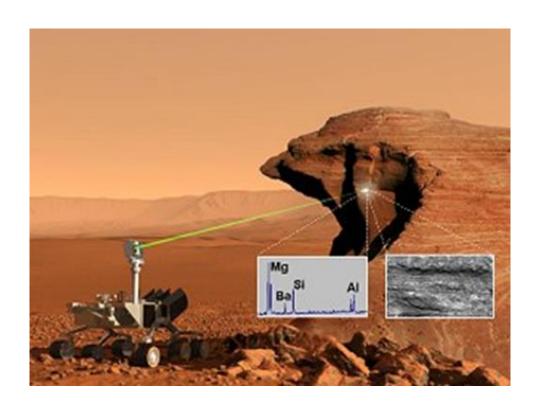
# M.O.R.E project Detection of organic Matter thanks to LIBS instrument S7 Final report



PRADELLE Mathis

MOYAL Samuel

GROSMAITRE Arthur





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## A. Introduction

#### 1. Context

#### a. LIBS in Martian Rovers

Laser-Induced Breakdown Spectroscopy (LIBS), also known as laser ablation spectroscopy, is a chemical analysis technique used in planetary exploration, including Martian rover missions. The technology was first incorporated into the ChemCam device of the Curiosity rover in 2012[1].

When used in Martian rovers, a laser is utilized to ablate a small sample of rock or soil on Mars' surface. When the laser strikes the sample, it generates a high-energy plasma. This plasma then emits light that is analyzed by a spectrometer to determine the chemical composition of the sample.



Figure 1 : Vue de la tête du rover Curiosity et de la ChemCam [1]

The use of LIBS in Martian rovers offers several advantages. It allows for rapid acquisition of elemental composition information about Martian rocks and soils without the need for sample collection and return to Earth. This enables scientists to obtain real-time data about the materials present on Mars, learn more about the planet's geological history, and choose the most appropriate sampling areas for return to Earth. It allows in-situ soil analysis without the need for larger analytical instruments, thereby reducing time and associated costs. Moreover, LIBS is non-destructive, meaning it does not damage the samples during analysis.



In summary, the use of LIBS in Martian rovers like Curiosity allows scientists to obtain information about the chemical composition of samples on Mars quickly and non-destructively, with the goal of selecting the most appropriate areas for material samples to return to Earth for comprehensive analysis. This contributes to advancing our understanding of the red planet and its geological history.

However, the spectra obtained from the device are complex. The challenge is to determine if the analysis of these spectra would allow the detection of organic matter. Applied to a Martian rock, a positive response would be an indication suggesting that life could potentially thrive on the planet.

#### b. Physical Principles of LIBS Technology

LIBS spectroscopy analysis involves the use of a pulsed laser focused on a material using a series of optics.[2] When the laser delivers sufficient energy, the material's surface is heated. If the laser's fluence (energy per unit area) exceeds the material's ablation threshold, the material is vaporized, forming a cloud of vapor that interacts with the laser and becomes ionized.

Under the influence of the laser's energy, the cloud of ionized vapors transforms into a micro-plasma at several thousand Kelvin. The chemical species present in the plasma (electrons, atoms, and ions) are excited. The creation of this micro-plasma generates a shockwave that ejects material and creates a crater.

The laser vaporizes the ejected particles while maintaining the excitation of the chemical species. The electron density and the size of the plasma increase, as well as its internal pressure. At this stage, various physical reactions specific to the plasma occur, gradually making it opaque to the laser.

The laser pulse ends, and the plasma enters a phase of spatial expansion under the influence of its internal pressure. During this phase, the plasma cools down and its electron density decreases.



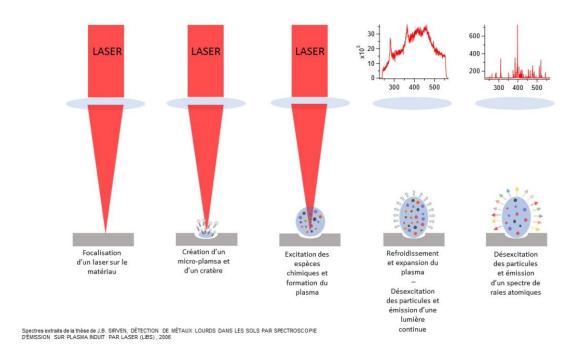


Figure 2 : Principe physique de fonctionnement du LIBS [3]

During the cooling process, the chemical species emit photons and de-excite, creating a continuous blackbody-type light radiation. As the electron density of the plasma decreases and it cools, the intensity of this radiation diminishes, giving way to a spectrum composed of atomic lines. The wavelengths of these lines are characteristic of the elements present in the analyzed material.

During the photon emission, internal exchanges occur within the plasma, leading to recombinations among the chemical species, including molecular recombinations that can manifest in the emission. The light emitted by the plasma is collected using an optical fiber connected to a spectrometer coupled with a detector. This system enables the recording of emission spectra in a range that typically spans from ultraviolet to infrared (200 to 950 nm), depending on the spectrometer used.

LIBS analysis involves interpreting these spectra by identifying the representative elements of the emission lines using a database. The position of the emission lines indicates the presence of the elements, and their intensities are proportional to their concentration in the plasma, and thus in the analyzed material.



