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# A novel short-wavelength near-infrared certified reference material from dysprosium and ytterbium oxides

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**Abstract:** This study involves the characterization of a new shortwave NIR wavelength standard solution to address the current limitations of shortwave near infrared (NIR) standard materials and to expand the spectral wavelength range of standard materials. Herein, an innovative use of a solution of dysprosium oxide and ytterbium oxide compounds dissolved in perchloric acid solution to calibrate and verify the NIR wavelength of a high-sensitivity ultraviolet-visible-near infrared spectrophotometer is reported. This standard material enables the near infrared wavelength to be accurately traced to the theoretical emission wavelength of the elements. In the study, cubic spline interpolation was performed on the SI traceable and validated instrument for the determination of peak wavelengths. The wavelength standard values of this standard material cover the shortwave near infrared region (700~1200 nm) with an uncertainty of 0.12 nm at a 95% confidence interval.

**Keywords:** Short-wavelength near-infrared; argon emission lines; wavelength calibration; rare earth elements; standard material. © 2024 ACG Publications. All rights reserved.

## 1. Introduction

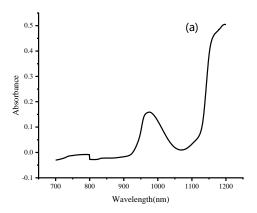
Near-Infrared (NIR) spectroscopy is part of vibrational spectroscopy, distinct from infrared or Raman, offering lots of unique and valuable advantages [1]. Over the past 20 years, with the help of significant advances in data analysis and background theory, NIR spectroscopy has made rapid progress across a wide range of application fields, while also driving the development of various NIR spectrometers and their applications too [2]. The accuracy of the wavelength in the measurements directly affects the overall performance of the near-infrared spectrometer and it is a key factor in ensuring reliable and precise measurement results [3].

Trivalent rare earth oxides are widely used in spectroscopic analysis due to their unique optical and electronic properties. The 4f electrons of their ions are shielded by the 5s and 5p electrons, making them less affected by environmental factors. The spectra of free ions resemble atomic linear spectra, with sharp spectral lines. For example, holmium oxide has long been a globally accepted solid or liquid standard substance for calibrating wavelengths in the ultraviolet-visible region (240 nm~650 nm) [6-12].

Compared to liquid standard substances, the sintering process of solid standards can often lead to minor peak shifts. Solutions, on the other hand, possess homogeneous and stable properties, making them less susceptible to external factors such as silica or polishing processes, and are therefore more suitable

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A new short-wavelength near-infrared certified reference material as a "benchmark." However, the challenge lies in addressing the absorption of  $H_2O$  in the short-wave near-infrared region, which can affect the accuracy of the standard substance, as shown in Figure 1a.



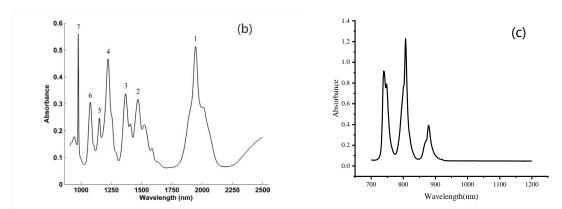


Figure 1. (a) Spectrum of H<sub>2</sub>O in the (700~1200) nm range

- (b) Spectrum of NIST SRM 2035b near-infrared wavelength standard material
- (c) Spectrum of Praseodymium-Neodymium (Pr-Nd) filter at near-infrared wavelength

Currently, available ultraviolet-visible-near-infrared spectrophotometers usually claim a wavelength range of (190~1100) nm in their manuals. While there are sufficient standard materials to calibrate the wavelength range of 190-800 nm, the same is not true for the short-wave NIR wavelengths in the range of (800~1100) nm, and there are very few suitable standard materials on the market to calibrate this spectral range [4]. In this field, one of the most widely used standard materials internationally is SRM2035b from the National Institute of Standards and Technology (NIST) in the United States [5]. This standard material is used for calibrations with peak wavelengths in the visible to near-infrared regions (330~2000) nm. According to the certificate of NIST SRM2035b, the spectral features whose positions are determined by a center of gravity (COG) or center of gravity algorithm are called "bands", while those determined by cubic polynomial fits are called "peak positions". As shown in Figure 1b, it is an absorption glass filter made of rare earth elements, designed for absorption in the NIR region, and is taken from the SRM2035b standard material certificate.

