Infrared and X-ray Diffraction Study of Symmetric Hydrogen Bond Formation in the Methane Clathrate

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The recent study of the methane clathrate under pressure has revealed two new structures in addition to the well known structure I clathrate. The highest pressure structure resembles a filled ice lattice and is denoted MH-III. This structure has been shown to be stable to pressures near 50 GPa. The open structure and consequent high compressibility of this clathrate means a centro-symmetric hydrogen bonds could be obtained at lower pressures than are required for the stable ice ice VIII phase in the pressure range above 2 GPa. In this study, we carried out infrared studies at ambient and low temperatures on mixtures of H2O and D2O in order to characterize this formation the centro-symmetric hydrogen bond. These studies were complemented by detailed theoretical calculations of the behavior of the MH-III clathrate using ab initio techniques.