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Laboratory astrochemistry of sulfur compounds – the importance of hydrogenation processes

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INTRODUCTION

Goal of laboratory astrochemical research

- Particle identification in interstellar medium
- Examination of the chemical processes
- Modelling space weather

Abundance of elements

- Most abundant: hydrogen (H)
- 10th most abundant: sulfur (S)
- “Missing sulfur problem”: theoretically predicted concentration >> detected
- Possible solution: sulfur as a compound

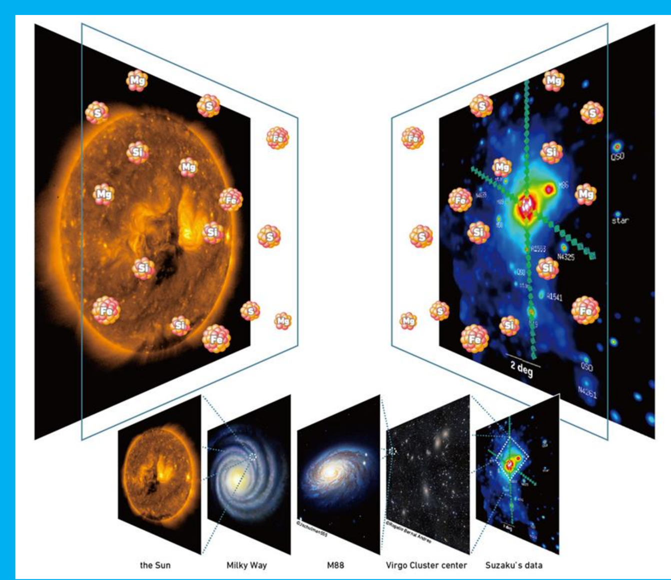


Figure 1: The composition of the universe according to Suzaku.

Thus the identification of possible carrier compounds is essential

AIMS

Figure 2: The structure of thioacetamide (CH_3CSNH_2)

- Identification of S compounds with spectroscopy in a controlled environment on Earth
- Study the simplest stable sulfur compound: thioacetamide (TA) (Fig. 2)
- Examine the hydrogenation processes of TA

METHODS AND MATERIALS

Using a dedicated experimental setup called Versatile Ice Zigzag Sublimation Setup for Laboratory Astrochemistry (VIZSLA)[1] (Fig. 3&4)

