Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Rotor in a Cage: Infrared Spectroscopy of an Endohedral Hydrogen-Fullerene Complex[1] TOOMAS RÕÕM, MIN GE, D. HÜVONEN, U. NAGEL, NICPB, Akadeemia tee 23, 12618 Tallinn, Estonia, S. MAMONE, A. DANQUIGNY, F. CUDA, M. C. GROSSEL, M. CARRAVETTA, M. H. LEVITT, School of Chemistry, Southampton University, Southampton SO17 1BJ, UK, Y. MURATA, K. KOMATSU, Institute for Chemical Research, Kyoto University, Kyoto 611-0011, Japan — We report the observation of quantized translational and rotational motion of molecular hydrogen inside the cages of C_{60}. Narrow infrared absorption lines at the temperature of 6 K correspond to vibrational excitations in combination with translational and rotational excitations and show well-resolved splittings due to the coupling between translational and rotational modes of the endohedral H_2 molecule. A theoretical model shows that H_2 inside C_{60} is a three-dimensional quantum rotor moving in a nearly spherical potential. The theory provides both the frequencies and the intensities of the observed infrared transitions. Good agreement with the experimental results is obtained by fitting a small number of empirical parameters to describe the confining potential, as well as the *ortho* to *para* ratio at 6 K and at elevated temperatures [S. Mamone, et al., arXiv:0807.1589v2].

[1]The support by the EstSF grants 6138 and 7011, the EPSRC, and the University Research Fellowship (Royal Society) is acknowledged.

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Date submitted: 21 Nov 2008 Electronic form version 1.4