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Title of Thesis: A Study of the Raman Spectrum of Simple Clathrate Hydrates of Hydrogen

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Abstract :

Clathrate hydrates are molecular structures in which water molecules form molecular cages that host other species of molecules. These structures are formed as a result of phase transition under specific temperatures and pressures. The shape and stability of the structure is dependent on the guest molecules. Clathrate hydrates are immensely present in nature, and are expected to appear in various applications like in transport, and storage of other molecules. They are also thought of as the future worldwide energy reservoir. Raman spectroscopy offers an effective way to understand the dynamics of such crucial structures. Raman spectroscopic measurements were obtained from samples of simple clathrate hydrates of hydrogen and hydrogen deuteride, using a novel cell that allowed us to witness the formation of clathrates, and perform in situ measurements upon them. Understanding the Raman spectrum will help unravel new and interesting traits of enclathrated molecules, as it reveals their quantum dynamics inside molecular cages. The cluttered region of the Raman spectrum assigned to the vibrational states with different occupancies have been analyzed, and a new interpretation of this region of the spectrum is proposed in this work, based on calculations of average occupancy per large cage for samples formed at different synthesis pressures, and subjected to heating and quenching cycles.

Keywords:

Clathrates; Clathrate hydrates; Raman spectroscopy; Vibrational spectrum.