# MODAL MINERALOGY OF IGNEOUS ROCKS WITH CHEMCAM AT GALE CRATER.

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**Introduction :** Analysis using laser induced breakdown spectroscopy (LIBS) technique provides compositional information about the surface under the targeted laser spot area. For the ChemCam instrument onboard MSL, the anamysis region is small but finite, typically equivalent to a disk of one to a few hundred $\mu$m in diameter for shots at a distance of 2 to 7 m from the rover masthead [*Maurice, 2012, LPSC 43, #2899*]. Since most igneous rocks are typically composed of several minerals, the average grain size relative to the laser spot size will have a significant effect on the results obtained. For example, each shot will most frequently sample single minerals (coarse granulometry), two to three minerals in varying proportions (granulometry roughly similar to the laser spot size), or more or less the same mixture (fine granulometry). From this, modal mineralogy(*) can easily be assess in the first case, needs some statistical work in the second one, and is mainly hidden to this technique in the third case.

(*) the modal mineralogical composition of a rock is its composition defined in term of actually present minerals, opposite to a normative mineralogy, which is a result of a calculation. This latter will not be used here.

This case study will consider measurements from sols 45 & 48 on the float rock named Jake_Matijevic, 14 laser location spots with 30 shots and therefore spectra at each spot. More precisely the data set consists in the series of said "CCS" spectra (denoised, dark and continuum removed, and aligned in wavelength). These data are represented as geometrical points in the « spectral space » (of 6144 dimensions), one point par spectrum. The present work mainly exploits the geometrical characteristics of the cloud of data points. Since the high-dimensionality of the spectral space (much more than samples…), perpendicular projections into a few well-chosen 2D and 3D sub-spaces will be used as tools for exploring it (after the choice of a given metric ; these are linear transforms). Use of the PCA technique either on correlations or on covariances, will help for this choice. In particular, it permits to define a subspace of the spectral space, later dubbed the « reduced spectral space », of 50 to 100 dimensions, which keeps most of the significant variability of the whole spectra set.

With such tools and data, observations are the following : the "cloud" of the 420 spectra is highly structured in the spectral space :

- the very first (one to three) laser shots of almost all locations result in LIBS spectra "gathered" around a relatively well-defined spectrum, that of the Gale crater dust ;
- for each targeted location, the remaining 28 or so spectra are clustered close to each other, relatively to the overall spread of the 420 spectra, therefore defining rather precisely each of the different target compositions. Moreover this spread is a good entry for estimating the uncertainties of a ChemCam measurement.

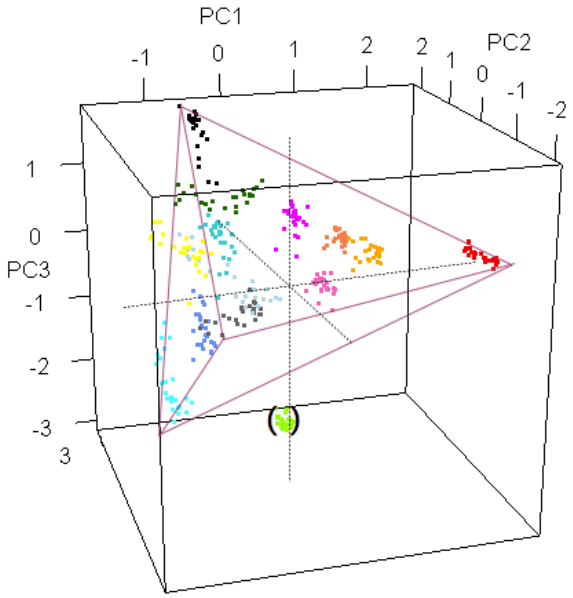


**Figure 1:** projection in a 3D subspace of the spectral space, of the cloud of 420 spectra points from the 14 targeted locations, coded each with a specific point color. The three chosen dimensions here are the 3 first principal components. The three dotted lines cross at (0,0,0) coordinates, which represents the mean spectrum. Axes are graduated in standard deviations around the mean. From spectra analysis and other projections, the green cluster is considered as a specific mineral. The remain-

ing 13 clusters spread inside a tetrahedron, with 4 clear end-members, considered as almost pure minerals.

**Discussion :**

- The center of the spectral cloud, such as the point representing the mean spectrum, average of the 420 spectra (minus the 20 or so dust ones), and shown with all-zero coordinates on PCA plots, is a priori the best approximation we get for the Jake_Matijevic whole-rock composition ;

- The dispersion of the targeted clusters is well explained by the micro-granular texture, with a grain size of the order of the laser spot size (within a factor of 2 to 3), about 300 $\mu$m at the rock distance for this measurement series ;

- The four or so « extreme » spectral points define the end-member compositions of this mineralogical assemblage. These end-members, though being the purest approximations of the minerals present in the assemblage (the so-called modal composition of the crystalline rock), are still most probably mixtures under the laser spot between one dominant mineral and one or a few others. With the first order assumption that measured spectra are linear combinations of pure mineral spectra, using mathematical techniques of unmixing mixtures, one can estimate these pure components spectra, and try to relate them to simple minerals.

- These calculated "pure-component" spectra are compared with a still preliminary database of truely measured mineral spectra. This is done using independent component analysis (ICA) and Sammon's map tools.

- The same work is done using the calculated major element compositions with the ChemCam PLS procedure. An adaptated version of PCA is used to explore the topology of the cloud of the 420 calculated major element compositions in the said « compositional space » (of dimension 10), in correspondence with that from the reduced spectral space. In particular, the comparison between the end-members estimated within the major element compositional space, with the calculated major element compositions of the spectral end-members permits to assess the validity of some of the underlying assumptions ; among these, is the level of departure to linearity of spectra combination for mineralogical mixtures under the laser beam.

- Independently to this, the same procedure of extrapolating the end-members in the compositional space is proceeded in order to infer pure mineralogical components, with the great advantage of a better knowledge of attended minerals for such a type of rock, but conversely the drawback of increased uncertainties due to the still preliminary spectrum-to-composition quantification procedure.

As a preliminary conclusion, one lesson is that the research of the modal mineralogy can be engaged directly in the spectral space, despite the absence of external knowledge such as from mineral peculiar compositions, but without recourse to the quantification step, and therefore without adding uncertainties other than that of measurements. However clear interpretation requires having access to the mineral spectra database, which is presently in construction.