COMMUNITY USER WORKSHOP ON PLANETARY LIBS (CHEMCAM) DATA

C-QuEST Software

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What is C-QuEST?

Definition

- ChemCam Quick Element Search Tool
- Library of ChemCam emission lines for 32 elements

Why use it?

- Search for specific element in spectral database
- Search for specific spectral range
- Visualize an elemental synthetic spectrum
LIBS emission lines database

Why doing an emission lines library?

NIST

Not LIBS specific
Vacuum and Ambient

CREOSA

LIBS specific
Helium

Emission lines are dependent on the experimental conditions
(Pressure, Laser Energy, ..)

Need for a specific Martian database
Subset of the NIST database
### Periodic Table

- **SELECT ALL**
- **CLEAR ALL**
- **Major**
- **Trace**
- **Organic (CHNOPS)**
- **Other**

<table>
<thead>
<tr>
<th>Database</th>
<th>Wavelength (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>NIST</td>
<td>UV (240-341)</td>
</tr>
<tr>
<td>Martian</td>
<td>VIS (381-469)</td>
</tr>
<tr>
<td></td>
<td>VNIR (471-905)</td>
</tr>
</tbody>
</table>

### Informations

- **Nb lines:** 0
- **Print**
- **Spectra**
Choice between NIST and ChemCam database

[Image of the C-QuEST software interface showing the choice between NIST and Martian (Agnes Cousin) databases.]
Search for a specific spectral range
Search for a specific element
The most intense one is at 455.53 nm. There are some interferences with Ti lines, but no confusion. This is the line that ensures the presence of Ba in a spectrum.

58: Cerium

82: Lead

90: Thorium

92: Uranium
### Periodic Table

Select the elements you want to analyze using the checkboxes provided. You can select all elements by clicking the "SELECT ALL" button or clear all selections by clicking the "CLEAR ALL" button.

### Wavelength (nm)

Adjust the wavelength range from 300 to 320 nm to filter the visible light spectrum.

### Databases

- **NIST**: National Institute of Standards and Technology database.
- **Martian (Agnes Cousin)**: Martian database specifically designed for Martian samples.

### Information

The information section displays the selected elements and their properties based on the chosen databases and wavelength settings.
C-QuEST

20: Calcium

Ca shows several important lines. Here are the most ones, observed for each spectral range:
- UV: 315.978 nm and 318.025 nm
- VIS: 393.477 nm, 396.959 nm and 422.792 nm are the most important among others
- VNIR: lot of Ca lines. The most easy ones to detect are the triplet at 610.441, 612.39 and 616.3 nm with an increasing intensity, and a second triplet at 644.085, 645.159 and 646.436-646.557 nm with a decreasing intensity.

All these lines are well defined with no interferences.

The most important Ca lines in all the spectrum are those at 393.477 nm and 396.959 nm, but they can suffer some auto-absorption effects.

20: Iron
Al will be the example

13: Aluminium
Al shows several lines in all the spectral range.
The most characteristic lines are:
- UV: 2 lines at 308.305 nm and at 309.36–309.37 nm which are neutral lines. These lines are often interfered by Ti lines, but are still well characterized.
- VIS: 2 lines are observed, which are the 2 most important lines of the Al. They are observed at 394.512 nm and 396.264 nm (neutral lines).
- VNIR: the most important ones are observed at 704.4 nm and 705.85 nm.
Information about main emission lines

13: Alumminium
Al shows several lines in all the spectral range. The most characteristic lines are:
- UV: 2 lines at 308.305 nm and at 309.36-309.37 nm which are neutral lines. These lines are often interfered by Ti lines, but are still well characterized.
- VIS: 2 lines are observed, which are the 2 most important lines of Al. They are observed at 394.512 nm and 396.264 nm (neutral lines).
- VNIR: the most important ones are observed at 704.4 nm and 705.85 nm.
List of emission lines by database, element, ionization stage, wavelength or intensity