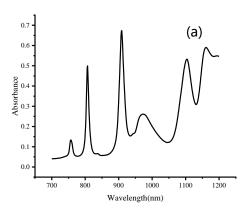
However, the Praseodymium-Neodymium (Pr-Nd) filter, which is one of the standards used for this purpose, has peak wavelengths at 740.8 nm, 748.8 nm, 807.3 nm and 879.6 nm (see Figure 1c), and in reality, this filter cannot evaluate the wavelength accuracy in the range of (900~1100) nm. On the other hand, the interference filters commonly used for this purpose can only provide a single standard value and since the interference filters are very sensitive to the incident angle of the light, their long-term stability is poor, which increases the measurement uncertainty budget and makes the instrument calibration more difficult.

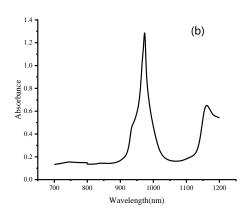
In this study, the characterization and certification of a rare earth element standard solution covering the range (700~1200) nm is reported to overcome the deficiencies of glass filter type wavelength standards and to calibrate short-wave near-infrared wavelengths.

## 2. Experimental

## 2.1. Selection of Candidate Substances

After obtaining the short-wave near infrared spectra of the compounds samarium oxide (Sm<sub>2</sub>O<sub>3</sub>), praseodymium oxide (Pr<sub>2</sub>O<sub>3</sub>), neodymium oxide (Nd<sub>2</sub>O<sub>3</sub>), ytterbium oxide (Yb<sub>2</sub>O<sub>3</sub>), dysprosium oxide (Dy<sub>2</sub>O<sub>3</sub>) and cerium oxide (CeO<sub>2</sub>) their suitability for our target region of 800-1200 nm was evaluated separately. Of these compounds, cerium oxide and praseodymium oxide were removed from the candidates without further examination due to the absence of absorption peaks in the target region. The presence of only one absorption peak around 1100 nm for samarium oxide and the fact that the peak shape of neodymium oxide was moderate, relatively flat and had no absorption peaks above 900 nm also caused the oxides of these two elements to be excluded from the evaluation. However, Dysprosium oxide (Dy<sub>2</sub>O<sub>3</sub>) exhibited symmetric and narrow absorption peaks in the range of 700~1200 nm (see Figure 2a). On the other hand, ytterbium oxide (Yb<sub>2</sub>O<sub>3</sub>) was found to have an absorption peak at 970 nm, effectively covering the water absorption "hump", and it was found that it did not show additional absorption in the rest of the range of 700~1200 nm (see Figure 2b). Therefore, it was considered that a new wavelength standard material could be developed by using the oxides of these two rare earths, and these two oxides were selected for the target wavelength range. Thus, the strong absorption peak of Dysprosium oxide provided precise wavelength calibration, while the 970 nm peak of Ytterbium oxide was intended to compensate for water interference in the near-infrared spectrum.





**Figure 2.** (a) Short-wavelength near-infrared spectrum of Dysprosium oxide (b) Short-wavelength near-infrared spectrum of Ytterbium oxide

## 2.2. Preparation of the Standard Material

The preparation was conducted at a controlled environment temperature of  $(20\pm4)$  °C. An XS205 model electronic balance from Mettler Toledo, Switzerland, was used to accurately weigh 4 g of dysprosium oxide (Dy<sub>2</sub>O<sub>3</sub>) and 4 g of ytterbium oxide (Yb<sub>2</sub>O<sub>3</sub>), both supplied by Adamas with a purity (mass fraction)  $\geq$  99.99%. The oxides were dissolved in a 10% perchloric acid (HClO<sub>4</sub>) solution, supplied by Sinopharm Chemical Reagent Co., Ltd., by heating and stirring until completely dissolved.

A new short-wavelength near-infrared certified reference material

The Milli-Q ultra-pure water system, manufactured by Millipore, USA, was used to prepare the water for the solution. After cooling, the solution's volume was adjusted to 50 mL with the 10% perchloric acid solution. Volumetric flasks and pipettes, all single-mark glassware verified and calibrated by an accredited metrological institution, were used for precise measurements. The solution was then transferred into a custom quartz cuvette made from JGS2 optical quartz glass with a path length of 1 cm. After sealing the cuvette, it was stored as depicted in Figure 3.



