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Application News

Spectrophotometric Analysis No.A423B

UV and NIR Spectra of Commercial Mineral Water Samples and Quantitation of Mineral Water Sample Mixtures by Multiple Linear Regression

Mineral water, consisting of raw water from naturally occurring springs or sources, is now available under many commercial labels. The mineral content in these different brands of water not surprisingly differs depending on their source. Here we investigated these mineral content differences using absorption spectra obtained from measurement of using an ultraviolet, near infrared spectrophotometer. Since the differences in the absorption spectra cannot be seen in the visible region due to the transparency of mineral water, the investigation was conducted in the ultraviolet and near infrared regions.

These days, chemometrics is often used for simultaneous quantitation of multiple constituents. An example of the effectiveness of chemometrics quantitation is presented here, in which we applied multiple linear regression to determine the mixture ratios of several commercial mineral water samples.

■ UV and NIR Spectra of Mineral Water Samples

The absorption spectra of four commercial mineral water samples (A water, B water, C water, D water) from different natural water sources were measured in the UV region from 190-250 nm using the UV-3600 spectrophotometer shown in Fig. 1. The results are shown in Fig. 2, and the measurement parameters used are shown in Table 1.

A 10 mm path length quartz cell was used for the measurement, and ion exchange water (TOC 6 ppb, resistivity 18.2 Ω) was used as the reference sample. The differences in spectral shape due to individual differences in mineral types and quantities are clearly seen.

Next we measured the absorption spectra of the same samples in the near infrared region of 1000-1800 nm. Measurement of each sample was conducted using air as the reference, and a 2 mm quartz cell filled the sample. The results are shown in Fig. 3. Fig. 4 shows a magnification of the absorption peak of water in the vicinity 1450 nm in Fig. 3, and Table 2 shows the measurement parameters used. It is clear that in the near infrared region, almost no differences can be seen among the absorption spectra of the mineral water samples.

Fig. 1 UV-3600 UV-VIS-NIR Spectrophotometer

Table 1 Measurement Parameters

Measurement Wavelength Range	: 190 nm - 250 nm
Scan speed	: Medium
Sampling Pitch	: 0.5 nm
Photometric Value	: Absorbance
Slit Width	: 2 nm

Table 2 Measurement Parameters

Measurement Wavelength Range	: 1000 nm - 1800 nm
Scan speed	: Medium
Sampling Pitch	: 1.0 nm
Photometric Value	: Absorbance
Slit Width	: 5 nm

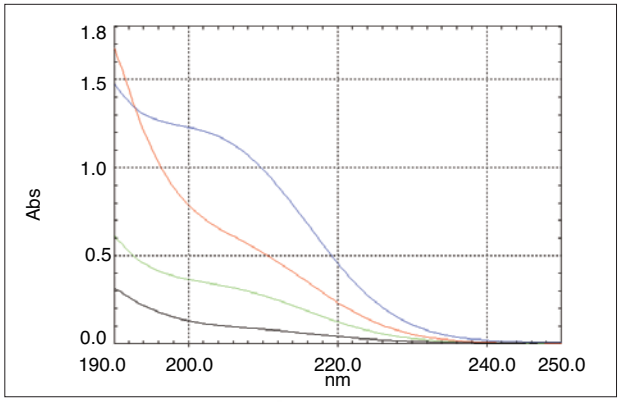

Fig. 2 Spectra of Four Mineral Water Samples (Red: A, Blue: B, Black: C, Green: D)

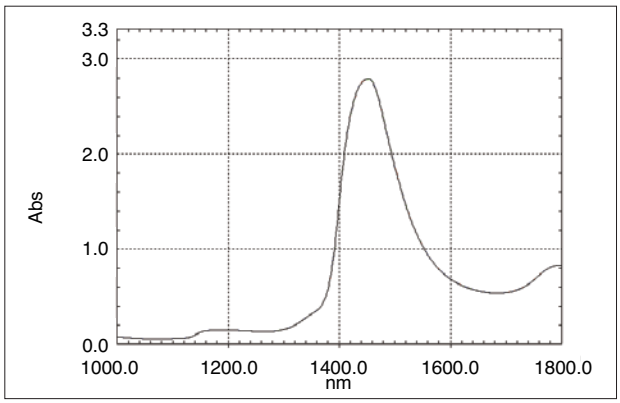

Fig. 3 NIR Spectra of Four Mineral Water Samples Measured with a 2 mm Quartz Cell

