reference 2.

[c] An information value is a value that may be of interest to the SRM user, but insufficient information is available to assess the uncertainty associated with the value. Information values cannot be used to establish metrological traceability.

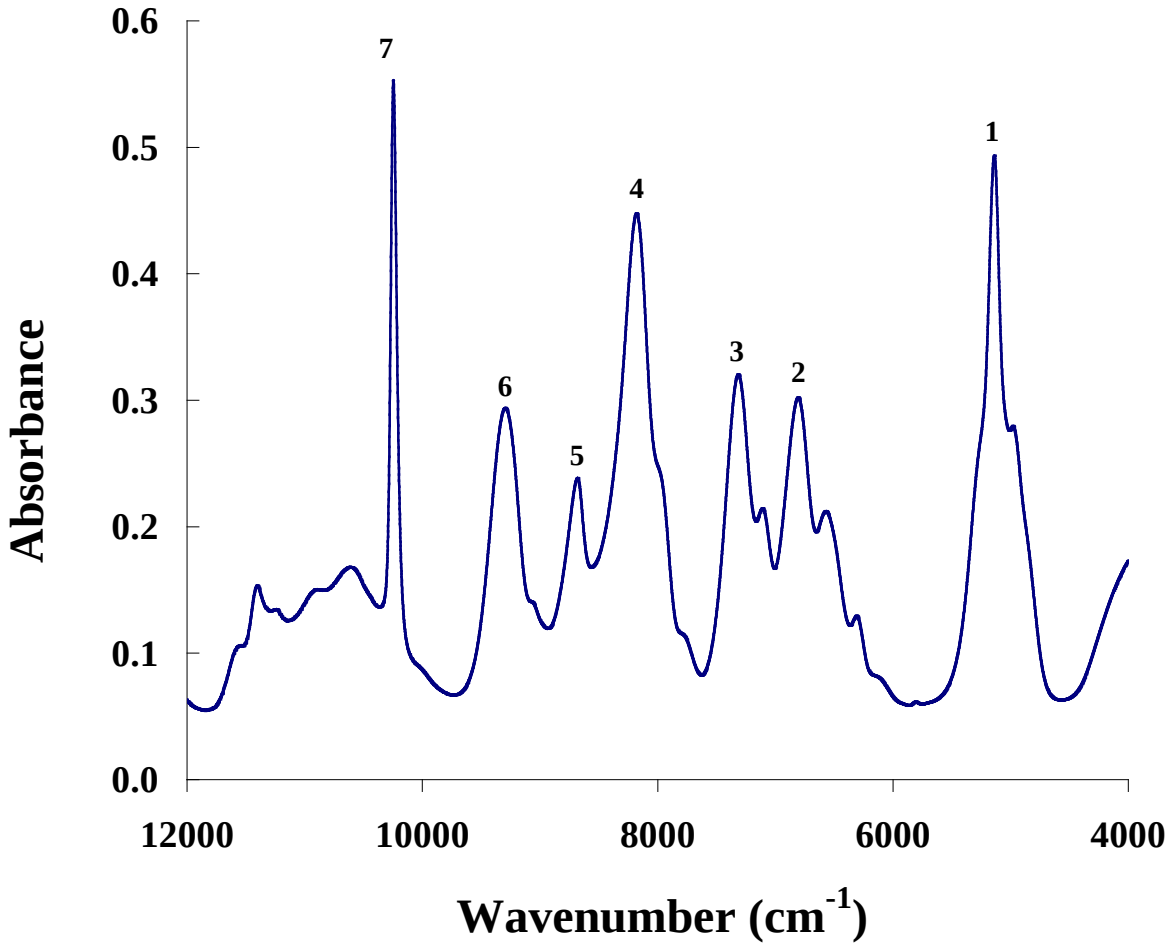

Figure 1. NIR Absorbance Spectrum of SRM 2065 with the band locations indicated.