#### 2. Problem statement

LIBS is primarily used to detect inorganic elements. Organic elements, namely carbon, hydrogen, oxygen, nitrogen, and sulfur, have different excitation and ionization levels compared to inorganic elements. As a result, they can be more challenging to detect and analyze using LIBS. There are several reasons for these difficulties.

First, organic molecules can exhibit complex structures, leading to complex emission spectra. Unlike inorganic elements that have characteristic emission lines, organic molecules may present a broad continuous spectrum with few distinct emission lines. This makes the identification and quantification of organic components more challenging to achieve accurately with LIBS [1].

Furthermore, when analyzing organic materials, there can be significant matrix effects from the compounds present in the sample.[2] These effects can mask or alter the spectral signatures of the organic elements of interest. It can be difficult to separate the signals of organic elements from background signals or interferences from other compounds present in the sample. This is notably accentuated by the shorter lifespan of elements like carbon in the plasma, which recombines more rapidly [1]. Therefore, the observation time of the plasma must be early in its lifetime.

Additionally, the precise identification of organic elements often requires specific calibration using reference samples containing the same organic compounds. This can be challenging due to the wide variability of organic samples and the need for a comprehensive and well-characterized database for calibration.

Despite these challenges, advancements are being made in the development of LIBS methods specifically tailored for the detection and identification of organic matter. Improvements in laser excitation techniques, light collection systems, and data analysis algorithms are underway to overcome these limitations and enhance the capability of LIBS to accurately identify organic matter.

Our objective is to determine to what extent and under what conditions organic matter could be identifiable in Martian minerals using a LIBS instrument.



## **B.** Development

## I. Méthodology

To address this issue, we sought to acquire a library of spectra through several samples. Then, by analyzing spectral data, we attempted to identify consistent indicators that allow for the detection of organic matter. As part of our project, we are using the TX1000 from iUMTEK [3], the company that provides us access to the LIBS.

We then established an experimental protocol to observe different spectra obtained through LIBS analysis.

#### a. Protocol

We proceeded as follows:

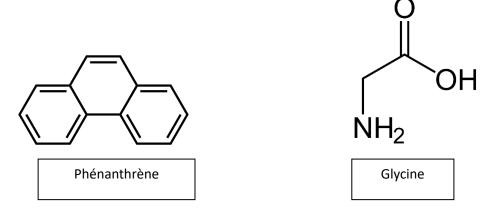
We aimed to use LIBS to study realistic samples prepared by us, where the nature of the organic matter varies, the matrix varies, and the mass concentration of the organic matter varies. The organic matter is initially dissolved in a solvent to facilitate mixing with the matrix.

Our project spanned over two years. In the first year, we focused exclusively on the nature and concentration of the organic matter. In the second year, we additionally changed the matrix.

#### b. Choice of organic matter

In view of the availability of organic products in the LGPM laboratory, we chose to study, on the one hand, phenanthrene and, on the other hand, glycine. Indeed, these two products consist of different organic elements: phenanthrene is composed of three aromatic rings and is therefore made up solely of carbon and hydrogen, while glycine, in addition to carbon and hydrogen, contains an amine group and a carboxyl group, and thus includes nitrogen and oxygen. This will allow for a preliminary study on the challenges of analyzing different organic chemical elements.





Moreover, these two molecules have the advantage of being in a powder form at room temperature, which makes the preparation of the samples easier.

#### c. Choice of the matrix

We favored a matrix in powder form to facilitate the mixture with the organic matter. Ideally, the matrix should contain as few elements characteristic of organic matter (C, H, O, N, S) as possible. Sand is a good candidate because it is primarily composed of SiO2. However, the characteristic line of oxygen may be distorted by the presence of the sand.

#### d. Choice of the concentration

The idea is to start with samples highly concentrated in organic matter and then gradually decrease the mass concentration until reaching the detection threshold. So, when referring to concentration, it concerns the ratio of the mass of organic matter to the mass of the entire product.

#### e. Choice of solvants:

The organic matter needed to be soluble in the solvents used. Moreover, these solvents should have a sufficiently low boiling point so that they evaporate relatively easily once the mixture of organic matter with the sand is completed, without deteriorating the glycine and phenanthrene during evaporation. Based on these criteria and the availability of solvents in the LGPM laboratory, distilled water with glycine and ethyl acetate with phenanthrene are good candidates, with respective boiling points of 100°C and 77.1°C.



#### f. Préparation of samples :

We prepared the samples in the LGPM laboratories.

Last year, we prepared a total of 9 samples.

They are distributed as follows:

- 1 control sample composed only of the matrix (sand)
- 1 control sample composed only of pure phenanthrene
- 1 control sample composed only of pure glycine.
- 3 samples with respectively 3%, 10%, and 30% by mass of phenanthrene
- 3 samples with respectively 3%, 10%, and 30% by mass of glycine

This year, we decided to go lower in concentration in view of the results obtained last year. Here are their distributions:

9 samples with respectively 3%, 1%, 0.5%, 0.2%, 0.1%, 0.05%, 0.02%, 0.01%, and 0.005% by mass of phenanthrene

9 samples with respectively 3%, 1%, 0.5%, 0.2%, 0.1%, 0.05%, 0.02%, 0.01%, and 0.005% by mass of glycine

2 control samples for which we corrected the preparation protocol compared to the previous year by following the same protocol as for the deposition of organic matter: sand put into solvents, respectively water and ethyl acetate, and then re-evaporated under the same conditions as the other samples.

