

From Infrared Spectra to Macroscopic Mechanical Properties of sH Gas Hydrates through Atomistic Calculations

Supporting Information

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Content:

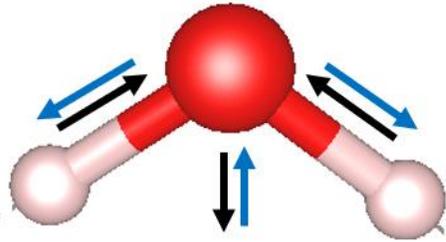
This file contains schematics of the main vibrational modes of water molecules and some guest vibrations in sH gas hydrates with average IR frequency values at 0 K and 0 GPa (unless otherwise stated). Molecules visualizations were made using VESTA* software.

Color code:

- Oxygen atom: red
- Hydrogen atom: white
- Carbon atom: brown
- Vibrations happening at the same time have the same color (black or blue).

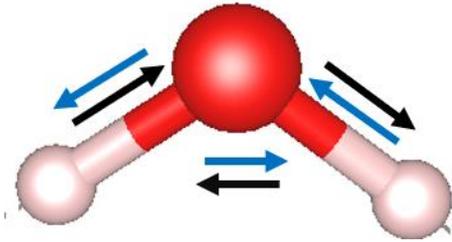
* K. Momma and F. Izumi, "VESTA 3 for three-dimensional visualization of crystal, volumetric and morphology data," J. Appl. Crystallogr., 44, 1272-1276 (2011).

