Europlanet TA Scientific Report

PROJECT LEADER

Project number: 22-EPN3-053
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TA Facility visited: TA2.12 ECRIS Laboratory, HU

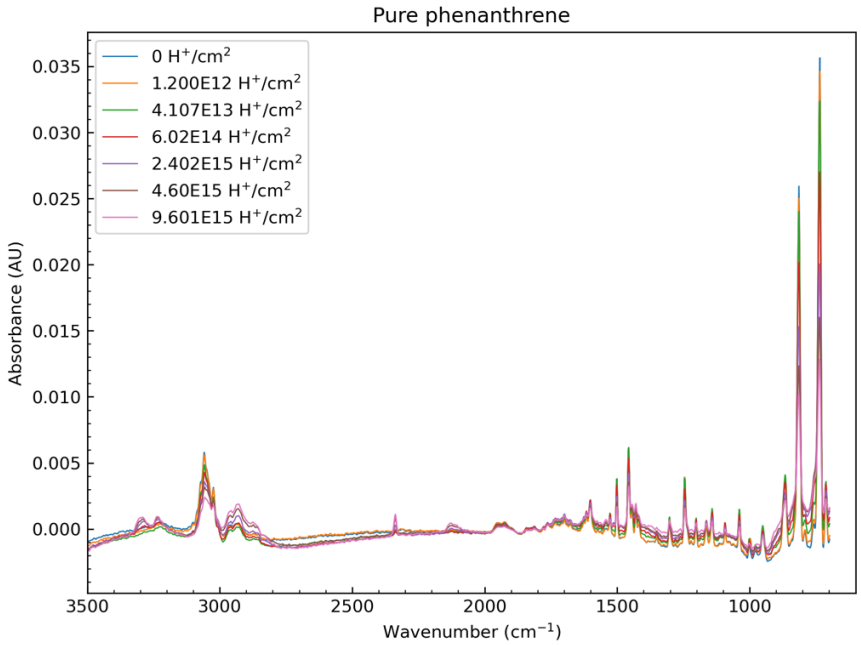
Project Title: *Proton processing of phenanthrene ice mixtures for application to Titan's lower atmosphere.*

Scientific Report Summary.
(plain text, no figures, maximum 250 words, to be included in database and published)

During this TNA visit, the three-ring PAH phenanthrene ($C_{14}H_{10}$), acetonitrile (CH_3CN) and their 1:1 mixture were irradiated using 10 KeV protons. The subsequent products of this processing were then measured using infrared spectroscopy (5000-700 cm^{-1}) and a quadrupole mass spectrometer. The aim of these experiments was to investigate 1) if energetic processing can modify the structure of solid hydrocarbons and 2) if proton irradiation could trigger the formation of new species. As a result of the TNA visit, we collected infrared spectra of at different proton fluences and then following this, infrared spectra during temperature-programmed desorption (TPD). We also obtained the residues after TPD for ex-situ analysis. The preliminary results show a) the puckering of phenanthrene solid, b) the formation of ethanimine (C_2H_5N) in acetonitrile solid, c) a complex behaviour of the 1:1 mixture, with puckering and formation of new hydrocarbon species.

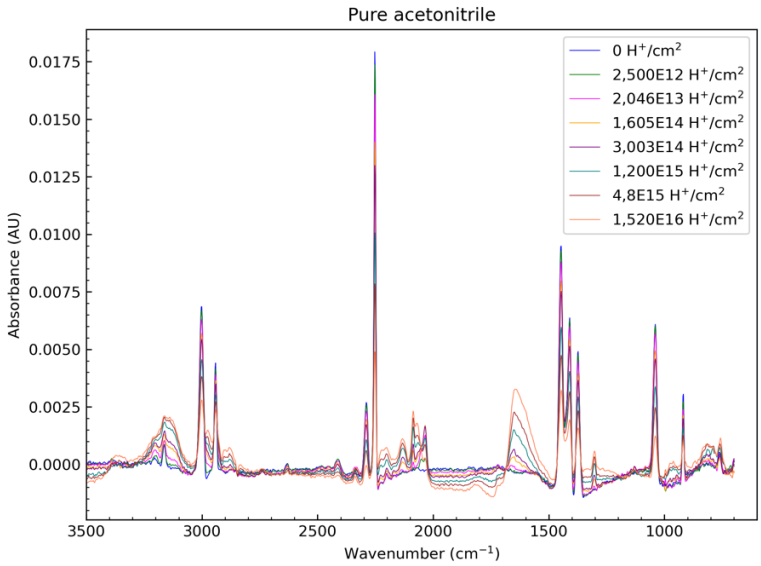
Full Scientific Report on the outcome of your TNA visit

During this TNA visit, the three-ring PAH phenanthrene ($C_{14}H_{10}$), acetonitrile (CH_3CN) and their 1:1 mixture were irradiated using 10 KeV protons. Acetonitrile was chosen as a substitute of HCN as a C=N containing molecule abiding laboratory safety rules. The subsequent products of this processing were then measured using infrared spectroscopy (4000-700 cm^{-1}) and a quadrupole mass spectrometer. The aim of these experiments was to investigate 1) if energetic processing can modify the structure of solid hydrocarbons and 2) if proton irradiation could trigger the formation of new species. The first day was started with deposition of phenanthrene, using the molecular evaporator, onto a 20 K window and then it was irradiated by 10 KeV protons. The irradiation was increased in steps with the infrared spectrum being taken after each. Once completed, the sample was linearly heated at a rate of 1 K/minute with a spectrum taken every 10 K to follow the evolution of the temperature increase and when molecules desorb from the surface. The IR spectra of the irradiated phenanthrene at different fluences are shown in the figure below.



