A PROCESS FOR LOW TEMPERATURE, LOW PRESSURE SYNTHESIS OFCLATHRATE HYDRATES

IITM Technology Available for Licensing

Problem Statement

- Clathrate hydrates (CHs) are crystalline inclusion compounds in which different guest molecules are encased in H-bonded water-cages, that requires high-pressures and moderate temperatures that enable their existence in marine sediments and permafrost region of earth.
- The presence of CHs in interstellar medium (ISM) is still in question due to the extreme high vacuum and ultracold conditions present there.

Technology Category/ Market

Category – Advanced materials

Applications – Energy resource, environmental engineering, Prebiotic Chemistry, Gas storage and separation

Industry - Chemical

Market -The global advanced materials market size was estimated at USD 61.35 billion in 2022 and it is expected to reach USD 112.7 billion by 2032, **at a CAGR of 6.27% from 2023 to 2032.**

Key Features / Value Proposition

Technical Perspective

- Discloses a process for synthesizing clathrate hydrates(CH) in ISM especially formation of methane, CO2, acetone and tetrahydrofuran hydrates in extreme low-pressure environments where CH are subjected to various chemical processes that act as sources for prebiotic molecules
- The present invention found that the molecular **mobility and interactions play crucial roles** in the formation of CHs, even though there is no external pressure to force cage formation.

User Perspective

- CHs can exist in extreme low-pressure environments present in the ISM, CH are ideal in Astrochemistry and Planetary Exploration, carbon capture and storage

Technology

The present invention discloses a process for synthesizing clathrate hydrates in interstellar environment at low pressure comprising:

Condensing the water vapor and guest molecule in vacuum

Annealing the condensed mixture

- The said interstellar environment is set at low pressure of 10^{-10} mbar and at cryogenic temperatures in the range of 10 K to 135 K
- The water vapor and guest molecule are condensed separately or together in an ultrahigh vacuum chamber
- The condensed mixture is gradually annealed to temperatures below the desorption temperature of guest molecule in vacuum for 0-48 hour
- The said the guest molecule includes methane, carbon dioxide, acetone and tetrahydrofuran.
- The clathrate hydrates includes methane hydrate, carbon dioxide hydrate, acetone hydrate, and tetrahydrofuran hydrate.

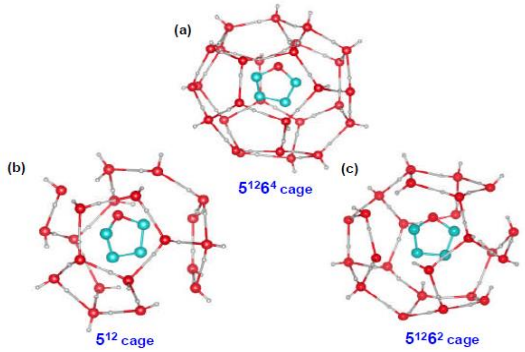

Fig 1.DFT-optimized structures of THF trapped within different CH cages, such as, (a) 51264 cage, (b) 512 cage, and (c) 51262 cage. Here, water cage and the guest molecule (THF) are shown. H atoms of THF molecules in all the structures are omitted for clarity. Color code used:cyan, C; red, O; gray, H.

