Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Interaction potential and IR absorption of endohedral H_2 in C_{60}[1]

TOOMAS ROOM, MIN GE, D. HUVONEN, U. NAGEL, Nat. Inst. of Chem. Phys. Biophys., 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. — We measured the IR spectra of a H_2 molecule trapped inside a C_{60} cage at temperatures from 6 to 300 K and analyzed the spectra by using a model of a vibrating rotor in a spherical potential. The electric dipole moment of IR transitions is induced by the translational motion of H_2. The rotation of H_2 is unhindered but coupled to the translational motion. The isotropic and translation-rotation coupling part of the potential are anharmonic and different in the ground and excited vibrational states of H_2. The vibrational frequency and the rotational constant of endohedral H_2 are smaller than in the gas phase. The assignment of IR lines to ortho- and para-H_2 is confirmed by measuring spectra of a para enriched $H_2@C_{60}$ and is consistent with the earlier interpretation of the low temperature IR spectra [S. Mamone *et al.*, J. Chem. Phys. **130**, 081103 (2009)].

[1]Support by the Estonian Ministry of Education and Research grant SF0690029s0 and SF grants ETF7011, ETF8170 and JD187 is acknowledged.

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Date submitted: 22 Nov 2010 Electronic form version 1.4