Using pynams for site-specific H diffusivity in clinopyroxene

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Quantifying the distribution and behaviour of hydrogen point defects (also called water or hydroxyl, here H) in nominally anhydrous minerals (NAMs) is an area of active research because of H's disproportionate effect on key physical and chemical properties and its potential to provide insight into fundamental Earth and planetary processes. Fourier Transform Infrared spectroscopy (FTIR) is the most commonly used tool for measuring H concentrations because of its relative ease of use, low cost, and ability to distinguish H incorporation sites. Over the past several decades, thousands of FTIR spectra have been collected, and the rate of spectra collection has increased with widespread availability of digital mapping stages and current efforts to systematically characterize H in various environments and experimental conditions.

I will demonstrate pynams, a free, open-source software package written in Python to quickly accomplish FTIR spectra interpretation tasks related to H in NAMs such as plotting, creating baselines, estimating H concentrations, generating H profiles, peak fitting with Gaussians, and applying the whole-block method to interpret diffusion data and perform tomographic inversions (Ferriss et al. 2015, *American Mineralogist*). The latest version of the code is publicly available on GitHub, a website for collaborative code development, at https://github.com/EFerriss.

Examples will focus on spectra from diffusion experiments to obtain site-specific H diffusivities in clinopyroxene. Site-specific diffusivities are necessary because bulk H diffusivities span 3 orders of magnitude with no clear correlation to sample chemistry and thus cannot be confidently applied to natural systems.