Experimentally, we weighed the masses of sand and organic matter to obtain these ratios. Then we solubilized glycine and phenanthrene in Erlenmeyer flasks in a minimum amount of solvent, respectively in distilled water and ethyl acetate. The Erlenmeyer flask is then tared on a scale to add the necessary mass of sand. The amount of solvent must still be sufficient to soak all the sand. We roughly mixed the sand now impregnated with the solute using spatulas or magnetic stirrers as soon as possible. Finally, we placed the Erlenmeyer flasks to slowly evaporate the solvent at a temperature around 50 degrees Celsius for one to two weeks before collecting the contents of the Erlenmeyer flasks into capped plastic containers.



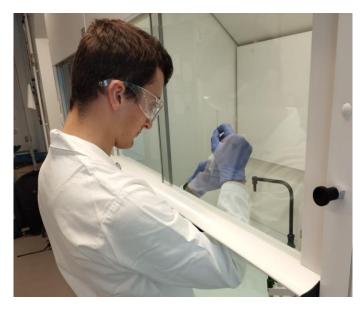


Figure 3 : Préparation of a phénanthrène sample



## II. LIBS experiment

#### a. Présentation of the instrument

The instrument used in this study (TX 1000 from iUMTEK) can analyze all types of samples (solid, liquid, and aerosols) and detect all the elements of the periodic table simultaneously. The heavier the element, the more easily it is detected. We had to optimize the device's parameters to obtain the most usable spectra possible. Care is taken not to change the device's parameters between two measurements to avoid distorting the results.



Figure 4: TX1000 device from iUmtek

#### b. Optimisation of parameters :

**Laser Energy:** It should be neither too low to achieve a stable plasma nor too high to avoid excessive pulverization of the powders.

**Detection Delay:** As organic elements have a relatively short lifespan in the plasma, the detection delay must be shorter than for the analysis of other types of elements.

**Number of Shots per Burst:** The aim is to minimize the dispersion of the powder while maintaining a usable signal. If the number of shots is too high, there's a risk of hitting the cap after forming a crater in the sample.

**Detector Gain:** Set to the maximum due to the small number of laser shots used. However, this increases the recorded noise.



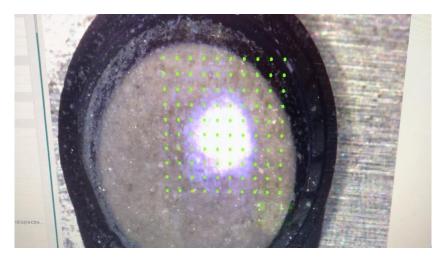


Figure 5: Shooting matrix during measurements

**Multiple Point Shots:** The shots are performed on a square matrix of 100 points to average the shots across the entire sample and thus reduce local noise, especially in the face of the low number of shots on each point. Also, this aims to compensate for the probable heterogeneity of the granular medium by multiplying the points of analysis.

For each sample, the repetitions are averaged, then a qualitative study is performed. The most significant emissions are identified on the spectra.

For all the samples, the powder is poured into the cap of the sample container. To meet the stated criteria, the chosen parameters are a gain of 200, a firing energy of 3.5 mJ, a detection delay of 150 ns, and the sampling is carried out according to a 10x10 matrix with a space of 0.75mm between each point on which a burst of 5 shots is performed.



## III. Analysis of the résults

#### a. Glycine

Recall of the main results of last year :

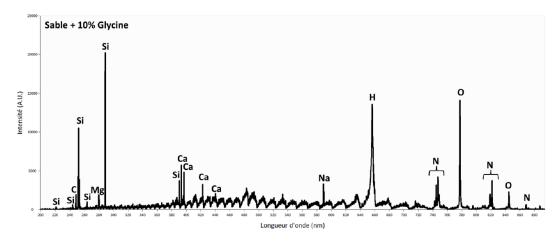


Figure 6: Graph showing the averaged spectrum of the sample containing 10% by mass of glycine

The detected elements Ca, Mg, Na are related to sample contamination (magnesium dust). With a weaker signal, we observe parasitic Al, Fe, Na, and Ti. Metals can, for example, come from the abrasion of the spatula by friction with the sand grains.

Silica is solely representative of the presence of sand.

The characteristic peak of the CN bond is related to:

- Recombinations between the carbon and nitrogen of glycine
- Recombinations between the carbon and nitrogen of the air.

The peak related to oxygen comes from the oxygen of glycine, the air, and the sand.

Since the O and CN peaks depend not only on organic matter, their study is of limited use for our project. Indeed, if the intensity of the CN bond varies in the samples, this could be due to the variation in the proportion of carbon and not necessarily of carbon and nitrogen of the organic molecule. However, variations in oxygen intensity can be due to the variation in the concentration of organic molecules, but too many interactions with the air do not allow its study without the risk of overinterpretation.



