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Low-temperature infrared spectroscopy of H_2 in solid C_{60}

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Diffuse reflectance infrared spectroscopy was used to probe the quantum dynamics of H_2 trapped in a C_{60} lattice. Because free H_2 is infrared inactive, features of the infrared spectra are induced solely through interactions with the host material and as such provide detailed information about the potential at the binding site. The design and construction of a cryogenic apparatus allowed the extension of previous room temperature measurements to temperatures as low as 10 K at pressures as high as 100 atm. The low temperature spectra contained much sharper peaks and a rich fine structure, enabling more precise determination of the details of the C_{60}-H_2 interaction potential. These studies of H_2 in C_{60} inform hydrogen storage materials research in a broader context, as illustrated by the diffuse reflectance spectra of H_2 in MOF-5.