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# Ramanalysis: Interactive Comparison and Matching of Raman Spectra

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Raman spectroscopy is an invaluable tool enabling rapid identification of many geochemically-relevant organic and inorganic compounds. However, identification of phases from their Raman spectra is still a manual, time-consuming process. Existing matching tools are either proprietary, consider only the largest peak, or attempt to match the shape of the whole spectrum, which can altered significantly by instrument-specific effects.

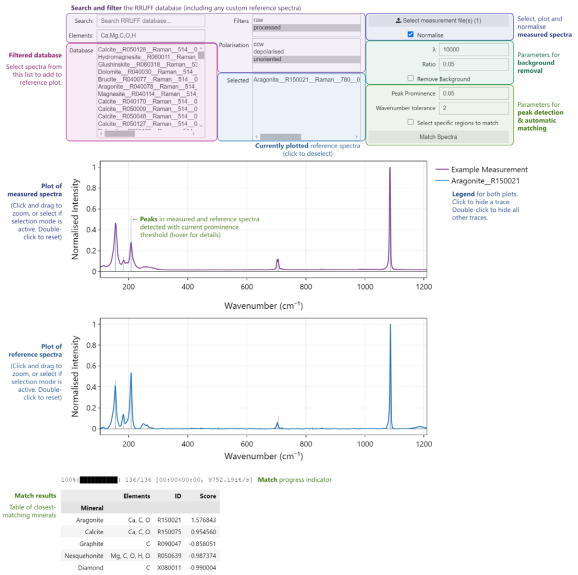
As an alternative, we present Ramanalysis: an interactive Python tool for plotting, comparing and automatically matching Raman spectra. Ramanalysis plots measured spectra in .txt or .csv format. Reference spectra are downloaded from RRUFF, an extensive online database of mineralogical Raman spectra [1], though custom reference spectra may also be added. The database can be searched by mineral name and/or chemical composition, and multiple reference spectra can be plotted on a linked x-axis for comparison with the measured spectra.

An asymmetrically-reweighted penalised least-squares fit may be used to subtract the background from spectra. After background subtraction, peaks are identified based on a prominence threshold. The matching algorithm assigns a score to each reference spectrum, based on the similarity in wavenumber and prominence of peaks present in both the reference and measured spectrum. The five minerals with the highest-scoring spectra are reported back to the user. If the measured spectrum contains multiple phases, a selection tool can be used to select only certain peaks to match. The matching algorithm was verified by matching the lower-quality data from RRUFF using the higher quality spectra in the database.

Ramanalysis was inspired by Raman Match [2] but features several improvements, notably the linked, rescalable x-axes to enable better comparison between spectra, the use of multiple peaks to match spectra, and the ability to select spectral ranges for multi-phase matching. The program is built using Jupyter Widgets and Plotly, enabling interactive use with zero code editing required, but can easily be extended or modified by users with a basic knowledge of Python programming. The source code is licensed under GPL-3 and is available at github.com/PeterMethley/Ramanalysis.

[1] Lafuente *et al*. (2015) *Highlights in Mineralogical Crystallography*, 1–30.

[2] Berrada *et al*. (2025); *American Mineralogist* 110, 25–33.




| Mineral | Elements | ID | Score |
|---|---|---|---|
| Aragonite | Ca, C, O | R150021 | 1.576843 |
| Calcite | Ca, C, O | R150075 | 0.954560 |
| Graphite | C | R090047 | -0.858051 |
| Nesquehonite | Mg, C, O, H, O | R050539 | -0.987374 |
| Diamond | C | X080011 | -0.990004 |