Figure 3. Sealed short-wavelength near-infrared wavelength standard solution material

## 2.3. Value Assignment of the Standard Material

The prepared standard material was subjected to wavelength scanning using the Cary6000i UV-Vis-NIR spectrophotometer, manufactured by Agilent Technologies, USA. The scanning parameters were set as follows: spectral bandwidth of 2 nm for the (700~850) nm range and 0.5 nm for the (850~1200) nm range, with a scanning interval of 0.1 nm. The scanning results revealed multiple sharp absorption peaks uniformly distributed across the 700 nm to 1200 nm range. Cubic spline interpolation was applied to calculate the maximum wavelength points of each peak, with a total of 80 interpolation points. The primary absorption peak wavelengths were determined as 757.09 nm, 806.77 nm, 908.89 nm, 973.74 nm, 1103.34 nm, and 1160.79 nm (see Figure 4).

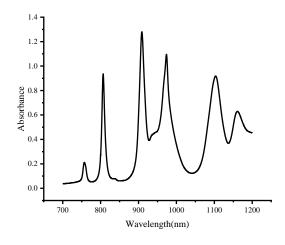


Figure 4. Spectrum of the Short-Wavelength Near-Infrared Wavelength Standard Solution Material

## 3. Results and Discussion

## 3.1. Verification of Calibration Instruments

The emission spectral lines produced by discharge lamps reflect the fundamental characteristics of elements and, as a basic physical standard, the measurement uncertainty of these wavelengths does not exceed  $\pm 0.001$  nm. Therefore, in general, the uncertainty of the peak wavelengths of the emission spectral lines generated by element lamps can be considered negligible [13].

The Cary 6000i UV-Vis-NIR spectrophotometer is equipped with a built-in low-pressure mercury lamp, which allows for self-calibration of the instrument's UV-Vis wavelengths. However, the low-pressure mercury lamp has virtually no emission spectral lines beyond 700 nm, making it inadequate for covering the measurement range of this standard material.

To address this limitation, our research group utilized the argon gas present in the mercury lamp to verify wavelengths in the (700~1200) nm range. Emission peaks from argon were selected at intervals of 100 nm for verification. The corresponding positions of the argon emission peaks, along with their uncertainties and relative intensity information, are summarized in Table 1, with data sourced from the NIST Atomic Spectra Database.

**Table 1.** Theoretical spectral data of argon emission peaks

Element	Theoretical Wavelengt h(nm)	Measured Wavelength (nm)	Error(nm)	Theoretical Wavelength Uncertainty (nm)	Theoretical Wavelength Relative Intensity	Electronic Configuration
	750.3869	750.38	-0.01	0.001	20000	3s2.3p5.(2P*<1/2>).4s
	811.5311	811.53	0.00	0.001	35000	3s2.3p5.(2P*<3/2>).4s
Ar I	912.2967	912.24	-0.06	0.001	35000	3s2.3p5.(2P*<3/2>).4s
	1047.0054	1046.96	-0.05	0.001	1600	3s2.3p5.(2P*<1/2>).4s
	1148.8109	1148.74	-0.07	0.001	400	3s2.3p5.(2P*<1/2>).4s

The scanning setup utilized the third light source without performing baseline calibration, with a single-beam mode and energy set to 5700. Both the detector switching and grating switching were configured to 850 nm, with a data interval of 0.01 nm to scan the five emission wavelengths of argon listed in the table.

The scanning spectrum (see Figure 5) indicates that the Cary6000i UV-Vis-NIR spectrophotometer has a resolution of 0.07 nm in the  $(700\sim1200)$  nm range. Therefore, using the error specification provided in the instrument manual (MPE:  $\pm0.1$  nm), satisfies uniform distribution, we calculated the uncertainty component introduced by the calibration instrument error.

