INFRARED SPECTROSCOPY OF H_2 IN METAL-ORGANIC FRAMEWORKS

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We present a novel use of diffuse reflectance infrared spectroscopy to study the quantum dynamics of molecular hydrogen adsorbed within a metal-organic framework (MOF) host. This technique is particularly useful in the context of hydrogen storage since it provides detailed information about the intermolecular potential at the binding site. Spectra consist of quite sharp bands associated with the vibrational, rotational, and center-of-mass translational 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 at least three different sites. The primary site has a binding energy of roughly 4 kJ/mole, while the secondary sites have a somewhat lower binding energy. All sites exhibit an ortho to para conversion rate on the order of 30-50 % per hour.