Atmospheric influence on chemical pathways of organics on Mars

Quantum chemical modelling of the spectroscopic and structural transformation of amino acids under air exposure

P. Mabey, F. Hofmann, A. Ragyanszki, A. Elsaesser, *Freie Universitaet Berlin, Arnimallee 14, 14195, Berlin, Germany / Zuse Institute, Takustr. 7, 14195 Berlin, Germany*

In Short

- With the ongoing search for life on Mars, space and ground based exposure experiments are becoming increasingly important.
- It is difficult to draw definitive conclusions from said experiments when risk of air contamination is high
- In particular, experiments at FUB have shown that the spectroscopic signature of thin films of alanine change from a broadband structure to sharp peaks within minutes of air exposure.
- The transition from an amorphous state to a zwitterionic crystal is brought about by this exposure. A better understanding of contamination procedures will allow us to recognize the signs in future experiments.

The search for life on Mars has been a fundamental objective of planetary exploration. Mars, with its similarities to Earth in terms of geological features and past potential habitability, presents a compelling target for investigating the existence of extraterrestrial life. Many teams are therefore actively engaged in identifying and studying biosignatures on its surface. These are indirect indicators or traces, typically organic molecules left by living organisms that can provide compelling evidence of biological activity, past or present.

However, Martian conditions have a significant negative impact on the preservation and detectability of these biosignatures. The harsh and inhospitable environment presents several challenges that can affect the stability and visibility of signs of life. One key factor is the thin atmosphere, which offers less protection against harmful radiation compared to Earth. High levels of particle and ultraviolet (UV) radiation can damage organic molecules, making them more vulnerable to degradation or alteration over time. This radiation can break chemical bonds and destroy or change the structures of organic compounds, potentially obscuring or erasing the evidence of past or present life.

For this reason, radiation exposure experiments, both on Earth as well as in space, are crucial to understanding the survivability of these compounds, their reaction products and therefore to identify suitable candidate molecules which can be searched for on the Martian surface. The space exposure experiments OREOcube and Exocube (PI: A.Elsaesser) are currently being developed by ESA and industrial partners to investigate the effects of such radiation on selected organic compounds in low Earth orbit and will be launched in 2025 [1,2]. In the context of these experiments, a ground simulation campaign performed at Freie Universitaet Berlin will provide crucial scientific support for these space missions. Samples will be exposed to simulated solar light and Martian conditions in dedicated planetary simulation chambers equipped with in-situ spectroscopic and mass spectrometric analytics to follow the degradation and photochemical kinetic pathways of selected organic molecules.

Most of these compounds exhibit strong reactivity with oxygen and water. Consequently, conducting these experiments requires stringent precautions such as the use of glove boxes and careful sample transfer procedures [3]. Despite these precautions, the risk of air contamination during these experiments remains a significant challenge. This research proposal aims to address the limitations posed by air contamination in drawing definitive conclusions from such experiments, with a specific focus on the spectroscopic signature of amino acid thin films. Radiation exposure experiments are prone to uncertainties and challenges due to the potential introduction of external substances, leading to air contamination [4,5]. Air contaminants can alter the behavior and spectroscopic signature of the target compound, consequently affecting the accuracy and reliability of the experimental results. Hence, understanding the impact of air contamination is crucial for obtaining conclusive outcomes from radiation exposure studies.

Previous experiments conducted at FUB have demonstrated that the spectroscopic signature of thin films of alanine undergoes a significant transformation from a broadband structure to sharp peaks within minutes of air exposure. Figure 1 shows the results. Initially prepared as a thin film in a nitrogen purged glove box, the alanine is completely separated from contaminants such as oxygen and water. In this state, an amorphous structure is observed, with broad spectral peaks. However, after only a few minutes of being removed from the glove box, the strucutre quickly changes to a zwitterionic crystal with sharper peaks. This observation highlights the role of air contamination in altering the molecular structure and properties of organics.

