Anharmonic vibration-translation-rotation of diatomic molecule encapsulated in hydrated clathrate cages

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Hydrate clathrates are crystalline compounds composed of water molecules that form cages in which small molecules are encapsulated, depending on the thermodynamic conditions of formation [1]. Two systems are studied: (i) Carbon monoxide hydrate, which can be considered an important component of the carbon cycle in the solar system, since CO gas is one of the predominant forms of carbon [1]. (ii) The H_2 clathrate hydrate, which is of great interest because of to its potential as a hydrogen storage material [2].

The aim of this work is to solve the time-independant Schrödinger equation, to calculate the anharmonic Vibration-Translation-Rotation (VTR) levels of diatomic molecules trapped in the clathrate hydrates. We will then calculate the vibrational shift of the diatomic molecules resulting from its encapsulation in the water cage.

In our calculations, we use a quantum dynamics code, ElVibRot [3], and two recent potentials [2,4]. (fitted with a neural network and derived from ab initio calculations at CCSD(T)-F12a) to evaluate the interactions between the trapped molecule (CO or H_2) and H_2O molecules. We will present our results of quantum calculations of the anharmonic levels of the VTR motions of H_2 and CO trapped in H_2O cages. We will then deduce the order of magnitude of the vibrational shift of them that has been measured experimentally [5] and also the influence of the 3-boby contributions on the VTR levels.

KEYWORDS: Diatomic**;** clathrate; vibration; translation; rotation; anharmonic.

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