## 3.2. Comparison of Cubic Spline Interpolation with NIST Method

In our study, we utilized cubic spline interpolation with 80 interpolation points to calculate the maximum wavelength points for each peak. One of the key advantages of this method is its ability to generate smooth and continuous curves across the entire data set, ensuring that the curve accurately passes through each known data point while maintaining natural connectivity and smooth transitions between intervals. This makes it particularly effective for capturing global trends in complex spectra, handling large data sets, and maintaining high interpolation accuracy.

In contrast, the two methods used by NIST in SRM 2035b focus on local peak and band detection but may be limited in their ability to capture general trends when dealing with large data sets. The first of these methods, the center of gravity (COG) or center of gravity algorithm, focuses on the general distribution of spectral bands by calculating the centers of gravity and, although it often achieves successful results, it has difficulty or may not capture the local details of complex or asymmetric peak shapes. The second method, the five-point cubic polynomial fitting approach, can accurately determine

A new short-wavelength near-infrared certified reference material peak locations using only five data points for localized fit, but its limited range makes it less flexible than cubic spline interpolation and it is not as effective in representing general trends.

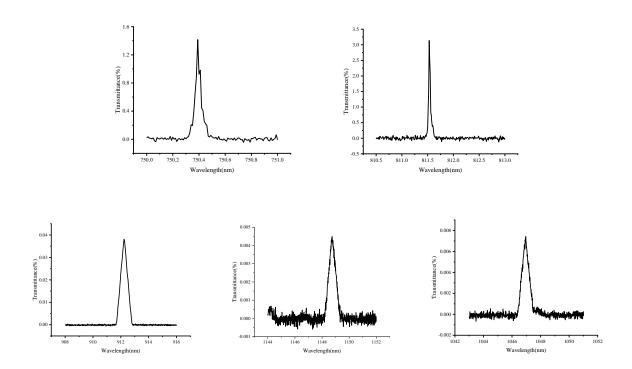


Figure 5. Measured Spectra of Argon at Five Wavelengths within the (700~1200) nm Range

Cubic spline interpolation offers several key advantages when compared to the methods employed by NIST in SRM 2035b. First, its global fitting capability enables a smooth fit across the entire spectral data, making it especially useful for analyzing continuous spectra or complex structures that include multiple peaks. This broad applicability allows cubic spline interpolation to capture the overall behavior of the data, whereas the NIST methods are more localized in their focus, potentially overlooking general trends. Furthermore, cubic spline interpolation excels in high-resolution analysis. By employing 80 interpolation points, it allows for a more detailed numerical examination of each peak, accurately capturing the peak itself as well as the variations surrounding it. This level of detail surpasses the five-point cubic polynomial fitting method used by NIST, which, though effective for localized peak detection, cannot provide as comprehensive a view of the spectral data. Lastly, cubic spline interpolation demonstrates greater flexibility and adaptability across different types of spectral data, whether they exhibit smooth or complex shapes. In contrast, the NIST methods, particularly when dealing with intricate or asymmetric peaks, may encounter limitations, making cubic spline interpolation a more versatile and powerful tool for spectral analysis.

In summary, our cubic spline interpolation method excels in preserving the integrity of global data while providing high-resolution interpolation of local details. It offers greater flexibility and adaptability compared to NIST's methods, making it particularly advantageous when precise descriptions of spectral behavior are required.

## 3.3. Assessment of Homogeneity

To test the homogeneity of the units, m units were selected. Using a highly precise experimental method, m sets of equally precise measurement data were obtained under the same conditions, as shown below:

1. 
$$x_{11}$$
,  $x_{12}$ , ..... $x_{1ni}$ , average value  $\bar{x}_1$   
2.  $x_{21}$ ,  $x_{22}$ , ..... $x_{2ni}$ , average value  $\bar{x}_2$ 

m.  $x_{m1}, x_{m2}, \dots, x_{mn_m},$  average value  $\overline{x}_m$   $= \sum_{k=1}^{m} \frac{\sum_{i=1}^{m} \overline{x_i}}{m},$ 

 $N = \sum_{i=1}^{m} n_i$   $Q_i = \sum_{i=1}^{m} n_i \left( \overline{x_i} - \overline{\overline{x}} \right)^2$ 

Between-unit sum of squares:

Within-unit sum of squares:

$$Q_{2} = \sum_{i=1}^{m} \sum_{j=1}^{n_{i}} (x_{ij} - \overline{x_{i}})^{2}$$

$$S_{1}^{2} = \frac{Q_{1}}{v_{1}}, \quad S_{2}^{2} = \frac{Q_{2}}{v_{2}}$$

$$F = \frac{S_{1}^{2}}{S_{2}^{2}}$$

 $v_1$ =m-1 (Between-unit degrees of freedom)  $v_2$ =N-m (Within-unit degrees of freedom)

According to the degrees of freedom  $(v_1, v_2)$  and the given significance level  $\alpha$ , the critical value  $F_{\alpha}$  can be obtained from the F-table. If  $F < F_{\alpha}$ , it is concluded that there is no significant difference between within-unit and between-unit variances, indicating that the units are homogeneous; if  $F \ge F_{\alpha}$ , it raises suspicion of systematic differences among the units. The between-unit heterogeneous standard deviation  $s_{bb}$  can be calculated using the following formula, which is equivalent to the uncertainty component  $u_{bb}$  caused by between-unit heterogeneous.

$$u_{\rm bu} = s_{\rm bb} = \sqrt{\frac{{S_1}^2 - {S_2}^2}{n}}$$

When the measurement method for homogeneity testing has poor repeatability, it may lead to  $S_1^2 < S_2^2$ . In this case, the standard deviation resulting from heterogeneous can be calculated using the following formula:

$$u_{\text{bu}} = s_{\text{bb}} = \sqrt{\frac{{S_2}^2}{n}} \sqrt[4]{\frac{2}{{v_{S_2}}^2}}$$

To assess the homogeneity [14], we randomly selected 11 bottles of the wavelength standard solution and performed three repeated measurements for each unit, recording the peak wavelengths. ANOVA was applied to test the homogeneity of the entire set of standard materials. The results showed that at a 95% confidence level, the calculated F values were all less than  $F_{0.05}(10,22)$ , indicating no significant difference between the units of data. This confirms that the standard material exhibits good homogeneity between units. Taking the peak at 973.74 nm as an example, the data and statistical results are shown are shown in Table 2 and Table 3.

Table 2.	Homogeneity test data	L

Unit No.	Value 1(nm)	Value 2(nm)	Value 3(nm)	Average value(nm)
1	973.75	973.76	973.75	973.75
2	973.77	973.76	973.74	973.76
3	973.75	973.74	973.73	973.74
4	973.75	973.75	973.76	973.75
5	973.73	973.72	973.75	973.73
6	973.75	973.76	973.74	973.75
7	973.74	973.75	973.73	973.74
8	973.76	973.74	973.73	973.74
9	973.74	973.75	973.75	973.75
10	973.76	973.74	973.75	973.75
11	973.75	973.74	973.74	973.74

**Table 3.** Homogeneity statistical results

$\mathbf{Q}_1$	$\mathbb{Q}_2$	$S_1^2$	$S_2^2$	F	F <sub>0.05</sub> (10,22)
$1.5 \times 10^{-3}$	$2.5 \times 10^{-3}$	$1.5 \times 10^{-4}$	$1.1 \times 10^{-4}$	0.35	2.30

## 3.4. Assessment and Monitoring of Stability

The linear model for stability evaluation is as follows:

$$Y = \beta_0 + \beta_1 X$$

 $\beta_0$ ,  $\beta_1$ : Regression coefficient;

X: Time;

Y: Certified value of the reference material.

For a stable reference material, the expected value of  $\beta_1$  is zero. The slope  $\beta_1$  and intercept  $\beta_0$ can be calculated using the following formulas:

$$\beta_1 = \frac{\sum_{i=1}^{n} (\mathbf{X}_i - \overline{\mathbf{X}})(\mathbf{Y}_i - \overline{\mathbf{Y}})}{\sum_{i=1}^{n} (\mathbf{X}_i - \overline{\mathbf{X}})^2}$$
$$\beta_0 = \overline{\mathbf{Y}} - \beta_1 \overline{\mathbf{X}}$$

 $X_i$ :The i-th time point;

Y<sub>i</sub>:The characteristic value of the reference material candidate at the i-th time point (the corresponding value on the fitted line);

 $\overline{X}$ : The average value of all time points;

