Infrared Spectroscopic Analysis of Solid-Phase Carbonic Acid

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Introduction

Carbonic acid (H_2CO_3) is a short-lived species in aqueous solutions on Earth; however, recent laboratory and astronomical studies have demonstrated that it can exist in a stable solid phase under astrochemical conditions. The investigation of such molecules is essential for understanding chemical processes occurring in interstellar ices, dense molecular clouds. Infrared (IR) spectroscopy provides a powerful tool for identifying molecules. Laboratory-based IR spectroscopic measurements are therefore crucial for interpreting astronomical observations and for building reliable astrochemical models.

Aims

The aim of this research was to investigate the formation, stability, and spectroscopic characteristics of carbonic acid in solid and gas phases under astrophysically relevant conditions. The study sought to determine whether carbonic acid remains stable during sublimation and whether it can be detected in the gas phase, thereby supporting recent astronomical observations and contributing reliable laboratory reference data.

Materials and Methods

Experiments were carried out using the VIZSLA (Versatile Ice Zigzag Sublimation Setup for Laboratory Astrochemistry) ultra-high-vacuum simulation chamber.

- Designed to mimic the conditions prevailing in space
- Studies molecules in a simulation chamber where astrophysical conditions (low temperature, ultra-high vacuum) can be created

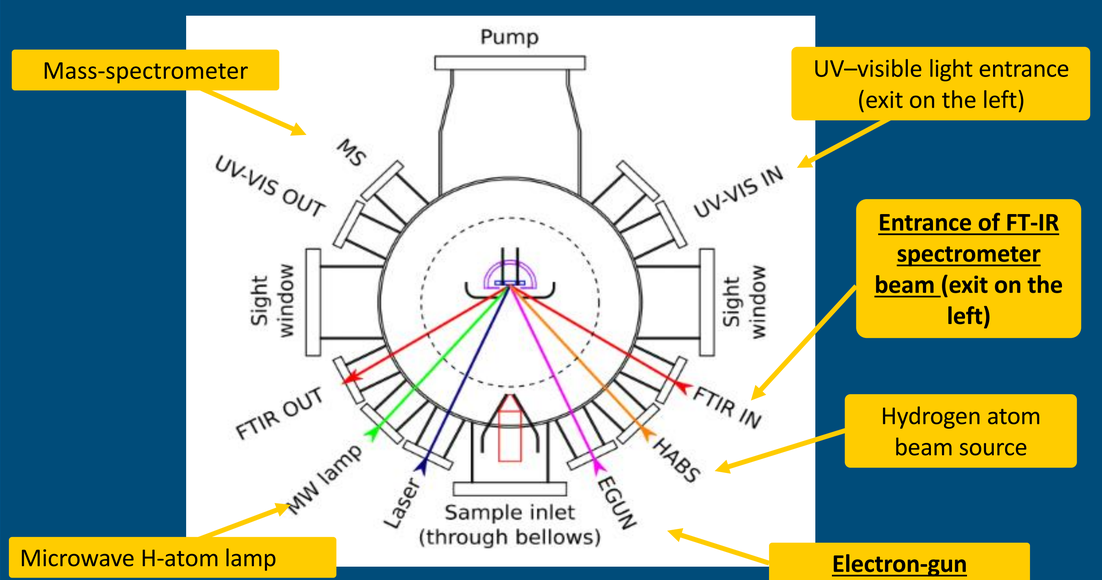


Figure 1: VIZSLA (top view)[1]

Identification using Fourier-transform infrared (FT-IR) spectroscopy:

sample is irradiated with IR light →
it absorbs some light →
results are displayed on a spectrum

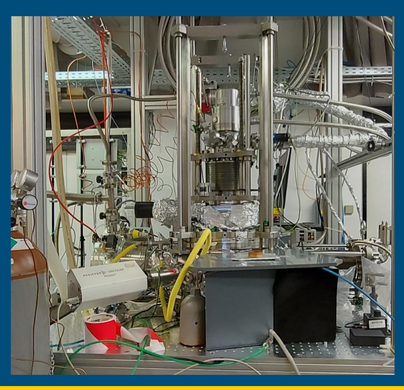


Figure 2: VIZSLA (side view, own photo).

