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Hydrogen-Deuterium exchange monitored by ATR-FTIR spectroscopy

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Measuring the extent of isotopic exchange is a common means for the determination of self-diffusion coefficients in any type of medium (gas, liquid, amorphous solid, crystalline solid). For rapidly diffusing species such as hydrogen in condensed phases, real time methods involving vibrational spectroscopy can be used by taking advantage of the large relative mass difference between ¹H and ²H, resulting in large differences in the band positions of their vibrational modes. We demonstrate rapid isotopic exchange between D_2O liquid and H_2O vapor using ATR (attenuated total reflectance) in a FTIR spectrometer. Over the course of a few minutes several spectra were acquired of a D_2O droplet mounted on a diamond crystal. The progressive exchange reaction between the liquid phase and H_2O from the atmosphere was monitored by measuring the decreasing absorbance of the D-O-D bending and O-D stretching bands and the increasing absorbance of the D-O-H and H-O-H bending and O-H stretching bands as functions of time. Our results offer some intriguing insights into the structural characteristics of water as inferred by this exchange process.