- 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

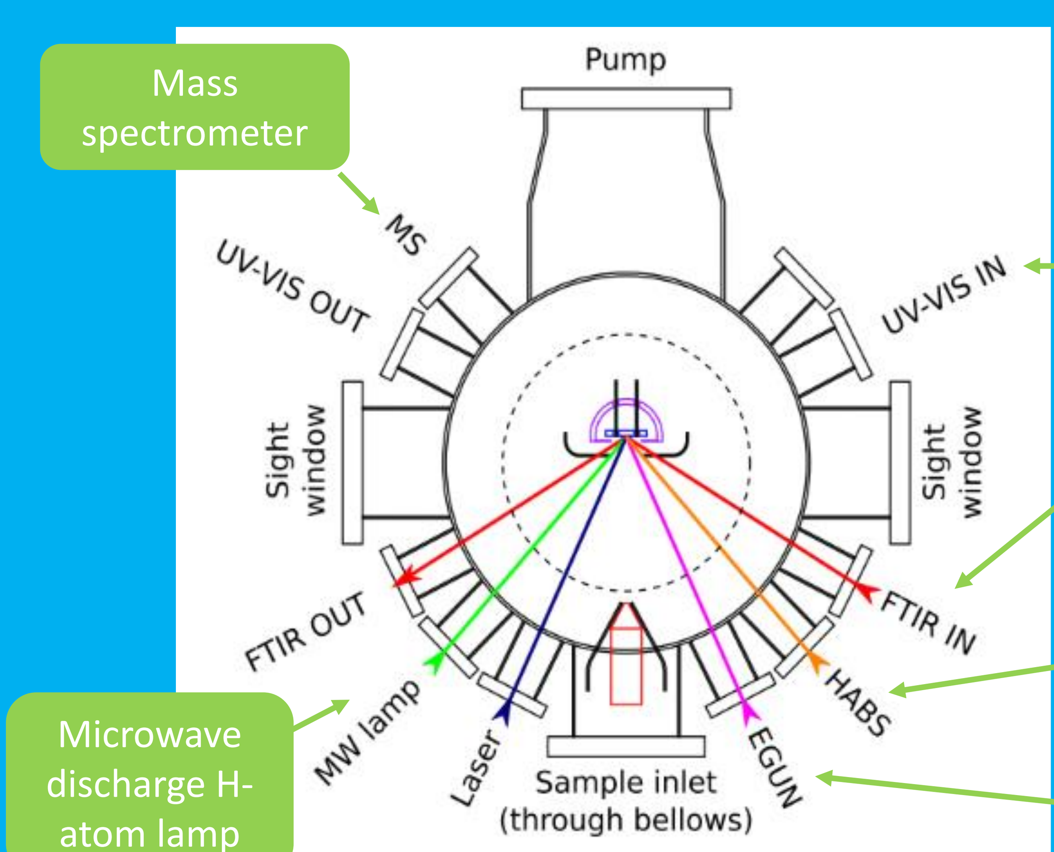


Figure 3: VIZSLA (top view)[1]

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

- The sample is irradiated with IR light
- It absorbs some light, and the results are displayed on a spectrum

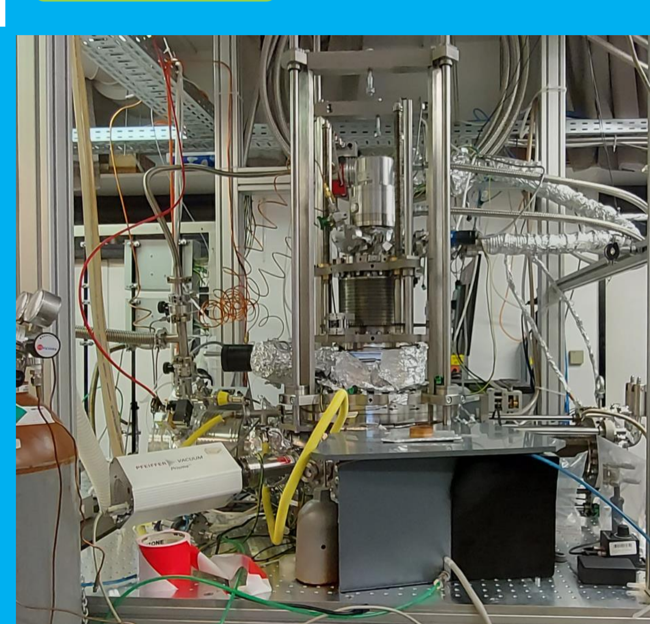


Figure 4: VIZSLA (side view, own photo).

TA ice in argon matrix was examined

- TA was isolated in a solid argon matrix at 15 K temperature
- The sample was irradiated with UV radiation (Lyman-alpha)
- UV radiation created by deexcitation of hydrogen in MW lamp

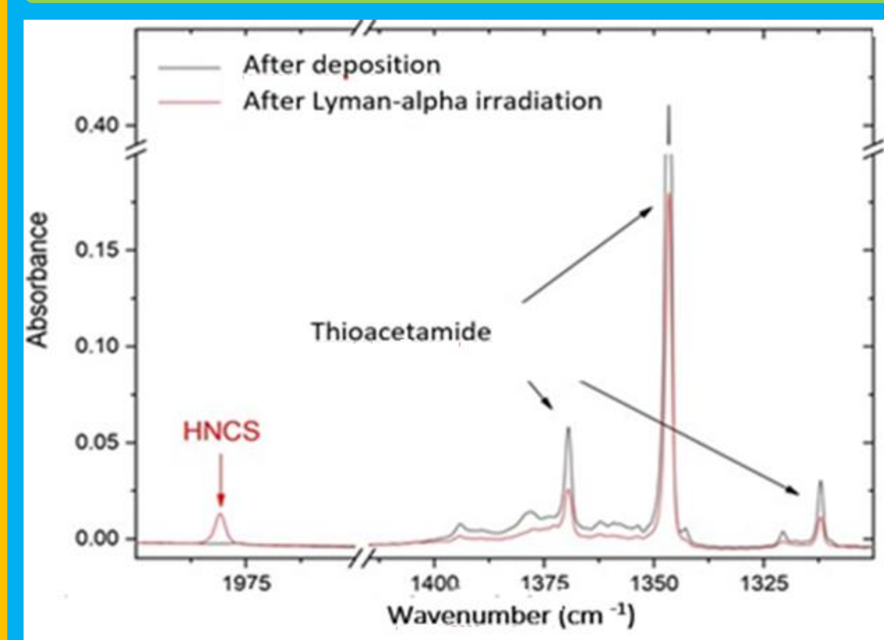
Pure TA ice (in amorphous form) was examined

- TA ice created by depositing TA vapor on a 10 K gold plated silver substrate
- The sample was bombarded with H atoms during deposition
- The H atoms were generated by HABS containing a tungsten filament heated up to 2073 K

In both cases ‘blank’ experiments were recorded (i.e. no H-atom bombardment / no UV radiation); furthermore, temperature-programmed desorption (TPD) was carried out (1K/min)

RESULTS

Figure 5: Segment of the sample’s IR spectrum after deposition and after irradiation.



