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Low Temperature & High Pressure Ethylene Oxide Hydrate Formation

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Abstract

Gas hydrates are crystalline, solid structures that are commonly formed in natural gas pipelines. They form when water and natural gas combine at the low temperatures and high pressures. The formation of these hydrates can cause blockages in the pipeline. In order to reduce their prevalence, we are researching the infrared spectroscopy of ethylene oxide deuterate, formed at 120 K, between 2200 and 3600 cm^{-1}. The IR spectra confirm reorientation of an initially disordered amorphous sample into a more structured crystalline hydrate. Understanding the structures and conditions that these gas hydrates form allows for new techniques to mitigate them to arise in the petroleum industry.

Background/Introduction

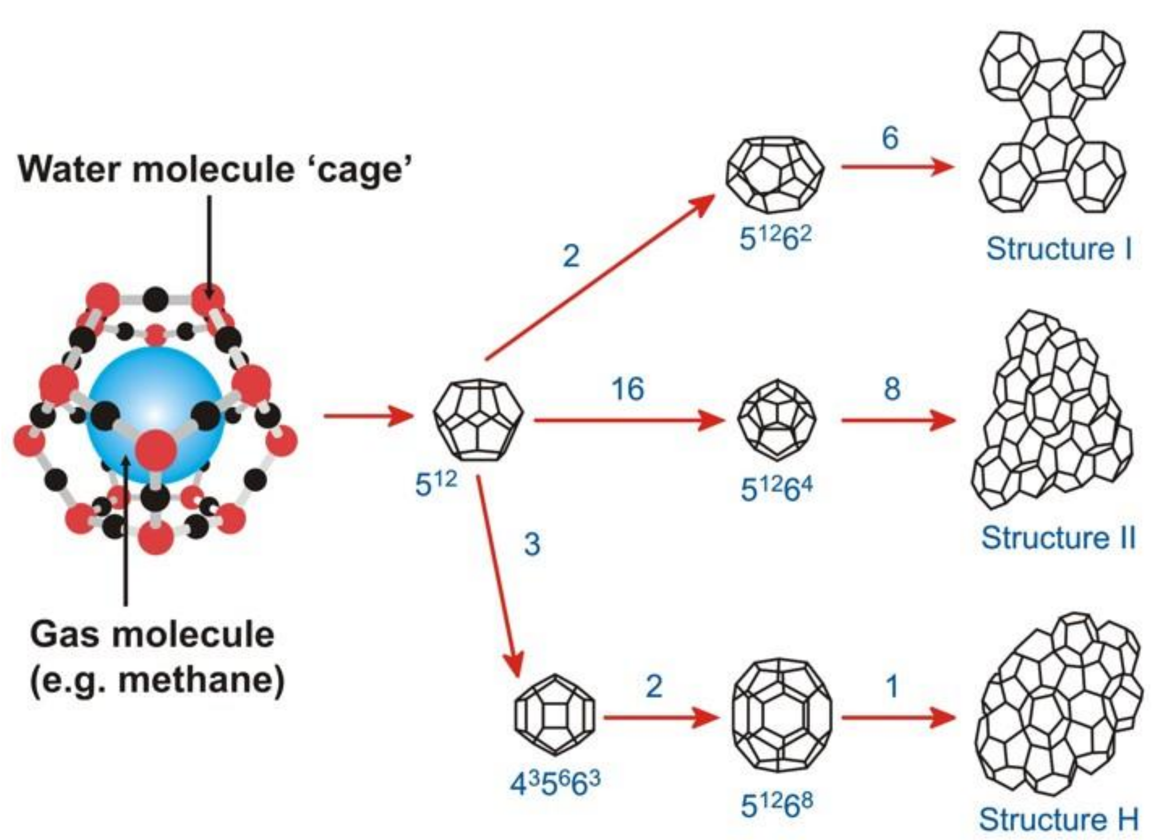

Figure 1: Gas Hydrate Cage Structures

Gas hydrates, also known as clathrate hydrates, are water molecules connected in a three dimensional cage structure. The cage is held together through hydrogen bonds. These hydrates have small gas molecules (methane, ethylene oxide, carbon monoxide) which are encapsulated in the middle. There are three types of structures: Type I, Type II, and Type H. The main focus in this lab is to create 5^{12} and $5^{12}6^2$ structures in order to create a Type I structure.

Goals for Fall Research

- Form Ethylene Oxide Hydrate and Deuterate
- Measure its infrared spectra over the CH range of Ethylene Oxide
- Calculate the structure of the 5^{12} and $5^{12}6^2$
- Calculate the infrared structure of the system and compare with measured data

Method & Results

Experimental Method:

Formation of Hydrate & IR Spectroscopy

1. 20 Min deposit of ethylene oxide (4% in Ar) + D_2O onto a CaF_2 window held at 50 K.
2. Measure the amorphous in the IR.
3. Heat the sample to 120 K for 2 hours
4. Cool the sample to 4 K
5. Measure the hydrate IR

Computational Method

Optimized Structure Calculations

1. Optimize the structure of 5_{12} & $5_{12}6_2$ hydrates with ethylene oxide using Gaussian 16 on the Raj computation cluster
2. Run frequency calculations from these optimized structures to obtain IR