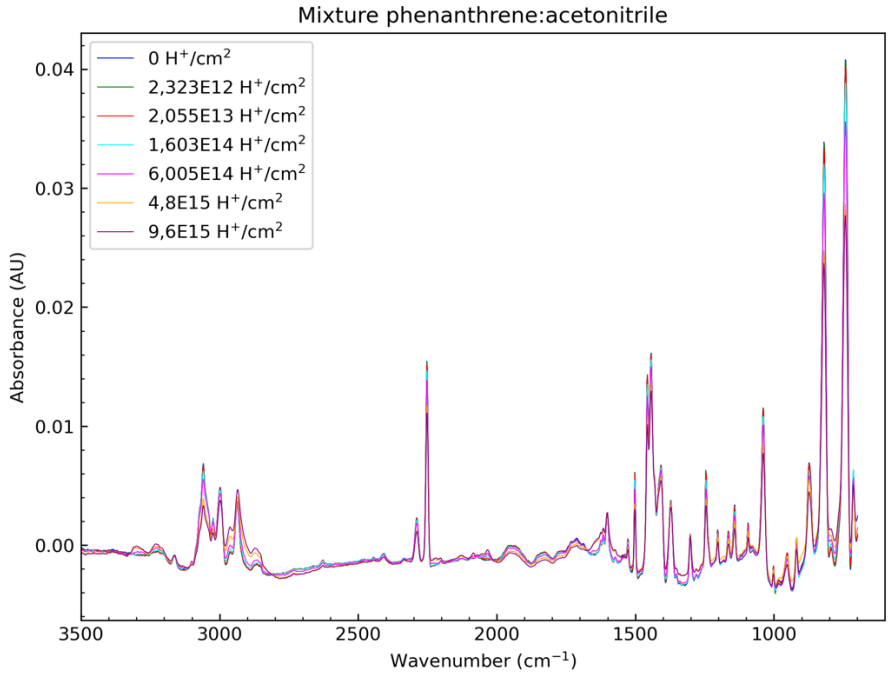
As phenanthrene is irradiated the amount of phenanthrene on the surface decreases as seen by the decreasing of the typical vibration bands of the molecule. The C-H out-of-plane bending modes at 810 and 735 cm^{-1} show a faster decrease with respect to the C-H stretch modes at 3000-3100 cm^{-1}. We preliminary interpret that as the result of "puckering" or compactification of the solid. Few bands – at 3300, 2900 and 2100 cm^{-1} – seem to gain strength upon irradiation. While the 3300 and 2100 cm^{-1} bands are likely due to water contamination, the 2900 cm^{-1} might be the result of additional H attaching to the phenanthrene, leading to the formation of aliphatic bonds. Additional work on background subtraction is needed to confirm this last assignment.

The same experiment was performed on acetonitrile. Below is a figure that shows the changes of irradiation for this ice.



The IR spectra of acetonitrile at different fluences show the expected decrease of the acetonitrile bands and the formation of new bands. The strongest one is at 1650 cm^{-1} and we preliminary assign it to the formation of ethanimine (CH_3CHNH). Analysis of the data is still ongoing and the routes of formation of the molecules shown in these spectra are being formulated.

The IR spectra of the 1:1 mixture of acetonitrile and phenanthrene upon irradiation is displayed below. There are a couple of minor bands appearing (e.g. around 2850 cm^{-1}), but the general behaviour suggests that phenanthrene might protect acetonitrile, quenching the formation of new molecules. A detailed analysis of the pure ices is fundamental to understand the behaviour of the mixture and it is underway.



- Give details of any publications arising/planned (include conference abstracts etc)

Planned to publish findings but still in early stages. It will form a significant part of a PhD thesis.

- Host confirmation

Please can hosts fill in/check this table confirming the breakdown of time for this TA project:

Dates for travel to accommodation for TA visit (if physical visit by applicant)	Start Date of TA project at facility	Number of lab/field days spent on TA Visit pre-analytical preparation	Number of days in lab/field site for TA Visit	Number of days spent in lab for TA Visit data analysis	End Date of TA project at facility	Dates for travel home (if physical visit by applicant)
Departed: 03-03-2024 Arrived: 03-03-2024	04-03-2024	0	5	0	08-04-2024	Departed: 08-04-2024 Arrived: 08-04-2024

Two visitors: Alessandra Candian and Annemieke Petrignani

The host is required to approve the report agreeing it is an accurate account of the research performed.

Host Name	**Dr. Zoltán Juhász / Atomki**
Host Signature	
Date	**15-04-2024**

- Project Leader confirmation

Do you give permission for the full version of this TA Scientific Report (in addition to the 250 word summary) to be published by Europlanet 2024 RI on its website and/or public reports? YES

Project Leader Name	**Dr. Alessandra Candian / UvA**
Project Leader Signature	
Date	**16-04-2024**