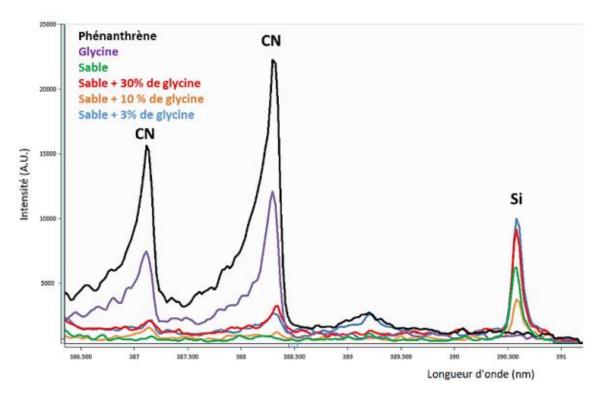


Figure 7: CN signal of glycine samples

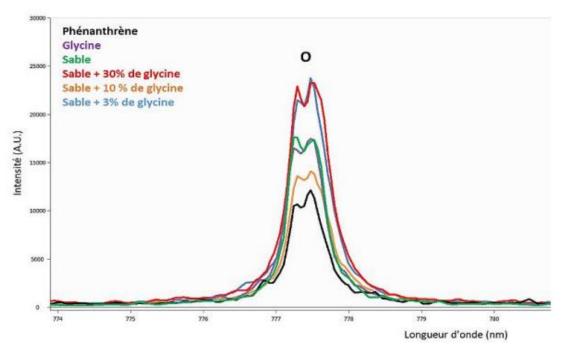


Figure 8 : Oxygène peak of glycine samples



That is why, to quantify the concentration of organic matter in relation to the matrix, we mainly focus on the peaks related to carbon and silicon.

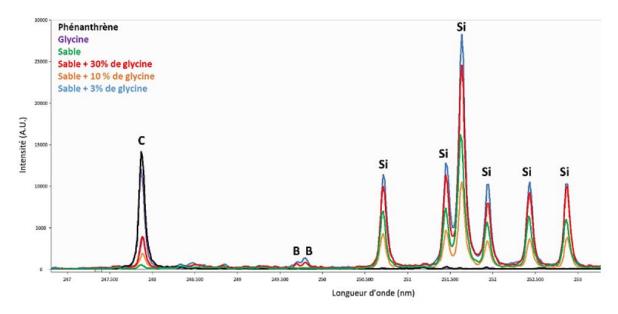


Figure 9: Averaged spectrum of pure phenanthrene samples, sand, and glycine at 3%, 10%, 30%, and 100% by mass, centered on the range [247nm; 253nm]

Generally, it is observed that the higher the concentration of organic matter, the higher the peak height related to carbon (and that related to the CN interaction) and the lower the peak height related to silica. However, this rule does not strictly apply to all samples as experimental conditions can slightly vary from one measurement to another. The main factor of this effect is the laser focusing, which is difficult to achieve precisely on a granular medium and therefore generates plasmas of variable intensity. Moreover, the background noise of the spectrum may have been removed differently from one spectrum to another, which can sometimes distort the relative height of the peaks.

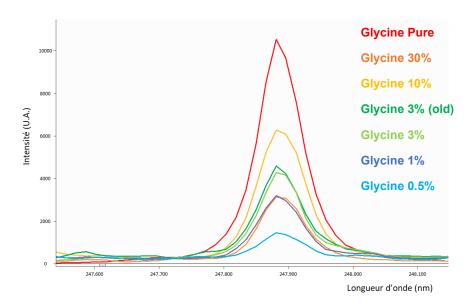
The relationship between peak height and concentration is not linear due to material-plasma interactions that vary depending on the concentration (matrix effects at low concentration, self-absorption at high concentration, etc.) [2]. A goal of the second year was therefore to perform more measurements to be able to plot a calibration curve to determine the detection threshold.

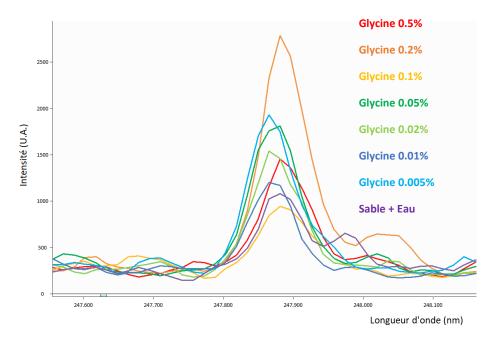
#### Second year results:

Based on the conclusions from the first year's experiments, we focused exclusively on the study of the carbon emission line at 247.9 nm in the second year. We conducted all the following measurements on the same day to ensure that the LIBS



device did not have measurement fluctuations due to external parameters such as temperature changes. Qualitatively, the intensity of this line is an increasing function of concentration in the range [1%, 30%]. In the range [0.005%, 1%], interpretation is more limited without data processing.





<u>Figure 10</u>: <u>Graphs showing the intensity of the carbon line at 247.9nm for different glycine concentrations</u>

Since we are interested in the detection of organic matter, and here carbon, we will consider the mass fraction of carbon in our sample, not the mass fraction of organic matter in the matrix.

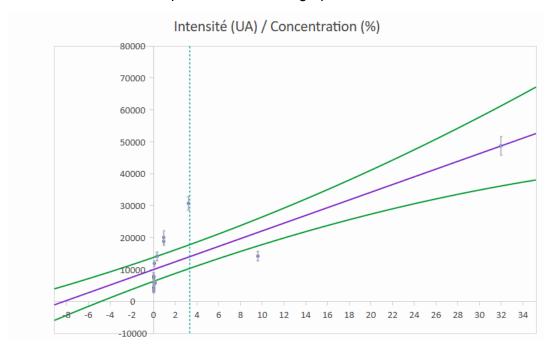


$$\frac{M_{2C}}{M_{glycine}} = 32\%$$

We thus obtain the following carbon concentrations:

% massique											
glycine	30	10	3	1	0,5	0,2	0,1	0,05	0,02	0,01	0,005
%massique C	9,6	3,2	1	0,32	0,16	0,064	0,032	0,016	0,0064	0,0032	0,0016

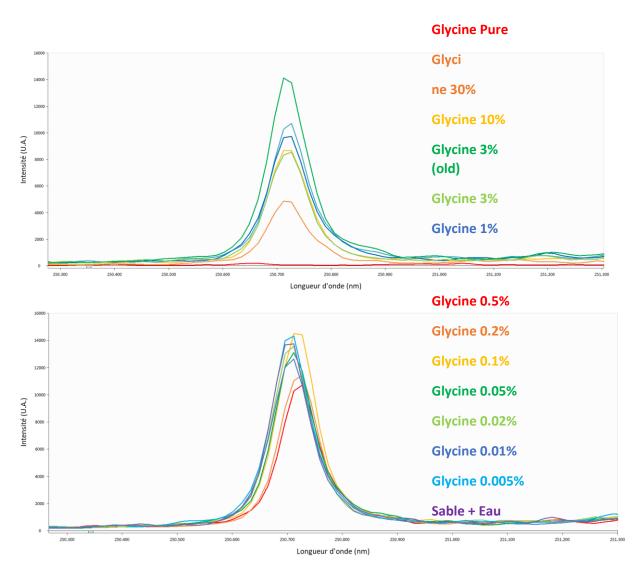
We perform a linear regression between the intensity of the carbon line as a function of the carbon concentration in our samples and obtain the graph below:



<u>Figure 11 : Graph showing the intensity of the carbon line at 247.9 nm as a function of the mass</u> concentration of carbon

We observe that there is no linear relationship between the intensity of the carbon line and the mass percentage of carbon in our sample in the considered concentration range. This can be explained by self-absorption phenomena in high concentrations [2]: ionized carbon elements collide with potential future ionized carbon elements, thereby reducing the number of ionized carbon releasing their characteristic energy during their de-excitation. Matrix effects can also contribute to this non-linearity. To minimize the effect of self-absorption, we decide to only consider carbon concentrations of approximately 3% or less. To detach as much as possible from the matrix effect, we normalize the intensities of the considered carbon line by the intensity of silicon at the line of 250.7nm [3]. Indeed, the graphs below highlight the fluctuations in the intensity of the silicon line while its relative concentration varies very little.





<u>Figure 12:Graphs showing the intensity of the silicon line at 250.7nm for different glycine concentrations</u>



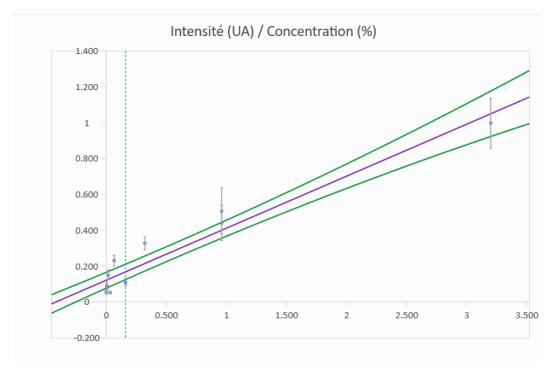


Figure 13 :Graph showing the intensity of the carbon line at 247.9 nm normalized by the intensity of the silicon line at 250.7nm as a function of the mass concentration of carbon in glycine samples

We find a pseudo-linearity between intensity and carbon concentration. But what about the detection limit? The post-processing software gives us a detection limit of 1600 ppm in carbon, while a more detailed observation of the curve suggests that a detection limit of around 500 ppm can be achieved by further increasing the number of shots. In practice, the non-linearity of the result obtained distorts the software data on the interpretation of this limit. In any case, this limit is not sufficient to allow this method to detect concentrations of organic matter of the order of a few ppm at most on Mars.

#### b. Phénanthrène

#### Recap of essential results from the first year:

The indicators suggesting the presence of organic matter that are visible are the peaks related to:

- C2: bonds in the radical compound of two carbons
- (
- CN: related to recombinations between the carbon and nitrogen of the air

Specifically for phenanthrene, it is observed that at high concentrations, it is possible to see a line at 516.5nm specific to bonds between two carbon atoms: the C2 bond. Although this gave good results during the first year of the project (figure below), reducing to lower concentrations quickly becomes unviable for several reasons. On one hand, the origin of the line being the interaction between multiple carbon atoms, it



becomes less systematic and reliable at low concentrations. Indeed, the probability of interaction becomes lower as the carbon concentration decreases. Unlike the C2 bond, the carbon of the CN bond can come from the solid molecule, so at low concentration, but the nitrogen from the atmosphere, so at very high concentration. This bond, therefore, remains more visible at low concentration since it requires one carbon and not two.

Thus, the carbon-carbon bond will not be further studied in the second year but could still provide additional information at high concentrations, which is excluded on Mars

#### Second year results:

In the same way as for glycine and for the same reasons, we focused exclusively on the carbon line for phenanthrene in the second year.