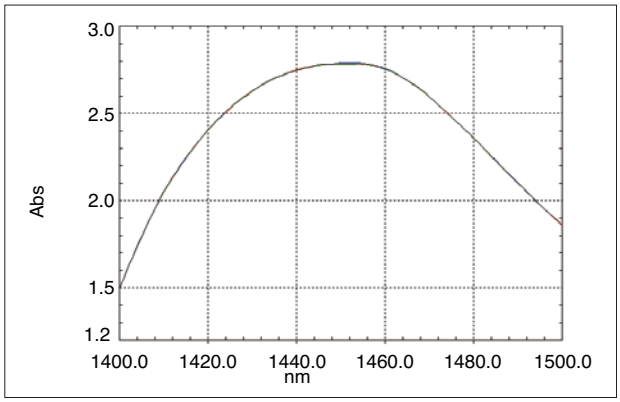

Fig. 4 Magnified Region of Fig. 3 Spectrum (Red: A, Blue: B, Black: C, Green: D)

■ Quantitation of Mixed Mineral Water Samples by Multiple Linear Regression

Mixed samples of mineral water were prepared using various ratios of A water, B water and C water, and the respective mixture ratios were determined by applying multiple linear regression to the obtained absorbance data.

Nine standard samples with varying mixture ratios, and 3 verification samples of known mixture ratios for verification were prepared, and the ultraviolet absorption spectra were measured. The mixture ratios of the standard samples and verification samples are shown in Table 3 and Table 4, respectively. The measurement results are shown in Fig. 5 (standard samples 1-5), Fig. 6 (standard samples 6-9), Fig. 6 (verification samples 1-3). The measurement parameters are the same as those shown in Table 1 on the previous page.

The number of wavelength points used for the multiple linear regression must be greater than the "number of sample constituents," and less than the "number of standard samples-2." In the present case, the former is 3 and the latter is 7, so 4 wavelengths were used. The four wavelengths, selected on the assumption that they reflect the difference between each of the mineral waters, were 200 nm, 205 nm, 210 nm and 215 nm. A calibration model (multiple regression equation) was created for each constituent using the regression analysis function of the Excel®(1) spreadsheet software application. The multiple linear regression equation for each model is shown in Table 5. As an index of correlation between the actual measured value and the predicted value (value calculated using the multiple linear regression equation), the weighted correlation coefficient for the water models A, B and C were 0.999921, 0.999986 and 0.999973, respectively.

When the absorbance values for the verification samples at the 4 wavelengths are substituted in the obtained multiple regression equations, the mixture ratios of the constituents corresponding to each model are calculated. The quantitation results are shown in Table 6. Comparison with the values of Table 4 confirms that the results are good.

Here we demonstrated that multiple regression analysis using absorbance values at multiple wavelengths can be successfully used to perform simultaneous quantitation of multiple sample constituents.

Table 3 Mixture Ratios of Standard Samples

	A Water (%)	B Water (%)	C Water (%)
Standard sample 1	20	30	50
Standard sample 2	50	20	30
Standard sample 3	30	50	20
Standard sample 4	0	50	50
Standard sample 5	50	0	50
Standard sample 6	50	50	0
Standard sample 7	100	0	0
Standard sample 8	0	100	0
Standard sample 9	0	0	100

Table 4 Mixture Ratios of Samples for Verification

	A Water (%)	B Water (%)	C Water (%)
Verification sample 1	10	80	10
Verification sample 2	30	30	40
Verification sample 3	20	60	20