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Images

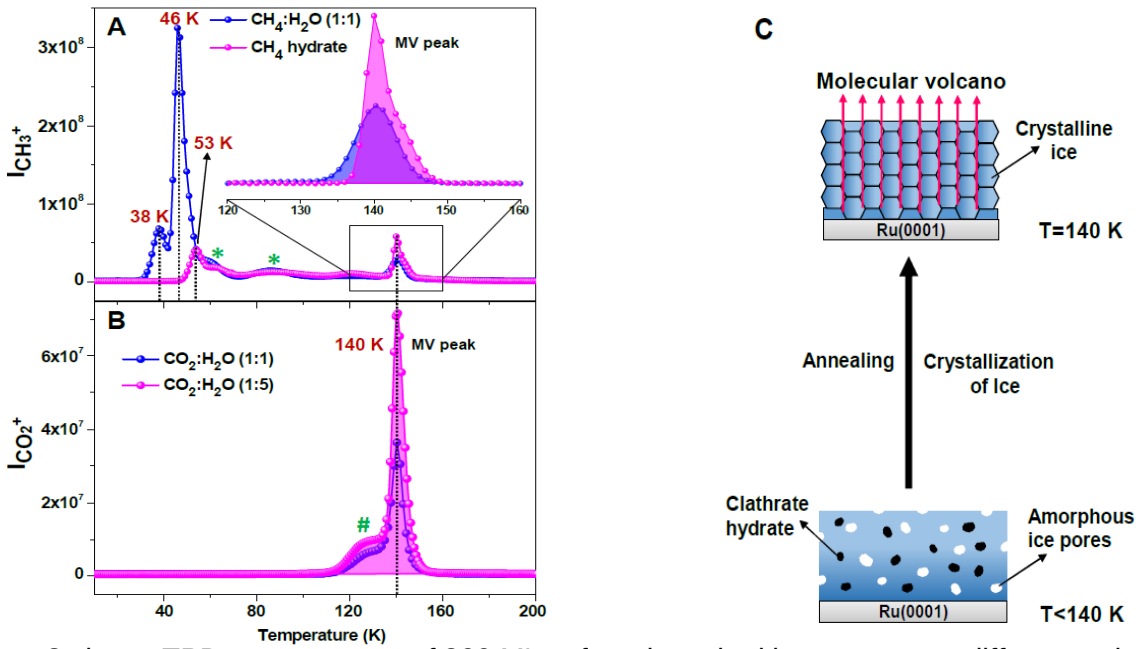

Figure 2 shows TPD mass spectra of 300 MLs of co-deposited ice systems at different ratio.

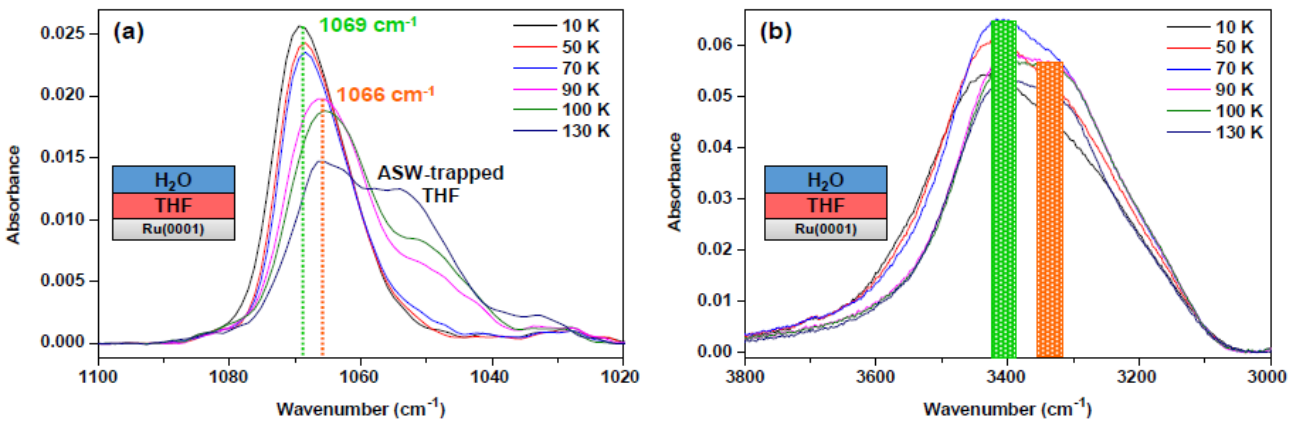

Fig. 3 Shows temperature-dependent RAIR spectra of 300 MLs of a THF@H2O mixture (1:1) in (a) asymmetric C-O stretching region, and (b) in O-H stretching region, which was sequentially deposited at 10 K on Ru(0001) substrate. The sequential deposition was carried by condensing 150 MLs of H2O film over the same coverage of THF film, thus making it a (1:1) mixture. This mixture was annealed at 2 K min-1 heating rate and the spectra were collected

Research Lab

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Intellectual Property

- **IITM IDF Ref. 1817**
- **IN 356814 –Granted**

TRL (Technology Readiness Level)

TRL-3,Experimental Proof of Concept

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