The primary objective of this research proposal is to investigate the hypothesis that exposure to air induces a transition from an amorphous state to a zwitterionic crystal in amino acid thin films. To achieve this, we propose utilizing quantum chemical modelling to simulate the molecular interactions and dynamics of amino acids in the presence of air contaminants. This study will employ state-of-the-art quantum chem-

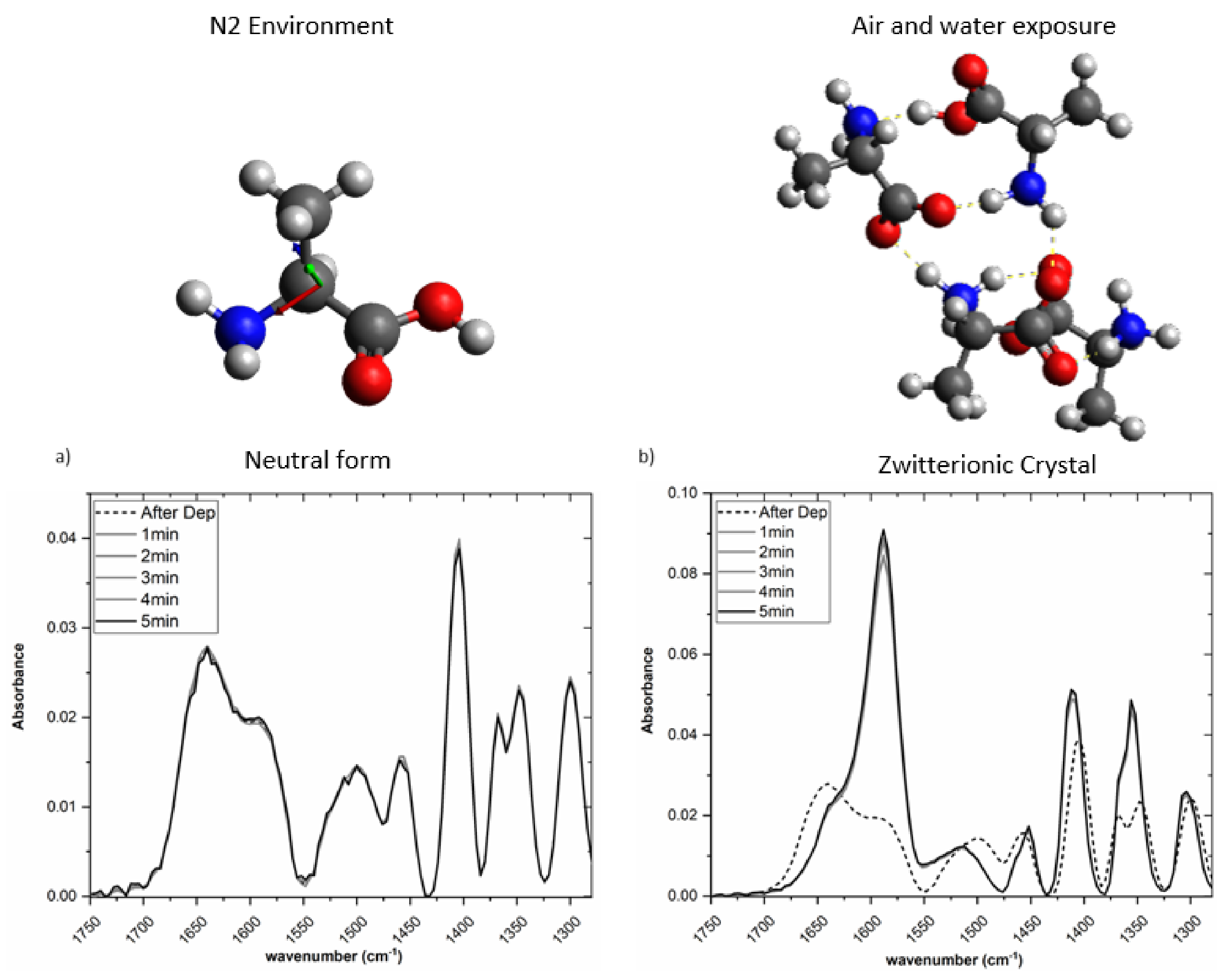

Figure 1: Alanine exposure experiment at FUB. Left: Alanine thin films in fully purged nitrogen environment several minutes after deposition. Right: Similar samples, but air exposed after deposition.

ical modelling methods, to simulate the behavior and spectroscopic changes of amino acid thin films upon air exposure. Quantum chemical calculations will allow for accurate predictions of molecular structures, electronic properties, and vibrational spectra. The obtained spectroscopic signatures from the quantum chemical modelling will be compared with experimental observations to validate the proposed hypothesis. This analysis will provide insights into the mechanisms underlying the changes induced by air contamination in amino acid thin films.

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https://www.physik.fu-berlin.de/en/einrichtungen/ag/ag-elsaesser/index.html

More Information

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