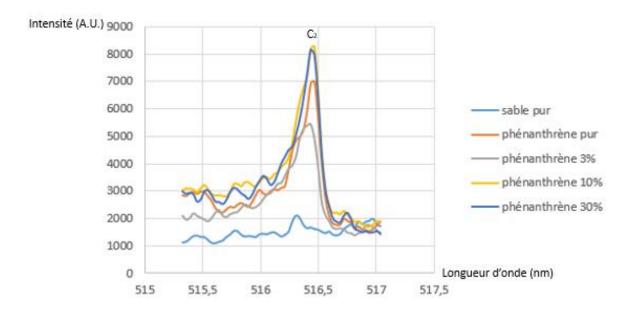
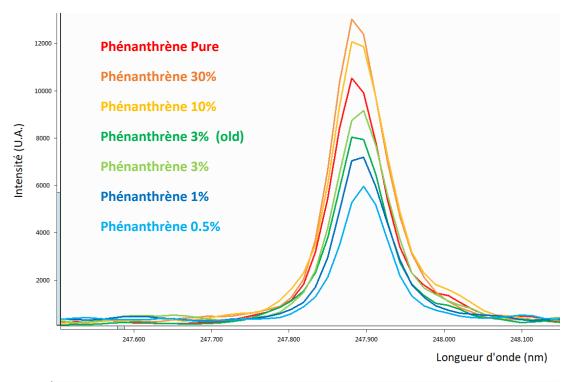
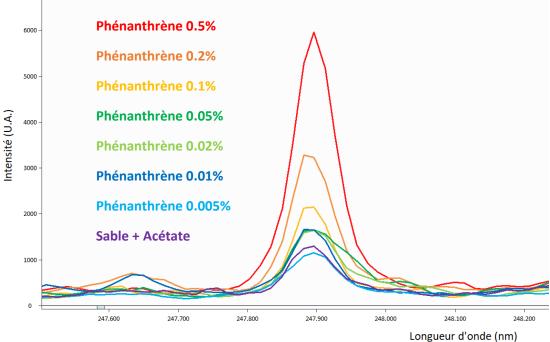


Figure 13:] Averaged spectrum of pure phenanthrene samples, sand, and phenanthrene at 3%, 10%, 30%, and 100% by mass, centered on the range [515 nm; 517 nm]







<u>Figures 14 : Graphs showing the intensity of the carbon line at 247.9nm for different phenanthrene concentrations</u>

At first glance, we obtain more satisfactory results than for the study of glycine: the carbon intensity is an increasing function of the phenanthrene concentration for the entire concentration range considered. This can be explained by the fact that phenanthrene is more carbon-concentrated than glycine. By the same calculation, we obtain the following table:



% massique											
phénanthrène	30	10	3	1	0,5	0,2	0,1	0,05	0,02	0,01	0,005
%massique C	28,2	9,4	2,8	0,94	0,47	0,188	0,094	0,047	0,0188	0,0094	0,0047

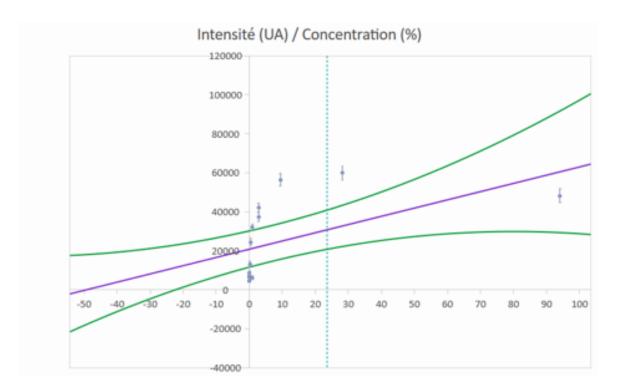
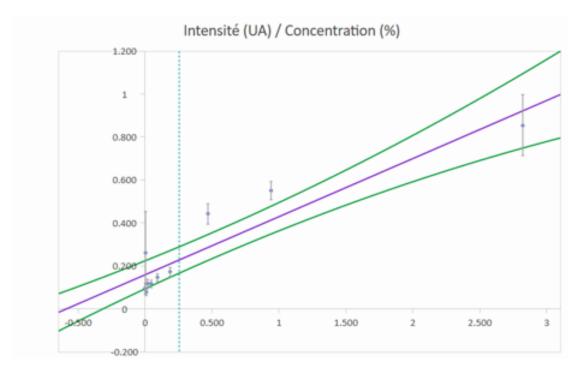


Figure 15 : Graph showing the intensity of the carbon line at 247.9 nm as a function of the mass concentration of carbon in phenanthrene samples

We encounter the matrix effects and self-absorption mentioned during the analysis of the glycine results. By the same process of normalization by the silicon signal and consideration of low considerations, we obtain the following regression:





<u>Figure 16</u>: Graph showing the intensity of the carbon line at 247.9 nm normalized by the intensity of the silicon line at 250.7nm as a function of the mass concentration of carbon in phenanthrene samples

Again, we obtain a relationship closer to linearity than before. However, the carbon detection threshold here is still not sufficient: about 2000 ppm according to the software, which is explained by some points with aberrant data and high uncertainties. By removing these points, it is possible to reduce the threshold by a few hundred ppm.

Finally, to test the consistency of the two sets of measurements, we tried to put on the same graph the normalized data of the two molecules on the same graph, the concentrations being converted to carbon concentrations (figure below). Then, we can observe two things:

- The data of the two molecules are consistent in that they give the same relative intensity on the carbon line at the same carbon concentration
- Increasing the number of data points reduces the detection limit calculated by the software, confirming what was already suspected: it is then proposed at 1200 ppm by the software. This confirms our visual observation for which our manually estimated limit is more of the order of about 500 ppm.