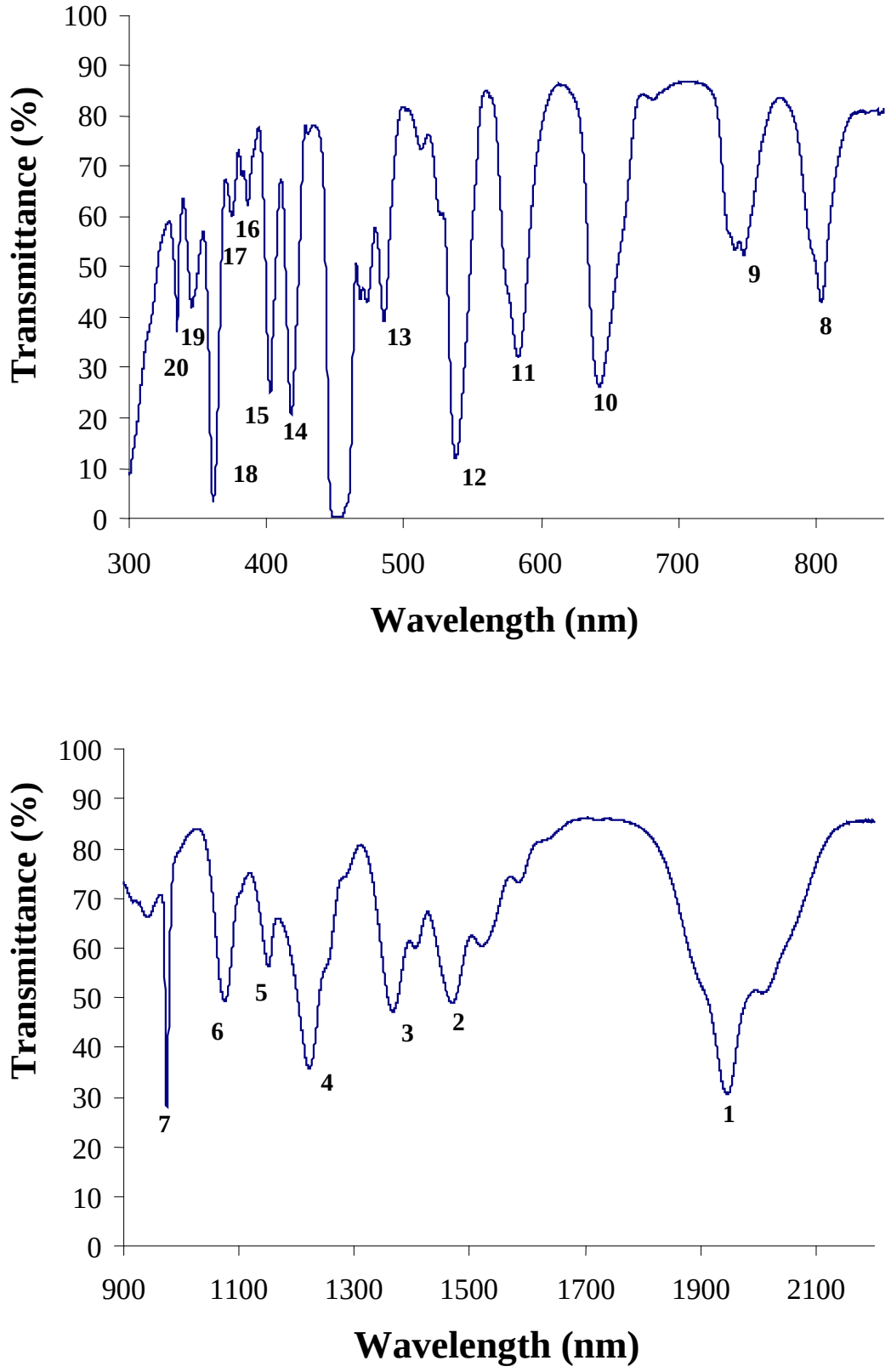

Figure 2. UV–Visible and NIR Transmittance Spectra of SRM 2065 in Air with the peak locations indicated.