HYDROGEN BONDING MANIPULATES ν(CH) INFRARED CROSS SECTIONS

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CH stretching moieties can be used in quantitative infrared spectra analysis to probe the concentration of species in confined environments. The Beer-Lambert law is often used to perform such analyses. A useful venue for this analysis is interpreting the presence of guest molecules in porous metal organic frameworks (MOFs), allowing time-resolved analysis of molecular transport. It is therefore critical to understand if molecules diffused into MOFs possess different infrared cross sections. Temperature programmed desorption mass spectrometry (TPD-MS) and temperature programmed Fourier transform infrared spectroscopy (TP-IR), combined with density functional theory (DFT), are used to compare the integrated ν(CH) intensities with the presence of analytes diffused into the MOF. Using temperature programmed techniques under ultra-high vacuum (UHV) conditions, we demonstrate nonlinear integrated infrared intensity in the ν(CH)/ν(CD) moieties of four separate analytes following diffusion into UiO-67 MOFs: acetone, acetonitrile-d_3, isopropanol and *n*-heptane. These results have implications on the use of integrated infrared intensity for discerning molecular transport kinetics into and out of environments capable of forming hydrogen bonds with guest molecules.