American Mineralogist, Volume 99, pages 1570–1579, 2014

WHAT LURKS IN THE MARTIAN ROCKS AND SOIL? INVESTIGATIONS OF SULFATES, PHOSPHATES, AND PERCHLORATES

Multivariate analysis of Raman spectra for the identification of sulfates: Implications for ExoMars†

GUILLERMO LOPEZ-REYES[1,*], PABLO SOBRON[2,3,4], CATHERINE LEFEBVRE[2] AND FERNANDO RULL[1]

[1]Unidad Asociada UVA-CSIC-Centro de Astrobiología, C/ Francisco Valles 8, 47151, Boecillo, Spain
[2]Space Science and Technology, Canadian Space Agency, 6767 Rte. de l'Aéroport, St. Hubert, Quebec J3Y 8Y9, Canada
[3]MalaUva Labs, 822 Allen Avenue A, St. Louis, Missouri 63104, U.S.A.
[4]SETI Institute, 189 Bernardo Avenue 100, Mountain View, California 94043, U.S.A.

ABSTRACT

We have built three multivariate analysis mathematical models based on principal component analysis (PCA), partial least squares (PLS), and artificial neural networks (ANNs) to detect sulfate minerals in geological samples from laser Raman spectral data. We have critically assessed the potential of the models to automatically detect and quantify the abundance of selected Ca-, Fe-, Na-, and Mg-sulfates in binary mixtures. Samples were analyzed using a laboratory version of the Raman laser spectrometer (RLS) instrument onboard the European Space Agency 2018 ExoMars mission. Our results show that PCA and PLS, can be used to quantify to some extent the abundance of mineral phases. PCA separated hydrated from dehydrated mixtures and classified mixtures depending on the phase abundances. PLS provided relatively good calibration curves for these mixtures. Upon spectral pre-processing, ANNs provided the most precise qualitative and quantitative results. The detection of mineral phases was 100% accurate for pure samples, as was for binary mixtures where the abundance of mineral phases was >10%. The outputs of the ANN were proportional to the phase abundance of the mixture, thus demonstrating the ability of ANNs to quantify the abundance of different phases without the need for calibration. Taken together, our findings demonstrate that multivariate analysis provides critical qualitative and quantitative information about the studied sulfate minerals.

Keywords: Sulfates, ExoMars, Raman spectroscopy, multivariate analysis, qualitative, quantitative