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Estimating modal mineralogy using Raman spectroscopy: Multivariate analysis models and Raman cross-section proxies

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Abstract

Raman spectroscopy is a powerful technique in the context of planetary exploration because it provides information on mineral identification, chemistry, and abundance. For Raman spectrometers with large spot sizes, multiple mineral phases can be investigated by collecting a single Raman spectrum. There is a lack of methodology for quantifying mineral species in mixtures due to the independent signal strengths of different materials in Raman spectra. Two techniques are presented in this work for quantifying common rock-forming minerals: partial least-squares multivariate analysis and a novel approach called Raman cross-section proxies (numerical metrics associated with specific Raman features). This paper targets 20 mineral species relevant to the mineralogy of the planet Mars. Mineral end-member samples and 187 binary mineral-mineral mixtures (mixture of two distinct minerals) are used for multivariate modeling. Eighteen diamond-mineral mixtures are used to derive Raman cross-section proxies. Mineral abundance proportions are predicted for the binary mineral-mineral mixtures with known mineralogical content to evaluate the efficacy of the two quantitative methods. Technique performance is mineral dependent. The root mean square error for unseen predictions (RMSE-P) using Raman cross-section proxies ranges from ±3.2–17.0 vol%. For the multivariate models, the cross-validated root mean square error (RMSE-CV) ranges from ±8.8 to 26.2 vol%. Although these error estimates are not directly comparable, they provide the most accurate error estimate currently available. Different scenarios may favor the use of one or the other of the two quantitative methods. This work provides fundamental groundwork that can be applied to common rock-forming minerals on terrestrial planets, including Mars. Quantification of mineral abundances aids in answering critical geologic questions related to ancient primary and altered rocks as well as planetary processes and conditions.

Keywords: Modal mineralogy, Raman spectroscopy, Raman cross-section