 $\overline{Y}$ : The average value of all time points;

n:Number of measurements

The standard deviation of 
$$\beta_1$$
, s( $\beta_1$ ), is calculated using the following formula: 
$$s(\beta_1) = \frac{s}{\sqrt{\sum_{i=1}^n (X_i - \overline{X})^2}}$$

s: Standard deviation of each point on the line is calculated using the following formula:

$$s^{2} = \frac{\sum_{i=1}^{n} (Y_{i} - \beta_{0} - \beta_{1} X_{i})^{2}}{n-2}$$

 $s^2 = \frac{\sum_{i=1}^n (\mathbf{Y}_i - \beta_0 - \beta_1 \mathbf{X}_i)^2}{n-2}$  The standard deviation s( $\beta_1$ ) can be used to make the following judgment using the t-test: if  $|\beta_1| < t_{\alpha,n-2} \cdot s(\beta_1)$ , it indicates that the slope is not significant and no instability has been observed.

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Maintaining the stability of the standard material is a crucial aspect of its development. Since the standard material may be subjected to transport during use, we studied its transport stability and long-term stability. The transport stability assessment used a simultaneous stability study method, measuring under repeatability conditions, meaning only one calibration was performed. The experiment simulated the environmental conditions that the units might encounter during transport. We divided the prepared standard material into six bottles, storing them at 50 °C and 4 °C for 0, 1, 3, 5, 7, and 14 days before testing. Each unit was measured three times. A t-test on the transport stability results indicated that at a 95% confidence level, the slope was not significant, and no instability was observed. This suggests that the standard material remains stable under transport conditions for up to 14 days, meeting practical transport requirements. Taking the peak at 973.74 nm as an example, the data and statistical results are shown are shown in Table 4, Table 5 and Table 6.

**Table 4**. Monitoring data of the transportation stability under 4 °C

Storage time(d)	value 1(nm)	value 2(nm)	value 3(nm)	Average value(nm)
0	973.76	973.74	973.75	973.75
1	973.74	973.72	973.76	973.74
3	973.73	973.75	973.74	973.74
5	973.75	973.76	973.73	973.75
7	973.74	973.73	973.75	973.74
14	973.76	973.74	973.72	973.74

**Table 5**. Monitoring data of the transportation stability under 50 °C

Storage time(d)	value 1(nm)	value 2(nm)	value 3(nm)	Average value(nm)
0	973.75	973.73	973.76	973.75
1	973.72	973.74	973.75	973.74
3	973.74	973.75	973.72	973.73
5	973.75	973.73	973.74	973.74
7	973.76	973.74	973.73	973.74
14	973.73	973.75	973.76	973.75

**Table 6**. Statistical results of the transportation stability

Tuble o. Blatistical i	Tuble 0. Statistical results of the transportation statistic						
	4 °C	50 °C					
$oldsymbol{eta}_1$	-3.8×10 <sup>-4</sup>	$4.1 \times 10^{-4}$					
$oldsymbol{eta}_0$	973.74	973.74					
$s(\beta_1)$	$3.9 \times 10^{-4}$	$4.0 \times 10^{-4}$					
$t_{0.95,4} \cdot s(\beta_1)$	$1.1 \times 10^{-3}$	1.1×10 <sup>-3</sup>					

The long-term stability assessment used classic stability study methods, measuring the units over time under the same conditions. We randomly selected one bottle of standard material for testing on the day of preparation and at 1, 2, 3, 4, 5, 8, and 12 months thereafter, repeating the measurements three times each time. The units were stored in a light-free environment at (20-25) °C. A t-test on the long-term stability results indicated that at a 95% confidence level, the slope was not significant, and no instability was observed. This indicates that the standard material remains stable when stored at room temperature for up to 12 months. The laboratory will continue to monitor the long-term stability of this standard material. Taking the peak at 973.74 nm as an example, the data and statistical results are shown in Table 7 and Table 8.