- Identification of decomposition processes of TA due to the UV irradiation was done with IR spectra (Fig. 5).
- The most common product was isothiocyanic acid (HNCS) denoted with red peak around 1980/cm.
- This could help us to identify sulfur compounds in space.

During TPD products sublimate (Fig. 6):

- HNCS still present at 38 K
- HNCS disappears at 50 K
- Further decomposition products sublimate at 100-150 K

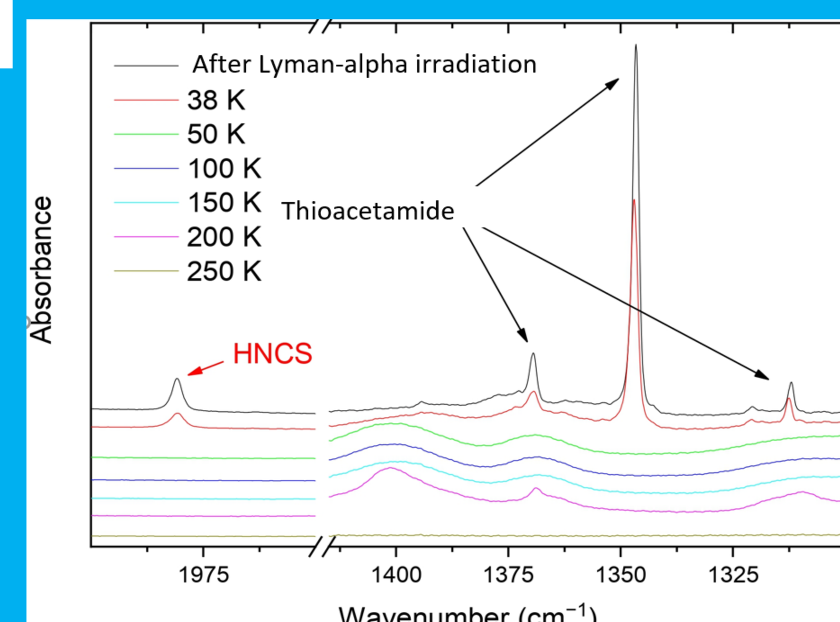


Figure 6: IR spectral changes upon the change of temperature.

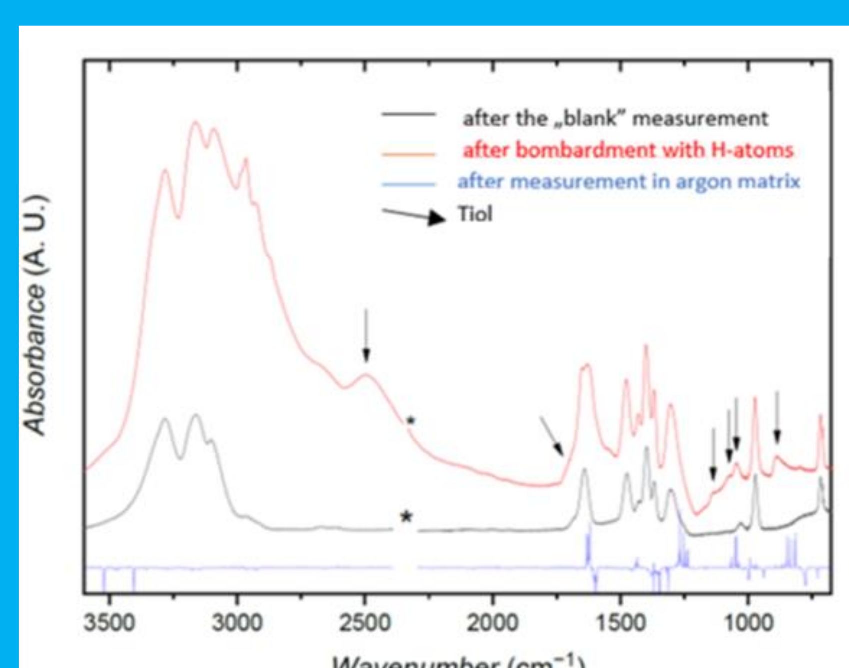


Figure 7: Segment of the sample’s IR spectrum after the „blank” measurement and after bombardment with H-atoms.

