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Infrared spectroscopy of trapped hydrogen in metal-organic-frameworks[1] STEPHEN FITZGERALD, KELTY ALLEN, PATRICK LANDERMAN, JESSE ROWSELL, Oberlin College — We present a novel use of diffuse reflectance infrared spectroscopy to study the quantum dynamics of molecular hydrogen trapped within metal-organic-framework (MOF) hosts. This technique is particularly useful in the context of hydrogen storage since it provides detailed information about the intermolecular potential at the binding site. The spectra consist of quite sharp bands associated with the quantized vibrational and rotational motion of the trapped hydrogen. The vibrational bands are redshifted relative to the gas phase while the rotational sidebands contain an additional fine structure due to the orientational dependence of the binding potential. Results on MOF-5 reveal the presence of two primary binding sites. The first saturates at a loading concentration on the order of 4 H_2 per Zn ion and has a binding energy of roughly 4 kJ/mole. The second has a somewhat lower binding energy. Both site produce an ortho to para conversion rate on the order of 30-50 % per hour.

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Stephen FitzGerald
Oberlin College

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