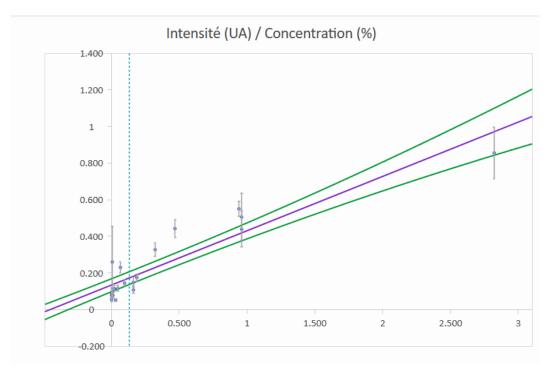


Figure 17: Graph showing the intensity of the carbon line at 247.9 nm normalized by the intensity of the silicon line at 250.7nm as a function of the mass concentration of carbon in phenanthrene and glycine samples

Finally, we also plotted the normalization curves of the CN line at 388nm of the two molecules by silica, which gave us coherent and similar results but with less precision at low concentration, especially for the detection limit. The study of the simple carbon line used above is therefore the most relevant.

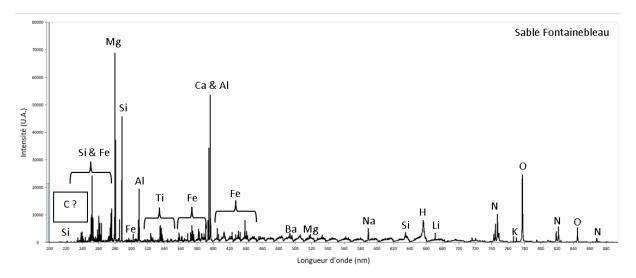


## IV. Additional studies (exclusive to the second year)

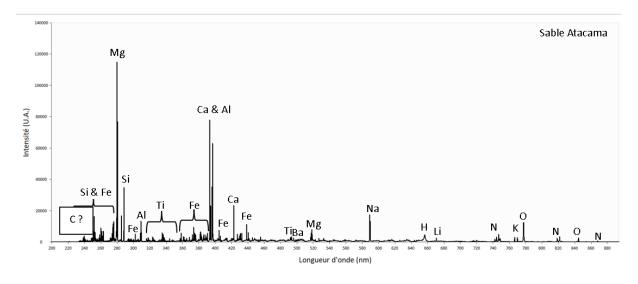
#### a. Study of other matrices

The study of raw matrices collected from different places on Earth has also shed light on LIBS phenomena. These samples consist of sand from Atacama, Thailand, Hawaii, Fontainebleau, and the laboratory sand we used as a matrix to create our glycine and phenanthrene samples.

Sands from Fontainebleau, Atacama, and Hawaii reveal that in the case of a strong presence of Fe, the C and CN signals available with the instrument are no longer clearly usable:

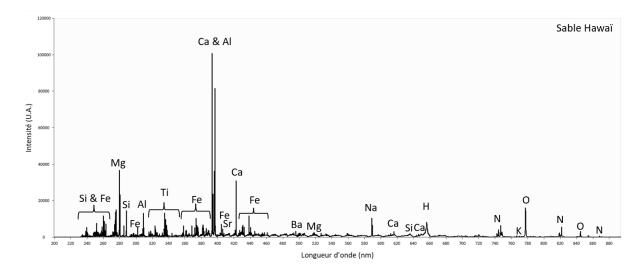


<u>Figure 18 : Emission spectrum of Fontainebleau sand - Detected elements: H, Li, Na, K, Mg, Ca, Ba, Ti, Fe, Al, Si, N, O, and B</u>





<u>Figure 19 : Emission spectrum of Atacama sand - Detected elements: H, Li, Na, K, Mg, Ca, Ba, Ti, Mn, Fe, Al, Si, N, O, and B</u>



<u>Figure 20 : Emission spectrum of Hawaii sand - Detected elements: H, Na, K, Mg, Ca, Ba, Ti, Fe, Al, Si, N, O, and B</u>

The study of Thailand sand highlights the phenomenon of artifacts or interferences that LIBS can suffer from [3]. Indeed, it is noted that the sample is very rich in calcium with the notable presence of fluorine, which is explained by a composition rich in shell or coral. This "too high" intensity saturates the detector and is materialized by the appearance of lines at wavelengths close to the wavelength corresponding to the deexcitation energy of ionized calcium. These energy peaks close to the main peak are therefore physically meaningless and are only diffraction orders of the central peak. They can obscure the detection of elements actually present in the studied sample.

In this case, the detection of carbon is complicated due to interferences related to the high intensity of calcium.



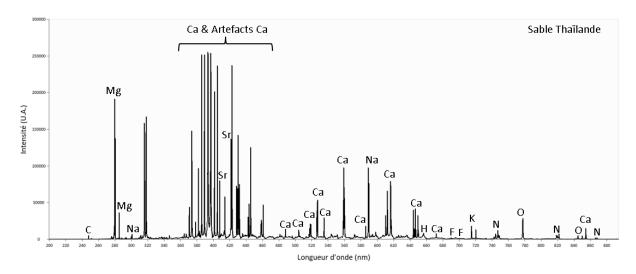


Figure 21: Emission spectrum of Thailand sand (Maya Bay) - Detected elements: H, Na, K, Mg, Ca, Sr, Al (traces), Si (traces), N, O, F, C, and CN (traces)

The analysis of the laboratory sand used in all our samples includes a lower presence of Fe, and no artifact phenomena: the C and CN signals are again available with the instrument, making the analysis we conducted coherent.

