QUANTUM TRANSLATION-ROTATION DYNAMICS OF HYDROGEN MOLECULES CONFINED IN THE CAGES OF CLATHRATE HYDRATES

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The coupled translation-rotation (T-R) eigenstates of a hydrogen molecule inside the small dodecahedral $(H_2O)_{20}$ cage of the structure II clathrate hydrate have been determined accurately by means of quantum 5D calculations, for *para*- and *ortho*-H_2[a], as well as *ortho*- and *para*-D_2[b]. In addition, the ground-state properties of two and three *para*-H_2 and *ortho*-D_2 molecules confined in the small cage have been calculated rigorously using the diffusion Monte Carlo method[b]. These calculations have provided a comprehensive picture of the quantum T-R dynamics of the encapsulated molecules. The translational modes exhibit negative anharmonicity; j is a good rotational quantum number, with the threefold degeneracy of the $j = 1$ level lifted completely. When two hydrogen molecules are confined, they are effectively excluded from the central region of the cage, and reside within a shell less than 2 bohrs wide. If time permits, the quantum dynamics results for multiple H_2/D_2 molecules inside the large $(H_2O)_{28}$ cage will be presented.

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[a] M. Xu, Y. S. Elmatad, F. Sebastianelli, J. W. Moskowitz, and Z. Bačić, *J. Phys. Chem. B* **110**, 24806 (2006)

[b] F. Sebastianelli, M. Xu, Y. S. Elmatad, J. W. Moskowitz, and Z. Bačić, *J. Phys. Chem. C* **111**, 2497 (2007)