Abstract Submitted
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Rotations and vibrations of water molecule inside the fullerene cage: infrared study of $H_2O@C_{60}$[1] TOOMAS ROOM, A. SHUGAI, U. NAGEL, NICPB, Tallinn, Estonia, S. MAMONE, A. KRACHMALNICOFF, R.J. WHITBY, M.H. LEVITT, Chemistry, Uni. of Southampton, UK, T. NISHIDA, Y. MURATA, Inst. of Chem. Research, Kyoto Uni., Uji, Japan, XUEGONG LEI, YONGJUN LI, N.J. TURRO, Dep. of Chemistry, Columbia Uni., New York — Water is the second molecule after hydrogen what has been trapped inside the cage of a C_{60} molecule by the molucular surgery method [Kurotobi and Murata, Science **333**, 613 (2011)]. We studied isolated water molecule isotopologs H_2O, D_2O, and HDO in the solid phase at cryogenic temperatures using IR spectroscopy. The water molecule rotation transitions were observed in the THz [Beduz et al., PNAS **109**, 12894 (2012)] and vibration-rotation transitions in the mid-IR range. The slow conversion between para and ortho water allowed us to record the time evolution of spectra and to separate ortho and para absorption lines of water. The similarity of the rotation spectrum of caged water to water in the gas phase indicates that water is free to rotate in the C_{60} cage even at temperature as low as 3 K. However, spectral lines show a splitting of about 0.5 meV what is not compatible with the icosahedral symmetry of C_{60}. Different models (e.g. crystal field effects in solid C_{60}, C_{60} cage distortions) will be discussed.

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