List of the Al lines present in the database between 300 - 320 nm

13: Aluminium
Al shows several lines in all the spectral range.
The most characteristic lines are:
- UV: 2 lines at 308.305 nm and at 309.36-309.37 nm which are neutral lines. These lines are often interfered by Ti lines, but are still well characterized.
- VIS: 2 lines are observed, which are the 2 most important lines of the Al. They are observed at 394.512 nm and 396.264 nm (neutral lines).
- VNIR: the most important ones are observed at 704.4 nm and 705.85 nm.
To print the list of emission lines.
To visualize the spectrum/spectra, only 1 database should be selected (NIST or Martian)
Spectral lines can be visualize with a Lorentz shape (~similar to a ChemCam spectrum) or as a Dirac, or both.
You can change the color of the spectrum/spectra.

- VIS: 2 lines are observed, which are the 2 most important lines of the Al. They are observed at 394.512 nm and 396.264 nm (neutral lines).
- VNIR: the most important ones are observed at 704.4 nm and 705.85 nm.
You can change the color of the spectrum/spectra.

Often interfered by Ti lines, but are still well characterized.
- VIS: 2 lines are observed, which are the 2 most important lines of the 394.512 nm and 396.264 nm (neutral lines).
- VNIR: the most important ones are observed at 704.4 nm and 705.85 nm.
To go back to initial color
Al will be the example
Example with several elements

C-QUEST

19: Potassium
The Potassium shows us generally 2 lines in the VNIR domain, located at 766.70 nm and at 770.11 nm. If these two lines are not observed, the sample does not contain K.

30: Calcium
Example with several elements

Specific range

The Potassium shows us generally 2 lines in the VNIR domain, located at 766.70 nm and at 770.11 nm. If these two lines are not observed, the sample does not contain K.
TIPS

• To visualize a synthetic spectrum, it is better to select only 1 spectral range (UV, VIS or VNIR):
  – Data acquired with commercial spectrometers without a demultiplexer (each spectral range acquired separately)
  – Total intensity from one domain to another can be different
Backup slides
Ground Station

ChemCam

- **Mast Unit**: Engineering & Qualification Model (EQM)
- **Body Unit**: Commercial spectrometers (same resolution as flight Model)

Mars

- 6 mbars
- Mars atmosphere (95.7% CO$_2$, 2.7% N$_2$, 1.6% Ar)

Conception with N. Striebig & B. Dubois

16 Mar 2014

ChemCam Community Workshop
Emission Lines Database Creation

Characterized sampled

Line identification with NIST

Processing

Line fitting

Database creation

<table>
<thead>
<tr>
<th>Element</th>
<th>Ext</th>
<th>OBS. Wave</th>
<th>OBS. Int.</th>
<th>Env.</th>
<th>Target</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al</td>
<td>I</td>
<td>257.570</td>
<td>143.582</td>
<td>MARS</td>
<td>Al/Si</td>
</tr>
<tr>
<td>Sr</td>
<td>II</td>
<td>421.682</td>
<td>327.219</td>
<td>MARS</td>
<td>Calib.</td>
</tr>
<tr>
<td>F</td>
<td>II</td>
<td>402.578</td>
<td>66.9510</td>
<td>MARS</td>
<td>Fluorine</td>
</tr>
</tbody>
</table>
### Type of target

<table>
<thead>
<tr>
<th>Pure targets</th>
<th>Geological targets</th>
<th>Specific Atmospheres</th>
</tr>
</thead>
<tbody>
<tr>
<td>C, Al, Si, Ti, Mn, Fe, Ni, Cu, Pb</td>
<td>H, Li, Be, B, F, Na, Mg, P, S, Cl, K, Ca, V, Cr, Zn, As, Rb, Sr, Cs, Ba</td>
<td>N, Ar, O</td>
</tr>
</tbody>
</table>

32 elements, 1336 emission lines