Report on the outcomes of a Short-Term Scientific Mission[1]

Action number: CA21126

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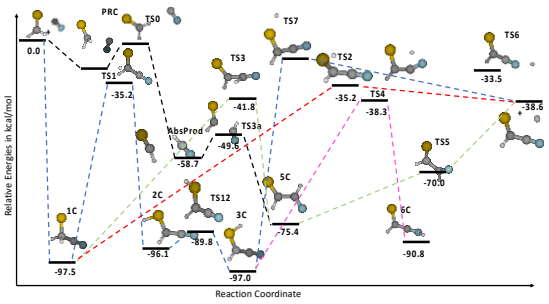
Details of the STSM

Title: **Formation and destruction of sulfur molecules in the interstellar medium**

Start and end date: 04/12/2023 to 14/12/2023

Description of the work carried out during the STSM

During this visit we have investigated in detail the possible reaction paths leading to the formation of the HCSCN molecule. We have identified a complex reaction mechanism involving several reaction-paths, and have computed all the transition states and reaction intermediates using DFT methodologies (wB97XD/6-311++G(d,p)). Our calculations show that the mechanism can occur without a reaction barrier which makes the mechanism energetically favourable at the low temperatures where HCSCN is detected. Currently we are employing MP2/aug-cc-pVQZ for geometry optimisations and frequency calculations, and CCSD(T) with the same basis set to retrieve accurate single point energies on the optimised structure. Calculations of the minimum energy paths and the potential energy V(R) of the very first step leading to the formation of CH2S+CN → CH2SCN are currently underway with the MP2/aug-cc-pVQZ model chemistry, which will be necessary for the capture theory rate constants calculations as a second step of this project.



[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.

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Description of the STSM main achievements and planned follow-up activities

Given the complexity of the reaction mechanisms encountered in the formation of the recently observed HCSCN molecule, during this STSM visit we were not able to investigate the other reactions such as S + CH2CN, nor the two ones leading to HCSCCH molecule. The current results are already of great interest and once MP2 and CCSD(T) calculations are terminated a very accurate picture of these reaction mechanisms can be used in astrochemical models, the subsequent computation of the reaction rate constants will provide an analytical function of temperature useful for Astronomers. A peer-review paper is planned as a result of the current project.

In the future we plan to tackle the remaining reactions separately as preliminary investigations have shown that they are also complex and exhibit several reaction paths like the one studied in this visit towards the formation of S + CH2CN → HCSCN + H , H2CS + CCH → HCSCCH, and S + CH2CCH → HCSCCH + H.

The extension of the calculations on the grain models will be of great interest to the astrochemical community.

The project will allow to develop a general computational procedure capable to predict energetics and kinetic data of paramount to astrochemical modelling. The importance of sulphur chemistry in astrophysics is timely as these molecules HCSCN and HCSCCH are precursor to biological molecules and research in this field is still incomplete. We will provide database for reaction properties for the current project and will investigate in the future as a continuation reaction mechanisms involving dust grains such as graphitic materials and probe their catalytic effects.

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