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
Choice between NIST and ChemCam database
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

Martian Fe I 300.039 76.994
Martian V II 300.070 522.527
Martian Ni I 300.337 11.184
Martian Fe II 300.352 258.952
Martian Ni I 300.451 236.055
Martian Mn I 300.854 28.107
Martian Fe I 300.902 86.970
Martian Cu I 301.172 8.228
Martian Mn I 301.204 41.185
Martian Mn I 301.226 41.185
Martian Ni I 301.288 288.071
Martian Fe III 301.405 10.424
Martian Mn I 301.555 43.700
Martian Ti I 301.807 2.619
Martian Ni I 302.002 39.155
Martian Mn II 302.080 476.444
Martian Fe I 302.137 204.569
Martian Fe I 302.152 132.304
Martian Fe I 302.195 132.304
Martian Mn I 302.363 182.195
Martian Fe I 302.672 60.710
Martian Ti II 303.061 2.221
Martian Mn II 303.194 594.236
Martian V II 303.433 886.474
Martian V II 303.470 886.474
Martian Mn II 303.623 360.566
Martian Zn I 303.666 36.211
Martian Cu I 303.698 8.539
Martian Fe I 303.827 46.509
Martian Ni I 303.882 11.184
Martian Mn I 304.148 334.049
Martian Fe I 304.252 28.551
Martian Mn I 304.564 209.186
Martian Ti II 304.757 1.760
Martian Mn I 304.793 209.186
Martian Fe I 304.849 11.184
Martian V II 304.911 1,097.2
Martian Mn II 305.154 349.718
Martian Ni I 305.170 189.878
Martian V I 305.428 117.904
Martian Ni I 305.520 41.308
Martian Mn II 305.525 42.538
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: a lot of Ca lines. The most easy ones to detect are the triplet at 610.441, 612.39 and 616.8 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.

26: 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

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 394.312 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).
- VNR: 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.
You can change the color of the spectrum/spectra.
To go back to initial color
Example with several elements

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.
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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 % CO₂, 2.7 % N₂, 1.6 % Ar)
Emission Lines Database Creation

Line identification with NIST

Characterized sampled

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>
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</thead>
<tbody>
<tr>
<td>Al</td>
<td>I</td>
<td>257.570</td>
<td>143.582</td>
<td>MARS</td>
<td>Al/Si</td>
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<tr>
<td>Sr</td>
<td>II</td>
<td>421.682</td>
<td>327.219</td>
<td>MARS</td>
<td>Calib.</td>
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<tr>
<td>F</td>
<td>II</td>
<td>402.578</td>
<td>66.9510</td>
<td>MARS</td>
<td>Fluorine</td>
</tr>
<tr>
<td>Type of target</td>
<td>Pure targets</td>
<td>Geological targets</td>
<td>Specific Atmospheres</td>
<td></td>
<td></td>
</tr>
<tr>
<td>---------------</td>
<td>--------------</td>
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<td></td>
<td></td>
</tr>
<tr>
<td><strong>Elements</strong></td>
<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>
<td></td>
<td></td>
</tr>
</tbody>
</table>

32 elements, 1336 emission lines