

## **SpecXY - a tool for working with spatial spectroscopic data**

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Spectroscopic techniques such as FTIR, Raman or hyperspectral imaging are important in modern geosciences. In recent years, there has been a shift from the exclusive use of single spot analysis to the use of 2-dimensional mapping. Maps help to reveal patterns in a sample that would not be detected by single point measurements. Filtering and extracting signal information from multiple combined pixels can help improving the signal-to-noise ratio and thus the precision of the data. However, the amount of data and information in the dataset increases significantly when maps are used instead of spot analyses.

To investigate large datasets, we have developed SpecXY, a user-friendly software solution for preparing, editing, extracting and comparing spatially resolved spectral datasets. SpecXY consists of two main modules for processing spectroscopic data. (1) The first module, SpecMaps, is designed for the investigation of spatially resolved spectroscopic data and allows various maps to be generated. This module provides a quick and efficient way to compare signals between different areas and extract average spectra for further calculations. It can be used to visualise and classify spectra, perform peak deconvolution from pixel spectra and to correlate spectral data with chemical data (e.g., from EMPA, LA-ICP-MS) or other numerical data of the same area. SpecMaps can handle any data type containing a map of wavenumber, energy, frequency, wavelength and intensity. (2) The second module, SpecDB, is designed as a spectra database with the ability to perform manipulations, advanced peak deconvolution, calculations (e.g., H<sub>2</sub>O quantification), match unknown spectra or visualise and compare important features in selected spectra.

In this contribution, we will present application examples of SpecXY using examples based on Fourier Transform Infrared (FTIR) spectroscopy data. A special attention will be paid to the investigation of H<sub>2</sub>O incorporation and distribution in clinopyroxene and multidimensional classification and correlation of complex datasets.