

# Supplementary Materials: Tools for remote exploration: a Lithium (Li) dedicated spectral library of the Fregeneda-Almendra aplite-pegmatite field

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## Continuum removal and feature extraction

The source code employed to remove the continuum and extract the main absorption features for the spectra collected using the SR-6500A equipment is given as an example. The process is similar for the spectra acquired with the ASD FieldSpec 4 and only minor changes are required: (i) when reading the original spectra files, only one header line needs to be skipped; (ii) these spectra already show absolute reflectance values, so there is no need to make the conversion.

```
# General imports
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import os

from pysptools.spectro import FeaturesConvexHullQuotient
from pysptools.spectro import SpectrumConvexHullQuotient

# State where to save the resultant spectra
path_results = '../results/'

# Create function to save the spectra
def save_fig(fig_id, tight_layout=True, fig_extension="tif", resolution=300):
    path = os.path.join(path_results, fig_id + "." + fig_extension)
    print("Saving figure", fig_id)
    if tight_layout:
        plt.tight_layout()
    plt.savefig(path, format=fig_extension, dpi=resolution)
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```
# Specify the path the folder containing the raw spectra
path_folder = '/.../'

# Find every file in the folder directory
spectra_paths = [os.path.join(path_folder, f) for f in os.listdir(path_folder) if
os.path.isfile(os.path.join(path_folder, f))]
spectra_paths.sort()
spectra_paths

# Get the name of the files
names = [os.path.splitext(os.path.basename(x))[0] for x in spectra_paths]

# Create a dictionary with all the spectra
spectra = {}
for i in range(len(names)):
    spectra[names[i]] = pd.read_table(spectra_paths[i],
        delim_whitespace=True, names = ('Wvl', 'Reflect. %'), skiprows=28)

# Plot the spectra and save the figure
for key, value in spectra.items():
    plt.figure()
    ax = plt.gca()
    spectra[key].plot(kind='line', x='Wvl', y='Reflect. %', ax=ax)
    plt.xlabel('Wavelength (nm)', fontsize=14)
    plt.xticks(size=14)
    plt.ylabel('Reflectance (%)', fontsize=14)
    plt.yticks(size=14)
    plt.title(key, fontsize=16, pad=10)
    ax.get_legend().remove()
    plt.show()
    save_fig(key)
    plt.pause(1)
    plt.close()

# Change the parameters for plotting the figures
params = {'legend.fontsize': 'xx-large',
          'lines.linewidth': 3,
          'lines.markersize': 13,
          'figure.figsize': (14,11),
          'figure.dpi': 300,
          'figure.titlesize': 'xx-large',
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        'axes.labelsize': 'xx-large',
        'axes.titlesize': 'xx-large',
        'axes.labelpad': 15,
        'axes.titlepad': 15,
        'xtick.labelsize': 'x-large',
        'ytick.labelsize': 'x-large'}
plt.rcParams.update(params)

# Remove the continuum
""" The FeaturesConvexHullQuotient function removes the convex-hull of the signal by hull
quotient"""
spectrum = list()
wvl_list = list()

for key, value in spectra.items():
    pixel = value['Reflect. %']
    pixel = pixel/100 # get absolute reflectance values
    wvl = value['Wvl']
    spectrum = pixel.tolist()
    wvl_list = wvl.tolist()
    spectra_features = FeaturesConvexHullQuotient(spectrum=spectrum,
        wvl = wvl_list, baseline=0.93)
    # plot the extracted features
    spectra_features.plot(path= path_results, plot_name= key, feature='all')
    # plot side by side original and corrected spectrum
    spectra_features.plot_convex_hull_quotient(path= path_results,
        plot_name= key + '_comparison')

# Get the statistics associated with each feature
b = {}
spectrum = list()
wvl_list = list()
for key, value in spectra.items():
    pixel = value['Reflect. %']
    pixel = pixel/100
    wvl = value['Wvl']
    spectrum = pixel.tolist()
    wvl_list = wvl.tolist()
    spectra_features = FeaturesConvexHullQuotient(spectrum=spectrum,
        wvl = wvl_list, baseline=0.93)
    b = spectra_features.features_all
    b_stats = pd.DataFrame(b)
```

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```
is_keep = b_stats['state']=='keep'
b_stats_keep = b_stats[is_keep]
b_stats_keep.to_csv(path_results+key+'.csv', sep=',', index =False)

# Export the continuum removed spectrum as *.txt, plot and save the spectra
b = {}
spectrum = list()
wvl_list = list()
plt.rcParams.update(plt.rcParamsDefault)
for key, value in spectra.items():
    pixel = value['Reflect. %']
    pixel = pixel/100
    wvl = value['Wvl']
    spectrum = pixel.tolist()
    wvl_list = wvl.tolist()
    spectra_remov = SpectrumConvexHullQuotient(spectrum=spectrum, wvl = wvl_list)
    conti_rem = spectra_remov.get_continuum_removed_spectrum()
    cont_corr = pd.DataFrame({'Reflectance':conti_rem})
    cont_corr.insert(0, 'Wvl', wvl)
    cont_corr['Wvl']=wvl
    cont_corr.to_csv(path_results+key+'_continuum_corr_spectra.txt',
                    sep='\t', index=False, header=False)
    plt.figure()
    ax = plt.gca()
    cont_corr.plot(kind='line',color= 'g', x='Wvl',y='Reflectance', ax=ax)
    plt.xlabel('Wavelength (nm)', fontsize=14)
    plt.xticks(size=14)
    plt.ylabel('Continuum removed reflectance',fontsize=14)
    plt.yticks(size=14)
    plt.title(key,fontsize=16, pad=10)
    ax.get_legend().remove()
    plt.show()
    save_fig(key + "_continuum_removed")
    plt.pause(1)
    plt.close()
```