- The starting materials were an ice mixture of carbon dioxide and water in a **3.5mol : 1mol** ratio which was deposited onto a gold-coated silver substrate at 10 K (-263°C).

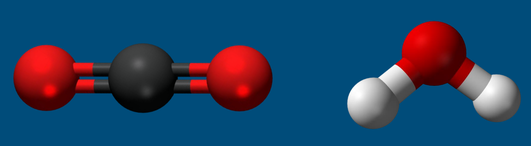


Figure 3: The models of water and carbon dioxide[2,3]

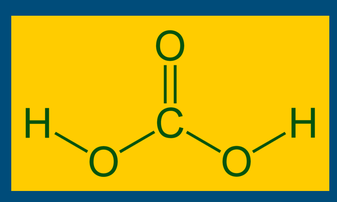


Figure 4: The structure of carbonic acid (H_2CO_3)

Operations:

- The samples were irradiated with 5 keV electrons to simulate cosmic radiation, and chemical changes were monitored using Fourier-transform infrared (FTIR) spectroscopy.
- Temperature-programmed desorption (TPD) experiments were also performed; these were done by heating the sample from 10 K to 300 K (-263°C to 27°C) at a rate of 1 K/min.
- In selected experiments, sublimated species were recondensed onto a secondary cold substrate and analyzed using argon matrix isolation.

Results and Discussion

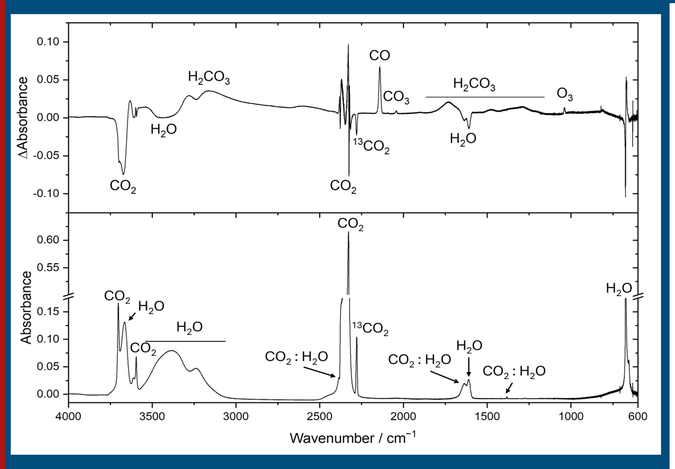


Figure 5: The IR spectra (bottom) and Electron-irradiated difference spectrum (upper) of the H_2O — CO_2 ice mixture

The difference spectrum shows the changes occurring due to irradiation:

- Peaks of initial materials decrease
- H_2CO_3 and other products appear

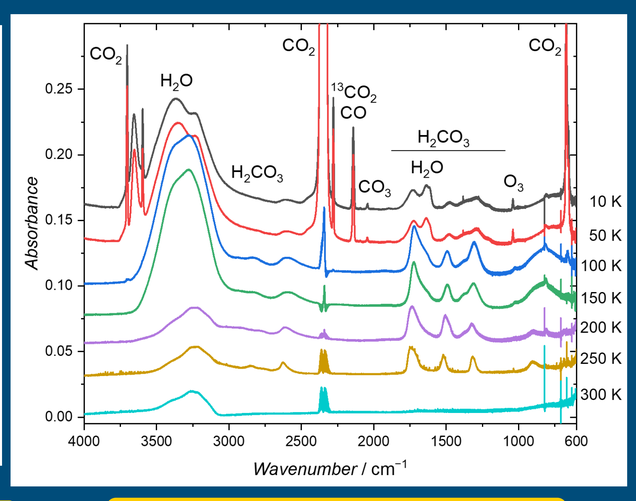
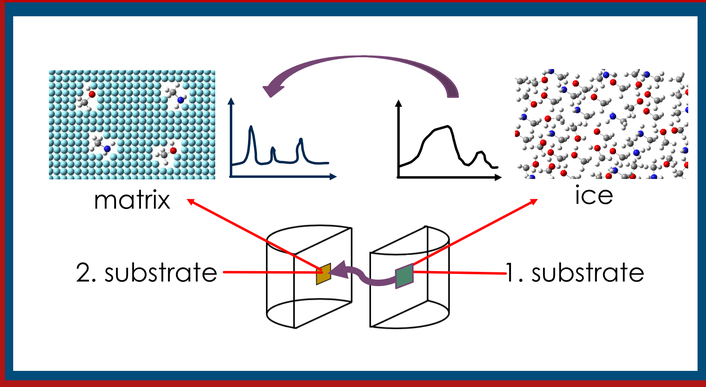


