American Mineralogist, Volume 98, pages 401–409, 2013

Quantitative analyses of powdered multi-minerallic carbonate aggregates using a portable Raman spectrometer

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Abstract

Mg-Ca carbonates are an important group of industrial minerals, which frequently occur intimately intermixed in natural settings and are traditionally assessed for phase purity by X-ray diffraction (XRD). In this study Raman spectroscopy is employed to quantify the modal abundance of hydromagnesite [$Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O$], huntite [$CaMg_3(CO_3)_4$], dolomite [$MgCa(CO_3)_2$], and magnesite [$MgCO_3$], in powdered mixtures constructed from fabricated reference materials. Particle size distributions were assessed by scanning electron microscopy and laser diffraction. Raman analyses performed using a portable instrument were conducted at 25 °C and at atmospheric pressure. XRD was employed to validate the accuracy and precision of Raman measurements. Monovariable and multivariable methods were employed to provide quaternary quantification from the spectroscopic data. For monovariable calibration the amplitude of the peaks was plotted against the measured weight ratios of the four mineral phases. Overlapping bands were resolved using the Gaussian Lorentzian method. Chemometric methods were used to perform the multivariable calibration. The overall lowest error on component values was obtained by principal component regression with application of standard normal variate correction. The quantifications derived by Raman spectroscopy and XRD show close agreement. Hence, evidence suggests that a reliable four-way calibration program to screen the purity of carbonate assemblages can be constructed, providing particle size effects are constrained and spectroscopic operating conditions are uniform.

Keywords: Portable, Raman spectroscopy, quantification, quaternary mixtures, carbonates