Table 5 Multiple Linear Regression Equations for 3 Models

Water Model A (%)	$R_A = 1073.318 \cdot A_{200} - 1614.381 \cdot A_{205} + 1120.181 \cdot A_{210} - 731.675 \cdot A_{215} - 24.416$
Water Model B (%)	$R_B = -541.210 \cdot A_{200} + 822.186 \cdot A_{205} - 91.882 \cdot A_{210} - 133.158 \cdot A_{215} + 3.725$
Water Model C (%)	$R_C = -532.109 \cdot A_{200} + 792.195 \cdot A_{205} - 1028.299 \cdot A_{210} + 864.833 \cdot A_{215} + 120.690$

(Note) A_{200}, A_{205}, A_{210}, and A_{215} are the absorbance values at the respective wavelengths, and R_A, R_B, and R_C are the respective mineral water mixing ratios.

Table 6 Quantitation Results for Verification Samples

	A Water (%)	B Water (%)	C Water (%)
Verification sample 1	10.38	79.90	9.72
Verification sample 2	30.12	29.96	39.92
Verification sample 3	20.41	59.68	19.91

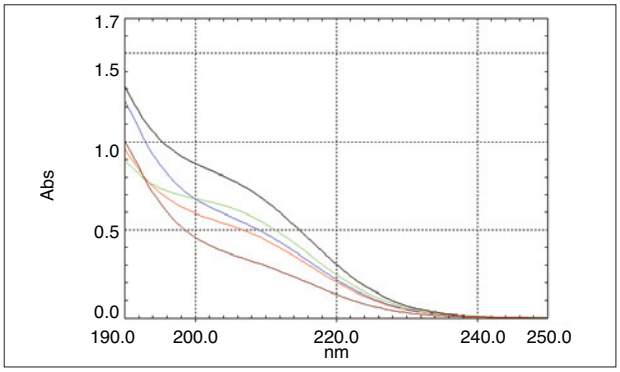

Fig. 5 Spectra for Standard Samples 1-5 (Red: 1, Blue: 2, Black: 3, Green: 4, Brown: 5)

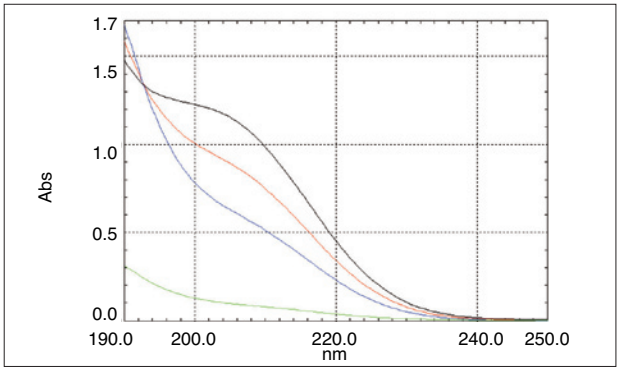

Fig. 6 Spectra for Standard Samples 6-9 (Red: 6, Blue: 7, Black: 8, Green: 9)

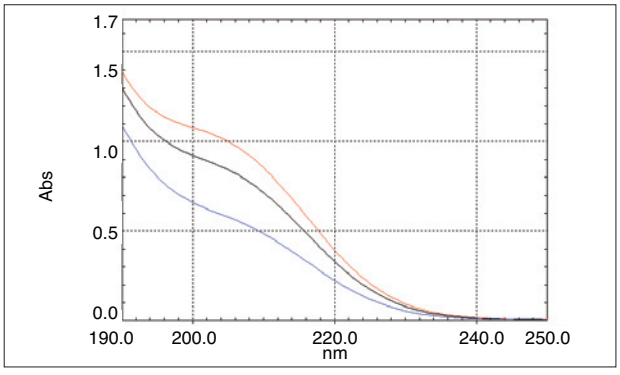

Fig. 7 Spectra for Verification Samples 1-3 (Red: 1, Blue: 2, Black: 3)

(1) Excel is a registered trademark or trademark of Microsoft Corporation.

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