

Abstract Submitted  
for the MAR11 Meeting of  
The American Physical Society

**Interaction potential and IR absorption of endohedral H<sub>2</sub> in C<sub>60</sub>**<sup>1</sup>  
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<sub>2</sub>  
molecule trapped inside a C<sub>60</sub> 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<sub>2</sub>. The  
rotation of H<sub>2</sub> 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<sub>2</sub>. The vibrational frequency and  
the rotational constant of endohedral H<sub>2</sub> are smaller than in the gas phase. The  
assignment of IR lines to ortho- and para-H<sub>2</sub> is confirmed by measuring spectra of  
a para enriched H<sub>2</sub>@C<sub>60</sub> and is consistent with the earlier interpretation of the low  
temperature IR spectra [ S. Mamone *et al.*, J. Chem. Phys. **130**, 081103 (2009) ].

<sup>1</sup>Support by the Estonian Ministry of Education and Research grant SF0690029s0  
and SF grants ETF7011, ETF8170 and JD187 is acknowledged.

Toomas Room  
Nat. Inst. of Chem. Phys. Biophys., Tallinn, Estonia

Date submitted: 22 Nov 2010

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