Ion-Molecule Reactions in Astrochemistry and the Study of Degradation Mechanisms of Space-Technology Materials

Nandana Pattathadathil, Daniela Ascenzi, Paolo Tosi, Luca Matteo Martini

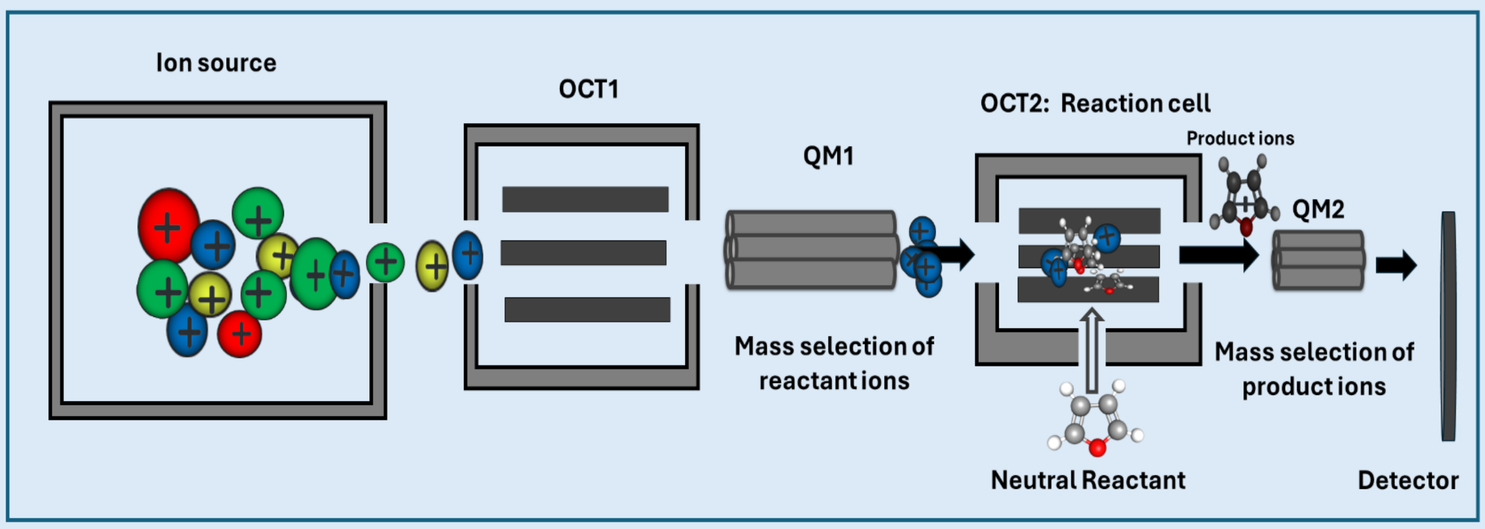
University of Trento, 39th cycle National PhD Program for Space Science and Technology

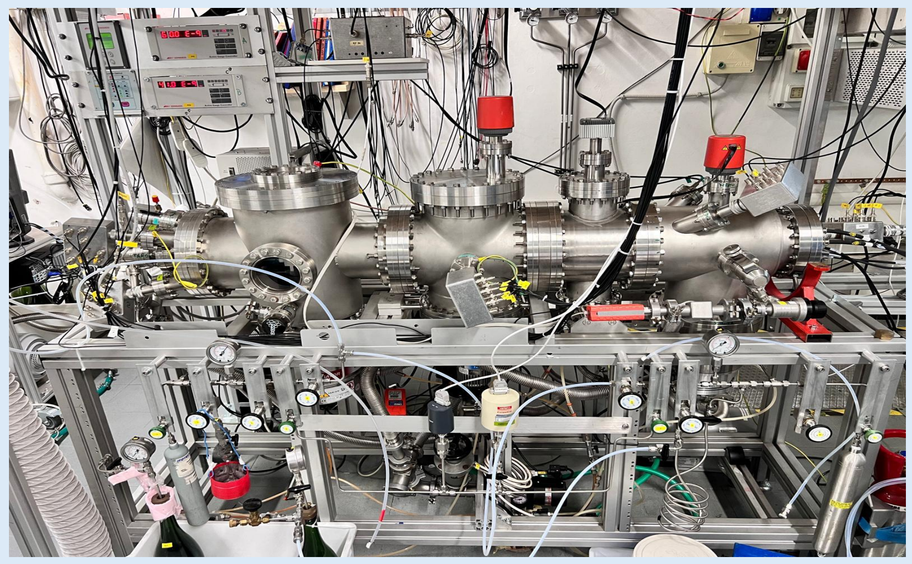
Abstract ID :248

Introduction

Polymers play a vital role in the aerospace industry, yet their vulnerability to atomic and ionic oxygen in space presents a significant challenge. Ground-based tests have confirmed that prolonged exposure in low Earth orbit (LEO) leads to degradation of the material. Protective measures have been explored, but a comprehensive understanding of the erosion mechanisms is lacking. In this project, we introduce a novel approach to delve into the chemical erosion caused by atomic oxygen ions (IO) at the molecular level. By deconstructing polymers into molecular moieties and subjecting them to single collision experiments, we aim to elucidate the underlying forces governing chemical attacks. Specifically, we will investigate reactions with the most representative moieties for the polymers, polystyrene, Kapton H and graphite. Our experimental setup, guided-ion-beam mass spectrometry(GIB-MS), will provide insights into reactive cross sections and product branching ratios. This pioneering endeavor marks the first comprehensive effort to address polymer erosion in space, with potential implications for aerospace materials science

