Laboratory astrochemistry of sulfur compounds – the importance of hydrogenation processes

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1. INTRODUCTION

The most abundant element in the universe is hydrogen, thus chemical processes that involve it are fundamentally important. Sulfur is also a common element, being the tenth most abundant one, making it relevant for studies. However, the theoretically predicted concentration of sulfur is three orders of magnitude higher than what has already been detected. This discrepancy in the sulfur budget is also called the 'missing sulfur' problem. Therefore, the identification of possible carrier molecules is of great importance.

2. AIMS

The present research focuses on studying the hydrogenation processes of the sulfurous compound thioacetamide (TA), which is a sulfur-containing analog of acetamide.

3. METHODS AND MATERIALS

For this, a dedicated experimental setup is used, specifically designed to simulate the conditions prevailing in space, called VIZSLA (Versatile Ice Zigzag Sublimation Setup for Laboratory Astrochemistry) [Figure 1].[1]

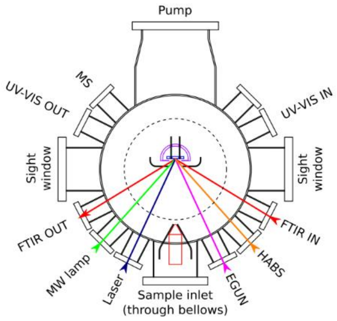

Figure 1: The VIZSLA experimental setup. FT-IR IN and OUT: entrance and exit of the IR beam of the FT-IR spectrometer. UV–VIS IN and OUT: entrance and exit of the light beam of the UV–Visible spectrometer. MW lamp: microwave-discharge H-atom lamp. Laser: port for laser irradiation. EGUN: electron gun. HABS: hydrogen atom beam source. MS: mass spectrometer

During the current measurements pure TA ices were examined, in amorphous form. This was done by depositing TA vapors on a low-temperature (10 K) gold-plated silver substrate. The sample was bombarded with H atoms during deposition, 'blank' experiment (without H-atom bombardment) was also performed for the sake of comparison. The H atoms were generated by the hydrogen atom beam source (HABS) device of the VIZSLA experimental setup. The changes were monitored using Fourier-transform infrared (FT-IR) spectroscopy.

4. RESULTS

Figure 2 shows the changes upon H-atom bombardment of the amorphous TA ice. The arrows show the position of new spectral features. The new bands disappear upon heating the sample, below the crystallization temperature.

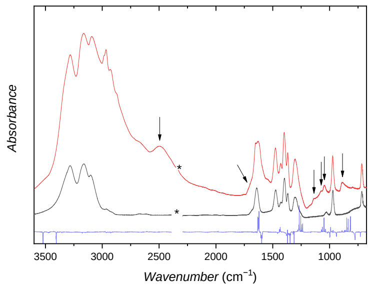

Figure 2: Sample IR spectrum of the 'blank' experiment (black trace) and after H atom bombardment (red trace).

5. DISCUSSION

After careful experimental as well as theoretical considerations, the appearing bands can be attributed to the formation of the higher-energy thiol tautomer of TA [Figure 3]. The unprocessed TA ice consists of only the more stable thione tautomeric form.[2]

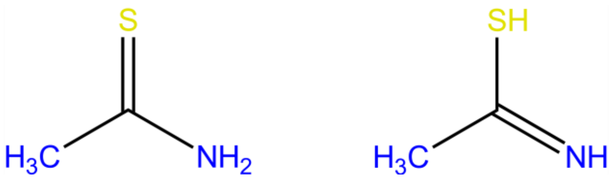

Figure 3: Thione (left) and tiol (right) tautomeric forms of TA.

6. CONCLUSIONS

Through these measurements, we can gain insight into the reactions between sulfur compounds and H atoms from an interstellar perspective.

7. ACKNOWLEDGEMENT

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8. REFERENCES

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[2] Góbi, S.; Reva, I.; Tarczay, G.; Fausto, R. (2020) J. Mol. Struct **1220**, 128719.