Raman Match: Application for automated identification of minerals from Raman spectroscopy data

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Abstract

Raman spectroscopy is a rapid, nondestructive analysis technique used in various scientific disciplines, including mineralogy, chemistry, materials science, and biology. The analysis of Raman spectra and the identification of specific substances in unknown samples can be complex and time-consuming due to the large database of Raman spectra. The Raman Match application was developed to simplify and automate the sample identification process through a search and match method. The application integrates the well-established RRUFF Raman database with the Python programming language. It provides a user-friendly graphical interface to load Raman spectra, identify and fit peaks, match peaks to the reference libraries, visualize the results, and generate publication-ready figures. The application offers a swift and automated method for mineral identification using Raman spectroscopy in laboratory and field settings and during planetary exploration missions to extraterrestrial environments with constraints on time and resources.

Keywords: Matching algorithm, peak identification, spectrum analysis, mineralogy, Raman database, Python