AUTOMATED AND SELF-REGULATED RAMAN SPECTRA ACQUISITION FOR SPACE EXPLORATION: EXOMARS RLS INSTRUMENT. G. Lopez-Reyes1, O. Peña Nogales1, A. Perez Oliveros1, A. Sanz1 and F. Rull1, 1Unidad Asociada UVa-CSIC-Centro de Astrobiología (C/ Francisco Valles 8, E-47151, Boecillo, Spain – lopezrge@cab.inta-csic.es).

Introduction: The RLS instrument is a Raman spectrometer which is part of the rover payload of ESA’s 2018 ExoMars mission. In order to optimize the spectra acquisition, RLS will be equipped with a set of algorithmic tools to automatically optimize the acquisition parameters taking into account the onboard available time and resources. The set of algorithms is aimed at providing a self-regulated and unsupervised method for the acquisition of Raman spectra, dealing with effects such as fluorescence and cosmic rays, and calculating the integration time (Ti) and number of accumulations (Na). All the algorithms are designed to adapt to the sample under study, to provide the best possible balance between performance and resources.

Materials and methods: To design and develop the algorithms, several sets of bulk and powdered (grain size <250 microns) samples were analyzed with the RLS ExoMars Simulator, which is a 532 nm Raman spectrometer with a 3-axis positioning system to emulate the operational framework of the Exomars rover [1]. The analysis and design of the algorithms here presented is being performed with Mathworks MATLAB, while implementation and testing is carried out with Microsoft Visual Studio and NI LabVIEW.

Automated Raman acquisition procedure: The general flowchart calculates the following parameters sequentially: 1-fluorescence quenching times, 2-detection and removal of cosmic rays and 3-calculation of Ti and Na. Fluorescence and cosmic ray removal (steps 1 and 2) are needed to ensure the quality of the reference spectra that will be used for the calculation of the acquisition parameters in step 3.

Self-regulated fluorescence removal algorithm. Fluorescence is a competitive effect that occurs when the laser excites fluorescence of the analyte or impurities, resulting in a general increase of the background level. This level can vary with time when continuously illuminated with the excitation source, by saturating the fluorescence energy states. The decreasing rate of the fluorescence level is thus related to the sample under analysis, and can vary highly among different samples. To evaluate the decreasing rate of the fluorescence, we selected a set of fluorescent samples and mixtures with different characteristics and background variation rates: fluorite, quartz, talc, and a mixture of alunite, calcite, epidote, magnesite and dolomite. The analysis of these samples showed that there is an inverse correlation between the SNR value and the background level of the spectrum. As time passes, the background level caused by fluorescence decreases, resulting in a higher SNR value. This effect is depicted in Fig. 1 for the main peak of alunite in the powdered mixture, and is also noticeable with non-fluorescent samples of the mixture (e.g., calcite).

Fig. 1. SNR and fluorescence background level evolution with excitation time

However, being the decreasing rates different for each type of sample, the final level of background that is achievable by its kind of sample is different, as shown in Fig. 2a. Under these conditions, it is complicated to extract, based on the absolute background level, an objective parameter for the algorithm to decide when the background has decreased to an acceptable level. To solve this issue, it was decided to use instead the decrement rate, which, as shown in Fig. 2b, converges for all samples. This way, when the decrement per second falls below a determined threshold, the algorithm decides to stop. We set it to 0.1%/s.

Fig. 2. Abs. background (a) and decrement rate (b) vs. time

Cosmic ray detection and removal algorithm. After the quenching of the fluorescence, two spectra are acquired that will be used as a reference for the calculation of Ti and Na of the final acquisition. In order to
The implementation of an autonomous Raman spectrometer as RLS requires that the system is provided with autonomous analytical tools. These will be used to objectively evaluate spectral characteristics during the acquisition process in order to optimize the performance of the instrument, while consuming the minimum quantity of resources. We have carried out a preliminary but extensive work to define the necessary algorithmic for an all-automatic and unattended Raman acquisition. The implementation of these tools on the RLS Exomars Simulator allows the testing and evaluation in an operational representative scenario.