Abstract Submitted
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Interaction of endohedral molecular hydrogen with C_{60}: infrared study[1] TOOMAS RÕÕM, MIN GE, D. HÜVONEN, U. NAGEL, NICPB, Tallinn, Estonia, S. MAMONE, M.H. LEVITT, M. CARRAVETTA, Southampton Uni., UK, Y. MURATA, K. KOMATSU, Kyoto Uni., Japan, XUEGONG LEI, N.J. TURRO, Columbia Uni., New York — We report on the dynamics of isotopically different hydrogen molecules, H_2, D_2 and HD, trapped in the molecular cages of a fullerene C_{60}[Min Ge et al., J. Chem. Phys. **134**, 054507 (2011), **135**, 114511 (2011)]. The infrared spectra were measured at temperatures from 5K to 300K and analyzed using a model of a vibrating rotor trapped in a spherical potential. The interaction potential was determined in the ground and in the first excited vibrational state of a hydrogen molecule. The isotropic part of the potential is similar for all three molecules studied. In HD@C_{60} we observe the mixing of rotational states and an interference effect of the dipole moment terms due to the displacement of the HD rotation center from the fullerene cage center. A three-site Lennard-Jones potential in the pairwise additive five-dimensional potential energy surface reproduces the hydrogen IR spectrum with great accuracy[M. Xu et al., J. Chem. Phys.**130**, 224306 (2009)].

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