

Included supplemental codes (.R files):

- “ramanFit”
- “example_peak_fitting”

Included example dataset (.csv file):

- “example_spectrum”

“ramanFit” returns the ν_1 fit parameters given inputs of measured Raman wavenumber and intensity. Wavenumber and intensity must be the same length. Wavenumber is in 1/cm units, and intensity is in arbitrary units. The start values for the optimization routine are based on typical measured values in this study using the WITec Alpha300RA. If an error message is received when running this function, the start values may need to be adjusted to typical values from your instrument.

“example_peak_fitting” shows one application of “ramanFit” by fitting one Raman spectrum and plotting the results.

“example_spectrum” is one Raman spectrum from an abiogenic aragonite given here as an example of the peak fitting function.