Report on the outcomes of a presentation and participation -

Inclusiveness Target Countries Conference[1]

Action number: "COST Action CA21126 – Carbon molecular nanostructures in space (NanoSpace)"

Grantee name: Boutheïna KERKENI

Conference Details

Conference title: 8th Workshop on Physical and Chemical processes of astrophysical interest: astrochemistry in the JWST era

Conference web-page: https://ipag.osug.fr/~faurea/stflorent/

Conference venue[2]: Saint Florent, Corsica, France

Conference start and end date: 08/06/2025 to 13/06/2025

Accepted contribution details

Title of the presentation: Unravelling the Reaction Mechanisms of CN and CCH with H_2CS: Implications for Sulphur Chemistry in the ISM

Co-authors: G. Ouerfelli, F. Dayou, C. Balança, and N. Feautrier

Other details of the presentation: specify here any additional details related to the contribution (e.g. title of the session / track of the conference programme in which the contribution is accepted)

Outcome of the conference participation

My oral presentation, entitled *"Unravelling the Reaction Mechanisms of CN and CCH with H_2CS: Implications for Sulphur Chemistry in the ISM"*, focused on the gas-phase formation of HCSCN and HCSCCH via radical–radical reactions and their relevance to the sulfur chemistry of dark molecular clouds, particularly TMC-1. The topic was well received, particularly for its connection to recently detected sulfur-bearing molecules, its potential relevance for interpreting future data from JWST, and its contribution to addressing the long-standing **"missing sulfur" problem** in interstellar chemistry.

The presentation allowed me to showcase the robustness of quantum chemical modeling in uncovering feasible reaction pathways and to emphasize the importance of including such reactions in astrochemical networks. The reactions presented stimulated discussion among

[1] This report is submitted by the grantee to the Action MC for approval and for claiming payment of the awarded grant. The Grant Awarding Coordinator coordinates the evaluation of this report on behalf of the Action MC and instructs the GH for payment of the Grant.
[2] For an online conference, specify virtual participation; for hybrid conferences, specify whether it is an in-person or virtual participation.

participants, and several colleagues expressed interest in the energetics and kinetic modeling aspects of my work.

Most notably, this conference facilitated new collaborative perspectives. I initiated aconcrete scientific connection:

- With **Dr. Francesca Tonolo** (Université de Rennes), we are planning to work together on **solving the master equation for complex reaction networks**, in order to obtain more accurate kinetic parameters under interstellar conditions. This collaboration will combine our expertise in theoretical chemistry and chemical kinetics, and aims to strengthen the reliability of rate coefficients used in astrochemical models.

Beyond these collaborations, the workshop provided the chance to engage with researchers working on complementary aspects of astrochemistry, including laboratory surface experiments and observational data interpretation. Although no formal projects were established with others at this time, the scientific exchange was stimulating and broadened the context of my work.

In summary, my participation enhanced the visibility of my research and laid the groundwork for promising future collaborations. It also allowed me to integrate my ongoing computational studies within broader observational and experimental frameworks relevant to sulfur chemistry in space.

Acknowledgement of inclusion of necessary supporting documents to claim the grant

I confirm that the following documents have been uploaded on e-COST as an integral part of this report:

- the certificate of conference attendance.

- the programme of the conference or book of abstracts / proceedings indicating the presentation (oral) of the grantee.

- copy of the given presentation (oral).