Main vibrational modes of water molecules in sH gas hydrates



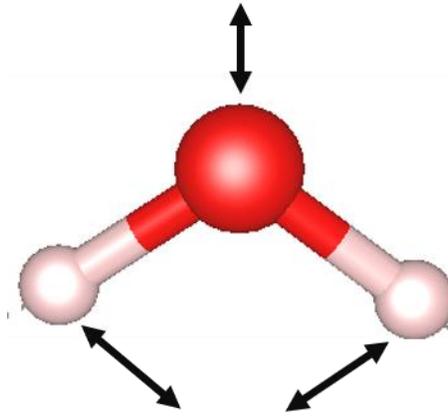
OH symmetric stretch

$\sim 3062 \text{ cm}^{-1}$



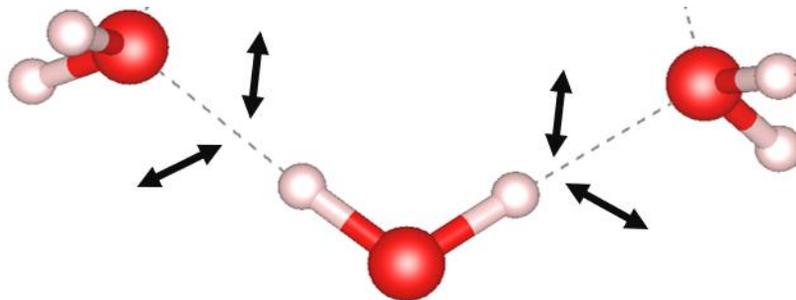
OH asymmetric stretch

$\sim 3268 \text{ cm}^{-1}$



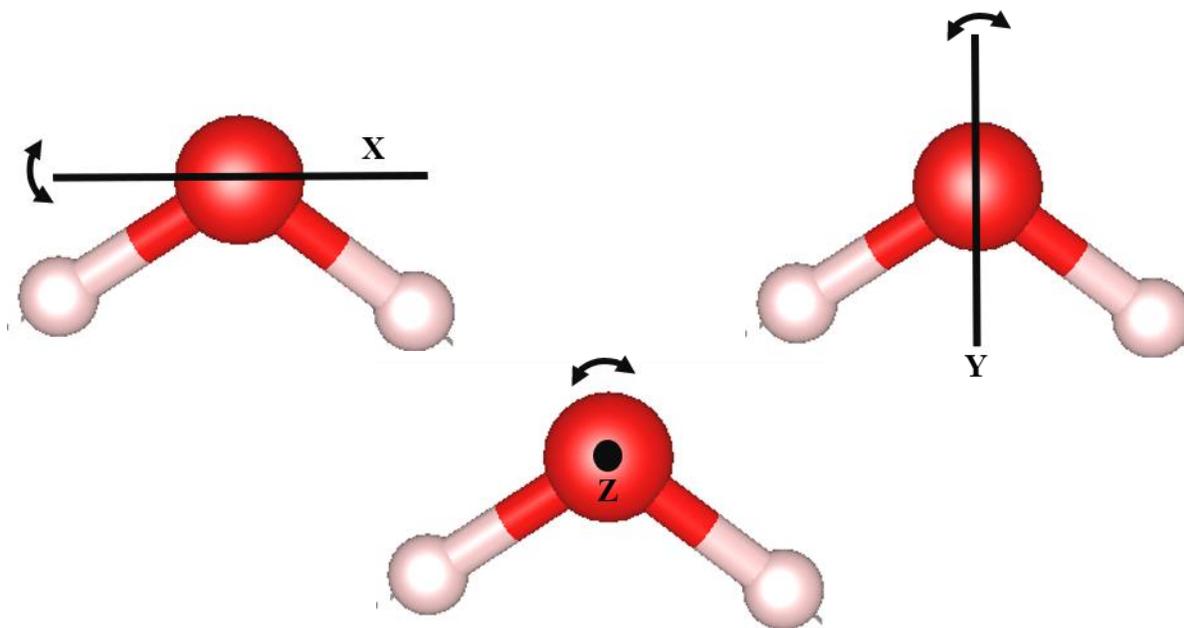
H₂O bending

$\sim 1633 \text{ cm}^{-1}$



Hydrogen bond stretching

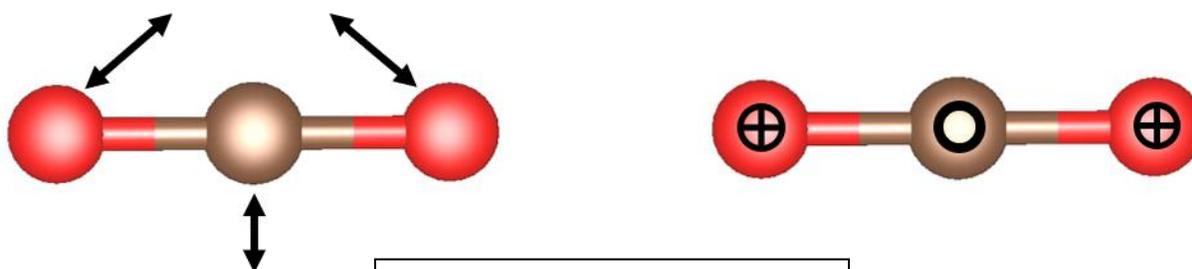
$\sim 192 \text{ cm}^{-1}$



H₂O libration modes
 ~ 648 cm⁻¹, 918 cm⁻¹

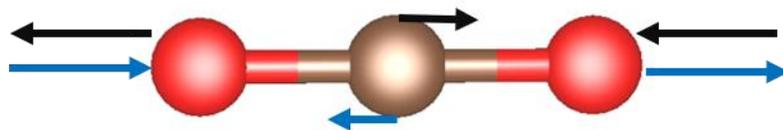
Selected vibrational modes of guest molecules encapsulated inside sH gas hydrates

Carbon Dioxide



CO₂ bending*
 ~ 610 cm⁻¹

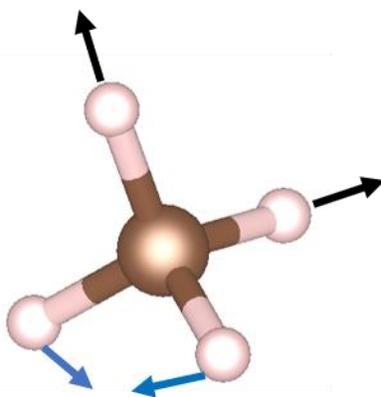
* Observed at pressures ≥1 GPa in sH gas hydrate



C=O asymmetric stretch

~ 2284 cm⁻¹

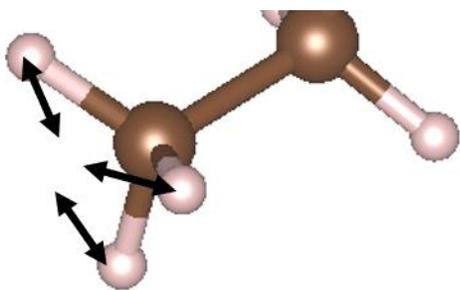
Methane



CH₄ asymmetric bending

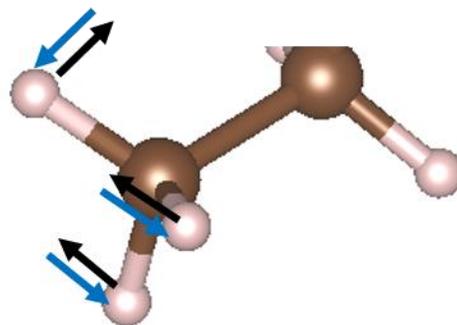
~ 1252 cm⁻¹

Neohexane



CH₃ symmetric bending

~ 1345 cm⁻¹



CH₃ asymmetric bending

~ 1432 cm⁻¹