Experimental Setup : GIB-MS & Methodology





Electron ionization ion source

- Two rhodium-tungsten filaments are placed in small compartments, and they emit electrons by thermionic effect.
- A cylindrical grid is placed and kept at a positive potential relative to the filament and in the region of the cylindrical grid Ions are created by the interaction between neutral particles and ionizing electrons.
- **We will use CO_2 as the precursor gas to produce O^+ ions, since using O_2 can reduce the lifetime of the filaments in the source [4]**

Quadrupole mass analyzer & Octopole ion beam guide

- Quadrupole mass analyzers are mass filters that allow only ions of a certain mass-to-charge ratio to pass.
- Electric fields create a stable path for ions of a certain m/z ratio so that only ions within a narrow mass region can pass through the device.
- RF electric potentials applied in opposite phases to alternate rods produce an inhomogeneous field to creates an effective radial potential well in the octopole

The Trento GIB-MS allow us to study the ion neutral reactions such as:

$$A^+ + B \longrightarrow P_i^+ + N_i$$

By measuring the **integral absolute reactive cross section** (σ_{ECM}) :

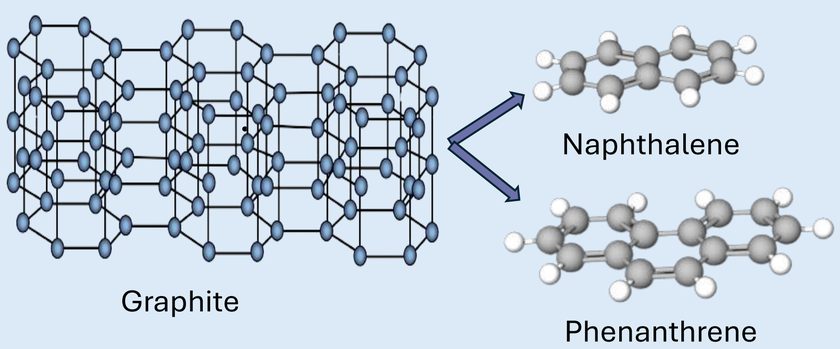
$$I(P_i^+) = I_0\left(1 - e^{-l.\sigma_i.n}\right)$$

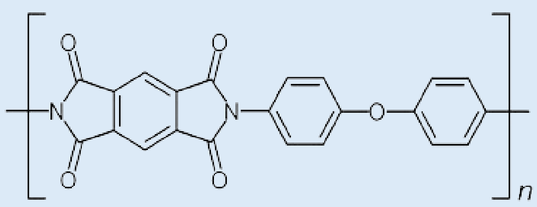
And **branching ratios (B.R)** for the products:

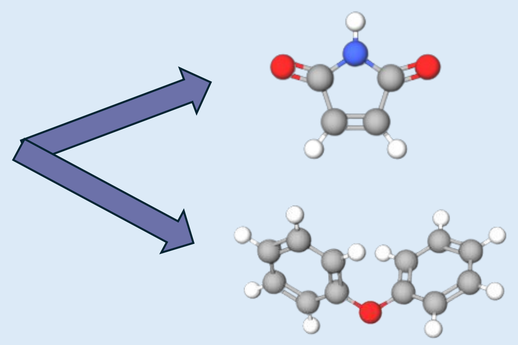
$$\text{B.R}(P_i^+) = \frac{P_i^+}{\sum_i P_i^+}$$

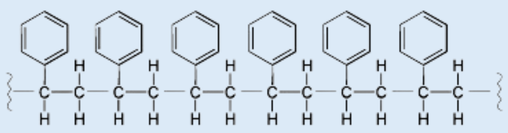
Research Objectives

Reactivity of O^+ ions with the small molecular building blocks of space technology polymers like graphite, polystyrene, Kapton H









- By measuring σ_{ECM} and branching ratios elucidate the mechanisms of chemical attack by O+ ions on space-technology polymers.
- Identify the specific vulnerable portions of polymer structures through single collision experiments.

References

1. Belic, D. S., Urbain, X., & Defrance, P. (2015). Electron-impact dissociation of ozone cations to O+ fragments. Physical Review A, 91(1), 012703.
2. Armentrout, P. B. (2000). Kinetic energy dependence of ion–molecule reactions: guided ion beams and threshold measurements. International Journal of Mass Spectrometry, 200(1-3), 219-241.
3. Gerlich, D. (2004). Applications of rf fields and collision dynamics in atomic mass spectrometry. Journal of Analytical Atomic Spectrometry, 19(5), 581-590.
4. Fishman, V. N., et al. "Selected Ion Flow Tube Studies of the Atomic Oxygen Radical Cation Reactions with Ethylene and Other Alkenes.
5. Doctoral Thesis of Andrea Cernuto
6. Caraiman, D., & Bohme, D. K. (2002). Periodic trends in reactions of benzene clusters of transition metal cations, M (C6H6) 1, 2+, with molecular oxygen. The Journal of Physical Chemistry A, 106(42), 9705-9717.

Acknowledgements

- This poster was produced while attending the PhD program in PhD in Space Science and Technology at the University of Trento, Cycle XXXIX, with the support of a scholarship financed by the Ministerial Decree no. 118 of 2nd march 2023, based on the NRRP - funded by the European Union - NextGenerationEU - Mission 4 "Education and Research", Component 1 "Enhancement of the offer of educational services: from nurseries to universities" - Investment 4.1 "Extension of the number of research doctorates and innovative doctorates for public administration and cultural heritage"

- Part of the research presented in the poster will be carried out within the National Recovery and Resilience Plan (NRRP), Mission 4, Component 2, Investment 1.1, Call for tender No. 1409 published on 14.9.2022 by the Italian Ministry of University and Research (MUR), funded by the European Union – NextGenerationEU– Project Title P20223H8CK "Degradation of space-technology polymers by thermospheric oxygen atoms and ions: an exploration of the reaction mechanisms at an atomistic level" - CUP E53D23015560001.