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Dynamics of endohedral hydrogen in C_{60}: Infrared study[1] MIN GE, U. NAGEL, D. HUVONEN, T. ROOM, Nat. Inst. of Chem. Phys. Biophys., Tallinn, Estonia, S. MAMONE, M.H. LEVITT, M. CARRAVETTA, Southampton Uni., UK, Y. MURATA, K. KOMATSU, Kyoto Uni., Japan, J.Y.-C. CHEN, N.J. TURRO, Columbia Uni., NY10027 — Infrared spectra of endohedral hydrogen isotopomers H_2, D_2, and HD were measured in the temperature range from 6 to 300 K. A model of a vibrating rotor in a spherical potential together with the translational motion induced dipole moment theory was used to explain the positions and intensities of IR absorption lines. By measuring spectra of a *para* enriched sample of $H_2@C_{60}$, we confirmed the assignment of lines to *ortho*- and *para*-H_2. Inside C_{60} cage the rotation of hydrogen is unhindered and the translation is quantized and coupled to the rotation. The isotropic and translation-rotation coupling part of the potential are anharmonic and depend on the vibrational states of hydrogen. The analysis of the isotopic effect on the IR transition intensities and interaction potential in the C_{60} cage is presented.

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