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Extracting structural disorder signatures from vibrational spectra using photoacoustic detection

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This work demonstrates that, in order for Fourier transform infrared (FTIR) spectroscopy to be an effective materials characterization tool, it is essential to evaluate which bands are affected exclusively by specimen differences, independent of the detection and data analysis methodologies. To do this, we compared standard optical detection with photoacoustic detection of FTIR spectra for two classes of benchmark samples: uniformly sized and shaped particles (silica spheres), and size-fractionated CaCO_3 (calcite) powders. Subsequent analyses focused on assessments of peak positions, relative intensities, and widths as a function of different sample and data collection parameters. By comparing these trends with other structural characterization data, we identify which spectrum features are uniquely related to structural disorder in the calcite powders. In doing so, we present a best-practices methodology for extracting specimen-specific features from FTIR spectra.

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