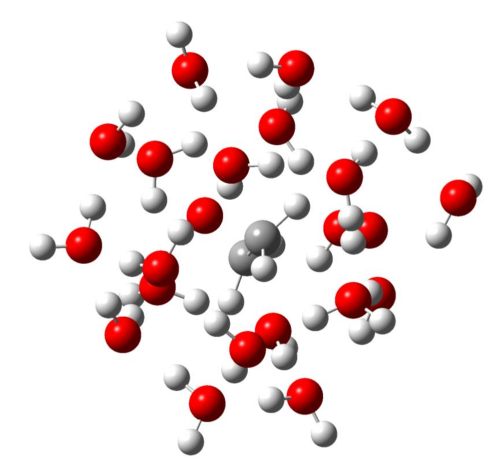

Figure 2: 5^{12} Ethylene Oxide Hydrate

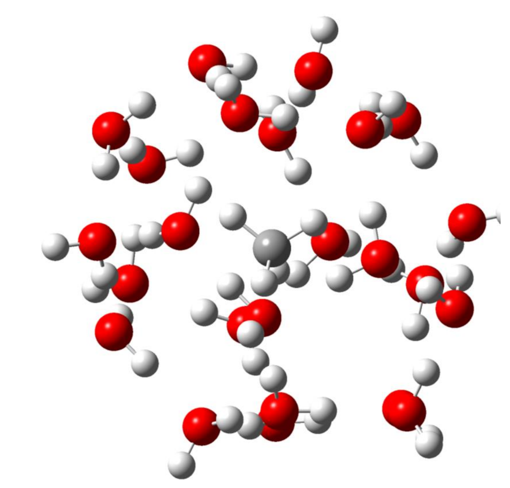

Figure 3: $5^{12}6^2$ Methane Hydrate

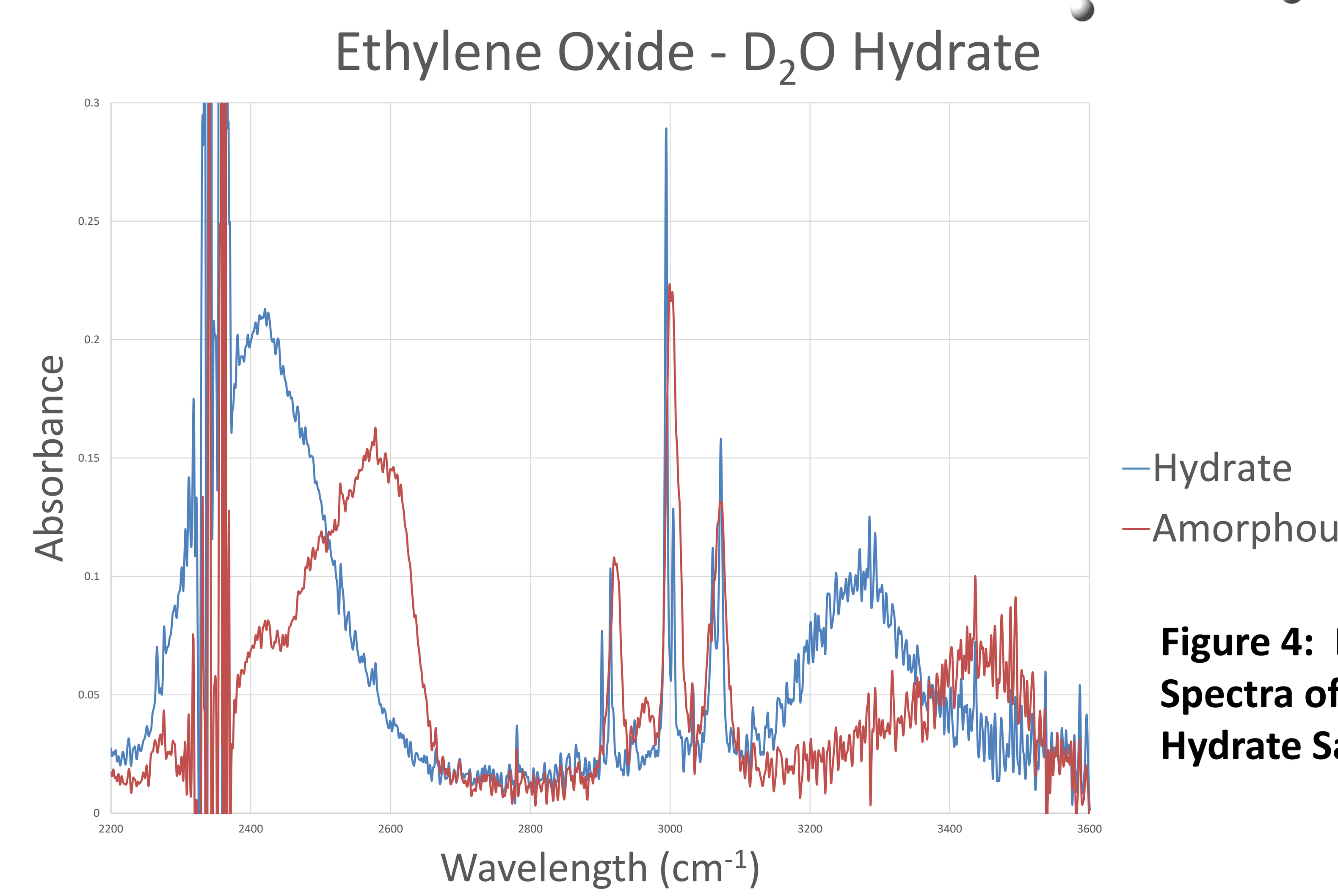

Figure 4: Experimental IR Spectra of Amorphous and Hydrate Samples

Conclusion/Next Steps

So far:

- Calculated 5^{12} Ethylene Oxide Hydrate
- Calculated $5^{12}6^2$ Methane Hydrate

Next Steps:

- Successfully optimize $5^{12}6^2$ ethylene oxide structure
- Successfully replace water with D_2O in 5^{12} & $5^{12}6^2$ structures

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