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Near-infrared signature of hydrothermal opal: a case study of Icelandic silica sinters

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Spectral criteria calculation procedures

$BDR_{5235/5100}$

Band depth ratio of the 5235 and 5100 cm^{-1} absorptions (BD_{5235}/BD_{5100})

This spectral criterion is similar to the $BDR_{1.91/1.96}$ of Rice et al. (2013) that quantifies the shape of the 5200 cm^{-1} absorption band (1.90 µm). To calculate this criterion, we first calculate the band depth of both components at 5235 and 5100 cm^{-1}, BD_{5235} and BD_{5100}. For both, we used the same method. For an absorption band centered at a wavelength λ_C with a minimum of reflectance R_C, R_C^* can be considered as the virtual reflectance at λ_C interpolated onto a linear continuum between two anchor points: S (λ_S , R_S) and S (λ_L , R_L). R_C* is then expressed:

$$R_C^* = a.R_S + b.R_L$$

with $a = 1 - b$; and $b = \frac{\lambda_C - \lambda_S}{\lambda_L - \lambda_S}$

The band depth of the absorption at λ_C (BD_C) is then expressed as:

$$BD_C = 1 - \frac{R_C}{R_C^*}$$

with R_C, the measured reflectance;
and R_C^*, the virtual reflectance.

For BD_{5235}: λ_C = 5235 cm^{-1} ; λ_S = 5495 cm^{-1} ; λ_S = 4705 cm^{-1} ; a = 0.671 ; b = 0.329
For BD_{5100}: λ_C = 5100 cm^{-1} ; λ_S = 5495 cm^{-1} ; λ_S = 4705 cm^{-1} ; a = 0.500 ; b = 0.500

$BDR_{4525/4425}$

Band depth ratio of the 4525 and 4425 cm^{-1} absorptions (BD_{4500}/BD_{4425})

This spectral criterion is similar to the $BDR_{2.26/2.21}$ of Sun & Milliken (2018) that quantifies the shape of the 4500 cm^{-1} absorption band (2.20 µm). To calculate this criterion, we calculate the band depth of both components at 4525 and 4425 cm^{-1}, BD_{4525} and BD_{4425}. The method for the calculation of each band depth is the same as explained above.

For BD_{4525}: λ_C = 4525 cm^{-1} ; λ_S = 4705 cm^{-1} ; λ_L = 4255 cm^{-1} ; a = 0.600 ; b = 0.400
For BD_{4425}: λ_C = 4425 cm^{-1} ; λ_S = 4705 cm^{-1} ; λ_L = 4255 cm^{-1} ; a = 0.378 ; b = 0.622

CRC_{5200} and CRC_{7000}

Concavity-Ratio-Criterion (CRC) of the 5200 and 7000 cm^{-1} absorptions

These two criteria were first defined by Chauviré et al. (2017) on transmission measurements. They quantify the shape of the high-frequency side of the 5200 and 7000 cm^{-1} absorptions respectively. Pineau et al. (2020) then adapted the calculation procedure for reflectance measurements.
For the absorption band at 5200 cm^{-1}, we chose two anchor points at $\lambda_S \approx$ 4700 cm^{-1} and $\lambda_L \approx$ 5400 cm^{-1}. Then, two band depth are calculated: BD_C is the real band depth of the low-frequency inflection point at 5100 cm^{-1}, and BD_C^* is the virtual band depth of the same inflection point using a linear continuum between the minimum of reflectance and the low-frequency anchor point at λ_L (the calculation method of band depths is explained above). The CRCc is calculated as:

$$CRC_C = \frac{BD_C}{BD_C^*}$$

The same calculation is applied for the absorption band at 7000 cm^{-1}, using anchors at $\lambda_S \approx$ 6000 cm^{-1}, $\lambda_L \approx$ 7700 cm^{-1}, and BDc = 6850 cm^{-1}.
The error in the CRC calculation is calculated empirically by shifting the two anchor points at λ_S and λ_L over 50 cm^{-1} (25 spectels), which generates 2809 distinct combinations for a single measurement. The CRC is calculated for each of the 2809 combinations. The retained value for the CRC is the average of all calculated values, and the error represents the standard deviation (1σ)

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