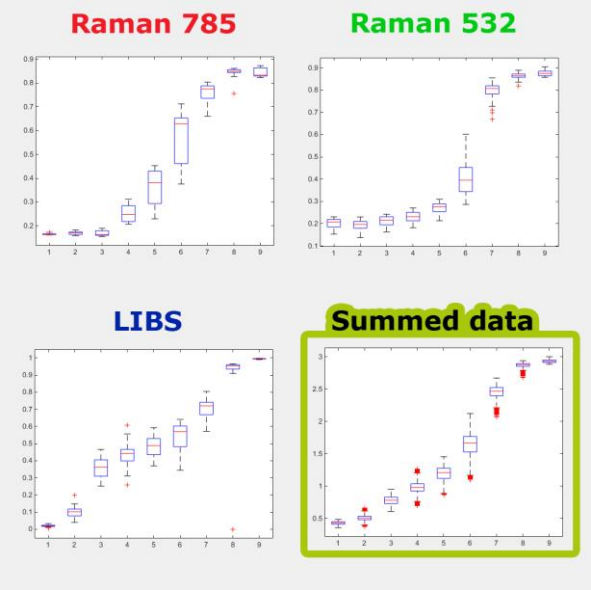
DATA FUSION OF RAMAN AND LIBS APPLIED TO PLANETARY EXPLORATION RELEVANT COMPOUNDS. Jose A. Manrique-Martinez[1,2], Guillermo Lopez-Reyes[1,2], Thomas Bozic[3], Andres Alvarez-Perez[1], Marco Veneranda[1,2], Jesus Saiz[1,2], Jesus Medina-Garcia[1,2], Fernando Rull Pérez[1,2]. [1]University of Valladolid, [2]Centro de Astrobiología, [3]University of Paris-Sud

Introduction: Raman and LIBS are two techniques that could share technical components, as both need a laser, spectrometer and detector. Also, these two techniques provide complementary information, while Raman spectroscopy provides molecular identification, LIBS provides elemental composition of the samples, allowing a good frame for collaborative chemometric analyses, and the development of combined instruments capable of performing both analyses on a sample, being especially interesting for solar System exploration[1].

About their application to the Exploration of the Solar System, LIBS have been used in the surface of Mars since Curiosity's landing in 2012 with ChemCam, while Raman is a future technique to be at the surface of the red planet with RLS (Exomars), Sherloc (M2020) and SuperCam (M2020), being this last one a combined Raman-LIBS instrument, and was included in the desirable payload for the Europa Lander mission.

In the present work we present the results of the analysis of binary and ternary mixtures of magnesium and sodium sulfates with magnesium chlorine, providing different scenarios where Raman and LIBS separately present different performances to quantify the amount of certain component in the mixtures. In the case of Raman spectroscopy, two different excitation wavelengths were used, 785 and 532 nm, using this experiment as well to evaluate the possible incidence of excitation source on the final results. Also, in the case of the 532 nm, the spectra were collected in automatic mode using an operation simulator for RLS instrument, introducing time constrains, and best possible parameters calculation for the acquisition.

The samples were physically mixed in different proportions to assess not only the detection limits of the Raman and LIBS techniques of these mixtures, but also to perform an investigation regarding the quantification of their mineral abundances. In order to do so, at a first stage separated univariate analysis were done calculating ad hoc indicators from the spectroscopical data. As a first glance to the fusion of the data, those indicators were later normalized and arithmetically combined to evaluate a final common indicator.



The second phase of the study implied separated multivariate analyses for both, binary and ternary mixtures [2]. During the last part of the present work, data fusion techniques were also applied to study the capability to improve the detection limits and/or quantification abilities of the techniques by merging the information from Raman and LIBS in the ternary and binary mixtures [3].

Acknowledgements: Authors would like to thank the Spanish Ministerio de Ciencia Innovación y Universidades for its funding under ESP2017-87690-C3-1-R, the University of Valladolid and Centro de Astrobiología for their support making possible this research.

References:

[1] Sobron, P., et al. (2013). Why Raman and LIBS for Exploring Icy Moons? 44th Lunar and Planetary Science Conference. Houston, Lunar and Planetary Institute: Abstract #2381.

[2] Lopez-Reyes, G., et al. (2014). "Multivariate analysis of Raman spectra for the identification of sulfates: Implications for ExoMars." American Mineralogist 99(8-9): 1570-1579.

[3] Sobron, P., et al. (2014). Data Fusion in Planetary LIBS+Raman Spectroscopy. 45th Lunar and Planetary Science Conference. Houston, Lunar and Planetary Institute: Abstract #2875.