Figure 6: The IR spectra of irradiated H_2O — CO_2 ice mixture during TPD

- At 200 K both precursors sublimate (CO_2 and H_2O)
- The remaining carbonic acid sublimates at 260–280 K (-13 to 7°C)



The carbonic acid on the 1st substrate sublimates during TPD then recondenses onto the 2nd substrate and is captured in an inert Ar matrix

Figure 7: The process of redeposition[1]

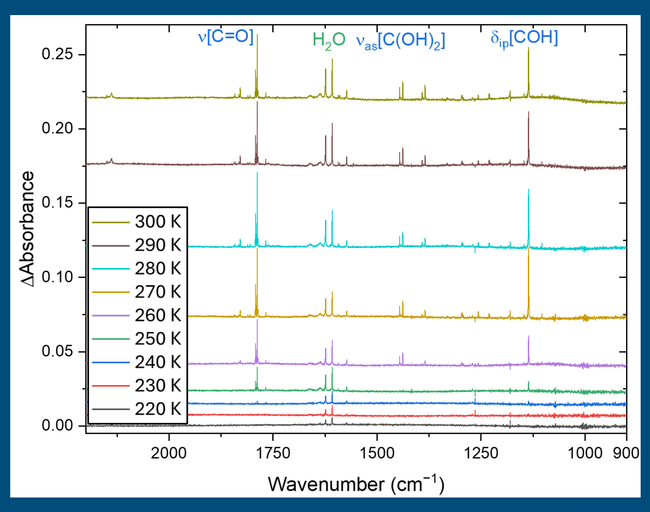


Figure 8: The difference spectra of the irradiated H_2O — CO_2 ice mixture taken during redeposition

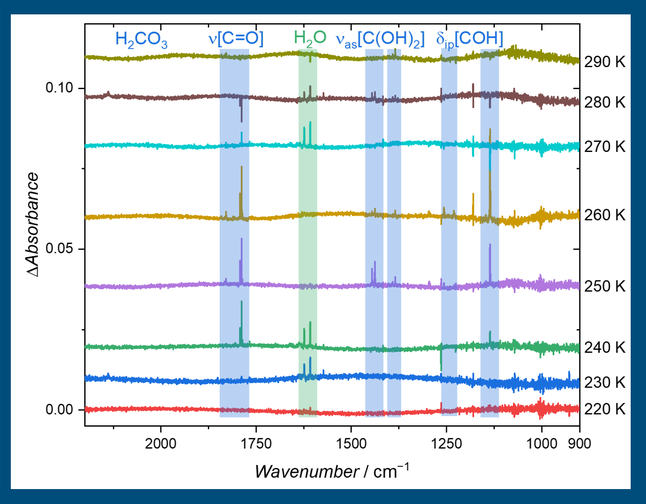


Figure 9: The difference spectra of the difference spectra of the H_2O — CO_2 ice mixture taken during redeposition

- The absorption bands of carbonic acid are clearly separated from water and carbon dioxide → **The molecule is stable in gas phase (when it sublimates to the other substrate)**

Conclusions

This study provides experimental evidence for the formation and stability of carbonic acid under simulated astrochemical conditions. The obtained infrared spectra and thermal behavior data contribute to the identification of carbonic acid in astronomical environments and improve our understanding of carbon chemistry in space.

Literature

[1]BAZSÓ, G.; CSONKA, I. P.; GÓBI, S.; TARCZAY, G. (2021) REV. SCI. INSTRUM. 92, 124104.
[2]https://commons.wikimedia.org/wiki/File:Carbon_dioxide_3D_ball.png
[3]https://en.wikipedia.org/wiki/Water#/media/File:Water-3D-balls-A.png