- Figure 7 shows the changes upon H-atom bombardment of the amorphous TA ice.
- The new peaks can be attributed to the formation of the higher-energy thiol tautomer of TA (Fig. 8). The unprocessed TA ice consists of only the more stable thione tautomeric form.[2]
- The tautomerization happens due to **H-atoms** and **not UV irradiation!**

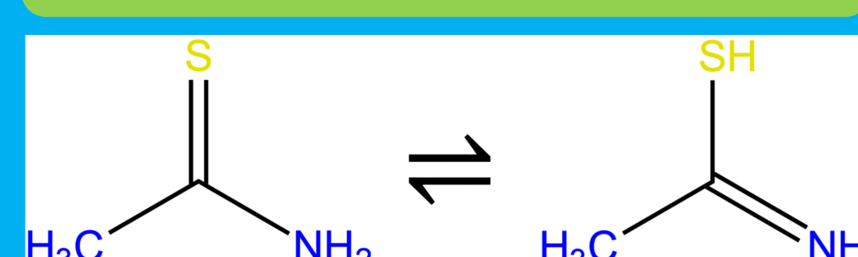


Figure 8: Thione (left) and tiol (right) tautomeric forms of TA.

- In Fig 9. the vertical lines show tiol peaks (c.f. Fig. 7.)
- During TPD the peaks of tiol gradually disappear from 100 K (blue curve). This can be explained by the thiol tautomers turning back into thione form.

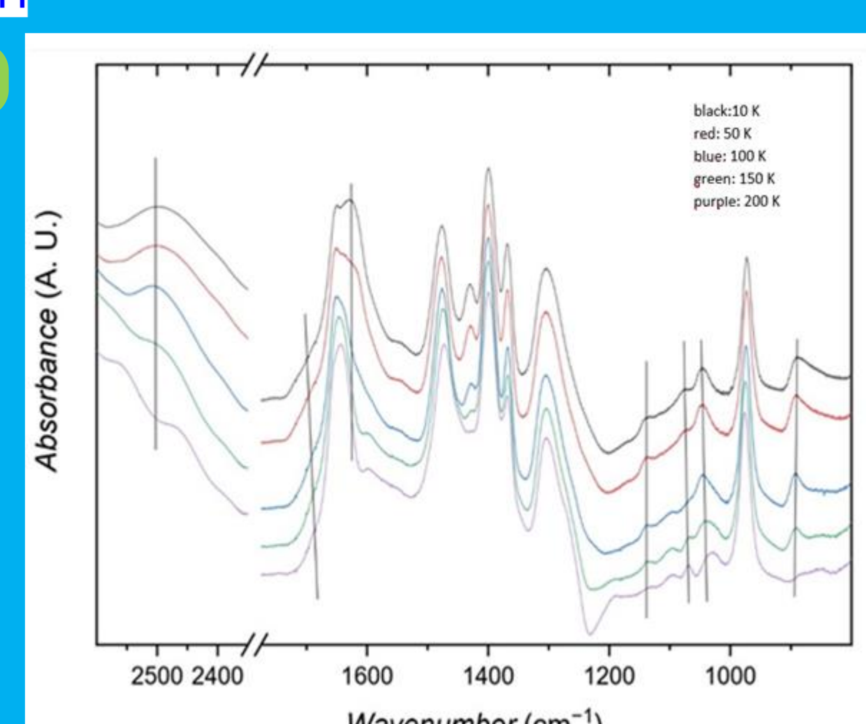


Figure 9: The IR spectral changes upon changing the sample temperature.

CONCLUSIONS

Through these measurements, we gain insight into the reactions between sulfur compounds and H atoms from an interstellar perspective. The processes without irradiation are important, because these reactions can take place in dense molecular clouds, due to high amounts of hydrogen atoms. The data can also be used by astronomers to identify sulfur compounds.

REFERENCES

[C] BAZSÓ, G.; CSONKA, I. P.; GÓBI, S.; TARCZAY, G. (2021) REV. SCI. INSTRUM. **92**, 124104.
[2] GÓBI, S.; REVA, I.; TARCZAY, G.; FAUSTO, R. (2020) J. MOL. STRUCT **1220**, 128719.