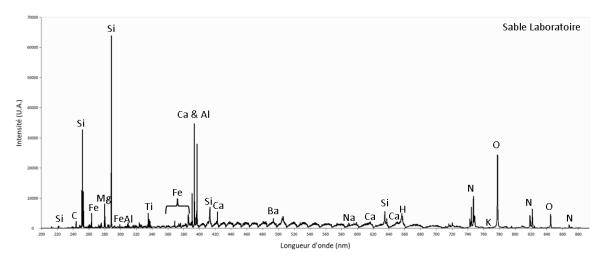


Figure 22: Emission spectrum of laboratory sand - Detected elements: H, Na, K, Mg, Ca, Sr, Al (traces), Si (traces), N, O, F, C, and CN (traces).

These results highlight the importance of the matrix on the detection of organic matter.

#### b. Use of Machine Learning for data analysis

Given the complexity of LIBS spectra, we had to choose to focus mainly on the carbon line. This univariate approach [4] does not take into account all the information contained in the spectrum but focuses only on a part. The spectra are too complex to



be processed as a whole by the naked eye. That's why scientists now use machine learning [2][4]. This new multivariate approach is based on the implementation of classification and prediction algorithms. The main techniques used are first dimensionality reduction techniques like Principal Component Analysis (PCA) or Linear Discriminant Analysis (LDA) [2][4]. Indeed, each LIBS spectrum can contain nearly a thousand wavelengths and thus be treated as a vector with nearly a thousand components. After being reduced, the data are divided into 3 classes. The training and validation data allow training and evaluating the model, whose relevance is evaluated by the test data. Partial Least Squares Regression (PLSR) is often used, but its efficiency is limited as a significant part of the observed phenomena has a non-linear dimension. That's why neural networks are increasingly used. [2][4]

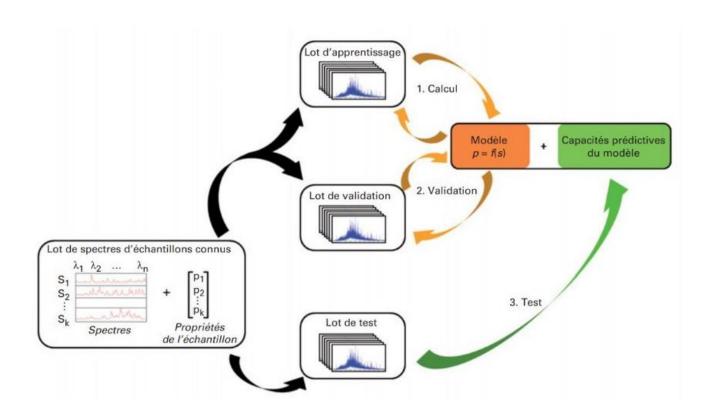


Illustration of the construction of the ML model [2]

We created a neural network that classified soils into twelve categories. Its accuracy was very good, which is promising. We also tried the Partial Least Squares method, which was less conclusive. We found our database online [5]. We reduced it with PCA then LDA. It would be interesting to adapt the algorithm to classify organic matter, but our experimental dataset is currently too small to do Machine Learning on it (not enough samples).



### C. Conclusion

#### 1. General overview

The results are partially satisfactory. On one hand, we managed to establish an almost linear calibration curve between intensity and organic matter concentration by freeing ourselves from matrix effects and self-absorption through normalization methods and concentration range selection. Nevertheless, this method allowed us to estimate a detection threshold for organic matter -here carbon- of the order of 1000 ppm. This has certain utilities in the world of industry, but concerning the detection of life on Mars, one could expect concentrations of organic matter of the order of a few ppm, far from the 1000 ppm. Moreover, we conducted all our measurements under the Earth's atmosphere: the composition of the Martian atmosphere is very different, with 96% carbon dioxide, making the plasma-atmosphere interactions different from ours. This explains why detecting organic matter with LIBS is a real challenge.

Technological advances are nevertheless made in this direction: improvements in laser excitation techniques, light collection systems, and data analysis algorithms are underway to overcome these limitations and improve LIBS's ability to accurately identify organic matter. In particular, the emergence of machine learning techniques for spectrum interpretation may allow a leap in the precision of sample detection. Classification works well, but quantification seems more complicated.

#### 2. Challenges and Improvement Perspectives

. We encountered several difficulties that could have slowed our project down and prevented it from finishing on time if we had not organized ourselves properly.

Firstly, our relative dependence on Kevin Boudoulec, a physicochemical analysis engineer at iUMTEK, to use the machine could be a constraint, especially for the host company. His specific expertise was indispensable to ensure the correct functioning of the device and a fair interpretation of the analyses. In his absence, we were only able to carry out data acquisitions without being entirely sure of our settings and without being able to interpret the results, although we gained autonomy and knowledge as we went along. Configuring the parameters during significant changes in the type of experiment proved complex, and we had trouble optimizing them without his help.

Then, we did not have easy access to the spectra from LIBS analysis, as they came from a specific software used by iUmtek, "Spectra," whose license is unaffordable for students, which took away our autonomy in interpreting the results.

However, despite these difficulties, we are delighted with our relationship with the staff at iUmtek, who generously welcomed us into their premises, and with Kevin Boudoulec, who shared his expertise with us.



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