<b>Table 7.</b> Monitoring data of the long-term stability of the refere
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Storage time(m)	value 1(nm)	value 2(nm)	value 3(nm)	Average value(nm)
0	973.75	973.74	973.73	973.74
1	973.72	973.76	973.75	973.74
3	973.76	973.73	973.72	973.74
5	973.74	973.75	973.76	973.75
7	973.73	973.74	973.75	973.74
12	973.72	973.73	973.76	973.74

**Table 8.**Statistical results of the long-term stability

 $oldsymbol{eta}_1$	$oldsymbol{eta}_0$	$s(\beta_1)$	$t_{0.95,6}\cdot s(\boldsymbol{\beta}_1)$
-2.8×10 <sup>-4</sup>	973.74	4.7×10 <sup>-4</sup>	1.3×10 <sup>-3</sup>

## 3.5. Uncertainty Assessment

The uncertainty of the peak wavelengths of the short-wave near-infrared standard material arises from three components: the uncertainty introduced by homogeneity, the uncertainty due to the long-term stability of the standard material, and the uncertainty introduced by the calibration instrument used to assign values to the standard material [15-16]. The calculation formula is as follows:

$$u_{\text{hom}} = u_{\text{bu}} = s_{\text{bb}} = \sqrt{\frac{s_1^2 - s_2^2}{n}}$$

$$u_{\text{lts}} = u_{\text{s}} = s(\beta_1) \cdot X$$

$$u_{\text{char}} = MPEV/\sqrt{3}$$

$$u_{\text{CRM}} = \sqrt{u_{\text{hom}}^2 + u_{\text{lts}}^2 + u_{char}^2}$$

By combining these components to calculate the combined standard uncertainty and then multiplying by the coverage factor k=2, we obtain the expanded uncertainty. The statistical results are summarized in Table 9.

**Table 9.** Peak wavelength values and uncertainties of the short-wavelength near-infrared wavelength standard solution material (nm)

Results	SBW	uhom	<i>u</i> lts	uchar	<i>u</i> crm	$oldsymbol{U}_{ ext{crm}}$
750.38	2.0	0.004	0.015	0.058	0.06	0.12
811.53	2.0	0.004	0.015	0.058	0.06	0.12
912.24	0.5	0.004	0.015	0.058	0.06	0.12
1046.96	0.5	0.004	0.015	0.058	0.06	0.12
1148.74	0.5	0.004	0.015	0.058	0.06	0.12

## 3.6. Principles and Traceability

For effective operations, process control, and reliable measurement results, maintaining accuracy and consistency is vital. Achieving this requires robust metrological methods based on certified reference materials (CRMs), following the guidelines of ISO 17034 and ISO 33405:2024[17,18]. CRMs are fundamental in ensuring quality assurance, supporting accurate research, validating test methods, and verifying outcomes. The certified values of the short-wavelength near-infrared (SW-NIR) standard material are obtained using a UV-Vis-NIR spectrophotometer. This instrument is calibrated with an atomic emission lamp, which serves as a reference for wavelength standards. The calibration of the spectrophotometer ensures that the wavelength measurements are traceable to the International System of Units (SI) through the SI unit meters (m).

## 4. Conclusions

According to ISO 33405:2024, the production and measurement of Certified Reference Materials (CRMs) used for material studies is extremely important. In this study, the NIR certified reference material developed and certified in accordance with the ISO 17034 standard successfully offers the following advantages to users.

- a) CRM provides precise wavelength positioning, which is necessary to calibrate the wavelength accuracy of near-infrared spectrometers, especially in the short-wave near-infrared region (700 nm–1200 nm). This provides more reliable and accurate measurements in spectroscopic analyses.
- b) It fills a critical gap in the availability of calibration materials for the 900 nm–1100 nm wavelength range, which is generally underrepresented in standard materials. By covering this range, CRM supports a wider range of analytical and research applications.
- c) CRM provides SI traceable certified values, ensuring that measurements are consistent and comparable over time. This increases the reliability and reproducibility of results in laboratories and industries using near-infrared spectroscopy.
- d) The material is permanently sealed and environmentally friendly, making it a sustainable option for laboratories and industries concerned about reducing waste and environmental impact while ensuring accuracy.
- e) Given its wide wavelength range and robust design, CRM is versatile and can be used in a variety of applications where near-infrared spectroscopy is widely used, such as medicine, material sciences, and environmental monitoring.

In conclusion, the CRM reported here is ready to be offered to users as a new material that increases accuracy for the NIR region of measurement, supports regulatory compliance, and helps improve the efficiency of calibration processes in a variety of industries.

## Acknowledgements

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## **Supporting Information**

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