LOW-TEMPERATURE INFRARED SPECTROSCOPY OF H_2 IN SOLID C_{60}

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Interstitial H_2 trapped in a C_{60} lattice forms an ideal case of a single isolated molecule confined within a cavity. Diffuse reflectance infrared spectroscopy is used to probe the quantum dynamics of the trapped hydrogen at temperatures as low as 10 K. Crystal field effects in conjunction with rotational translational coupling lead to a rich spectrum with multiply split peaks that are more than an order of magnitude sharper than at room temperature. Analysis of the data allows us to put much greater constraints on the parameters governing the fundamental C–H intermolecular potential.