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MD-GAS
Molecular Dynamics in the GAS phase

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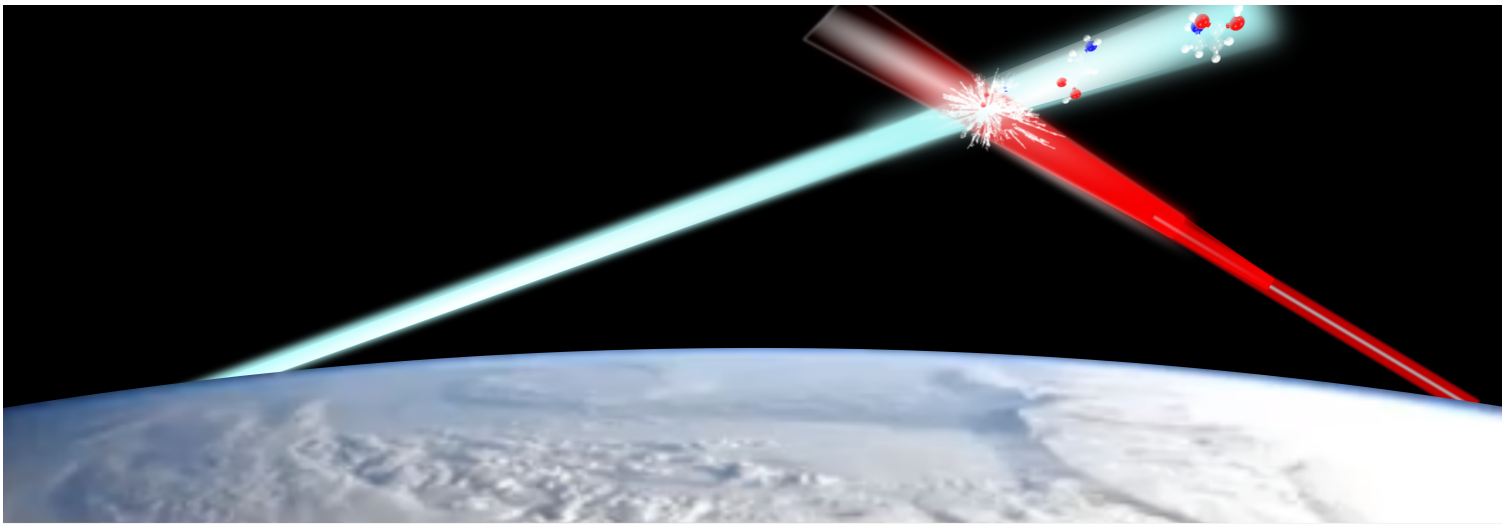
EUROPEAN COOPERATION IN SCIENCE & TECHNOLOGY

Working Group 1 & Working Group 2
Online Meeting

Book of Abstracts

15th-19th March 2021



MD-GAS COST ACTION

Molecular Dynamics in the Gas Phase

PROGRAM

Monday 15th March

Session 1 Chair: A. Cartoni

9:00 – 9:45 **T01 - Connection between cosmic rays, clouds and climate**
Henrik Svensmark……11

9:45 – 10:15 **T02 - Sunlight-Induced Nonadiabatic Dynamics of Atmospheric Molecules**
Basile Curchod……12

10:15 – 10:45 Meet the Speaker

10:45 – 11:00 Coffe break

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Mikael Ehm……13

11:30 – 12:00 **T04 - Competitive dehydrogenation and backbone fragmentation of super-hydrogenated PAHs**
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12:00 – 12:15 **T05 - Electron interactions with R134a (CF_3CH_2F) refrigerant gas**
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David Ayuso……27

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12:30 – 12:45 Meet the Speaker
E. R. Molina – P. Herczku – D. Ayuso

12:45 – 13:00 Meet the Speaker
D. Gupta – T. Luxford – H. Velásquez

13: 00 – 14:00 Networking Social Meeting

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Prince Tiwari……39

12:30 – 13:00 Meet the Speaker

TEMPERATURE INDUCED CYCLISATION MECHANISMS IN LINEAR DIPEPTIDES

L. Carlini[1], J. Chiarinelli, M. C. Castrovilli, G. Mattioli, E. M. Bauer, A. De Stefanis, V. Valentini, P. Bolognesi, L. Avaldi

CNR-Istituto di Struttura Della Materia (CNR-ISM), Area della Ricerca di Roma 1, Monterotondo Scalo, Italy

The linear (**ℓ-**) and cyclic (**c-**) dipeptides are prototype peptidesand may have played a key role in the origin of life [1]. Among the several processes that can induce the rearrangement of dipeptides from the **ℓ-** to the **c-**structure, the temperature is one of the least investigated and characterised. Nevertheless, understanding these temperature induced processes is crucial in several areas, from the synthesis of small molecules in the astrochemical harsh environment [2] to the development of innovative preparation methods of nanomaterials [3], as well as for practical purposes, such as the production of effusive beams for spectroscopic studies [4]. In this work we have investigated several **ℓ-** and **c-**dipeptides under controlled temperature and UHV conditions in a dehydrated environment, *i.e.* mimicking abiotic and hostile conditions in space. We combined Time-Of-Flight Mass Spectrometry (TOF-MS) in gas-phase with Thermogravimetric Analysis (TGA), Infrared (IR) and Raman spectroscopies in condensed phase. The observation that the mass spectra of **ℓ-**dipeptides contain features typical of both the **ℓ-**and **c-**structures [5], suggests that cyclisation may happen at some stage of the experimental procedure, driven by either the temperature, by the 'electrostatic forces' in the unstable zwitterion during sublimation or in the gas phase due to a fast rearrangement of the cation. In the case of L-Phenylalanyl-L-Alanine (PheAla), combining several experimental approaches and theoretical calculations, we provide evidences that an irreversible cyclisation mechanism driven by temperature happens in the condensed phase under UHV conditions. This process, that turns the fragile **ℓ-** into the more stable **c-**structure, does not require the presence of activating agents, chemical precursors or water molecules, and may have provided an effective channel protecting the peptides for the emergence of life in harsh chemico-physical conditions, as the hostile astrochemical environment.

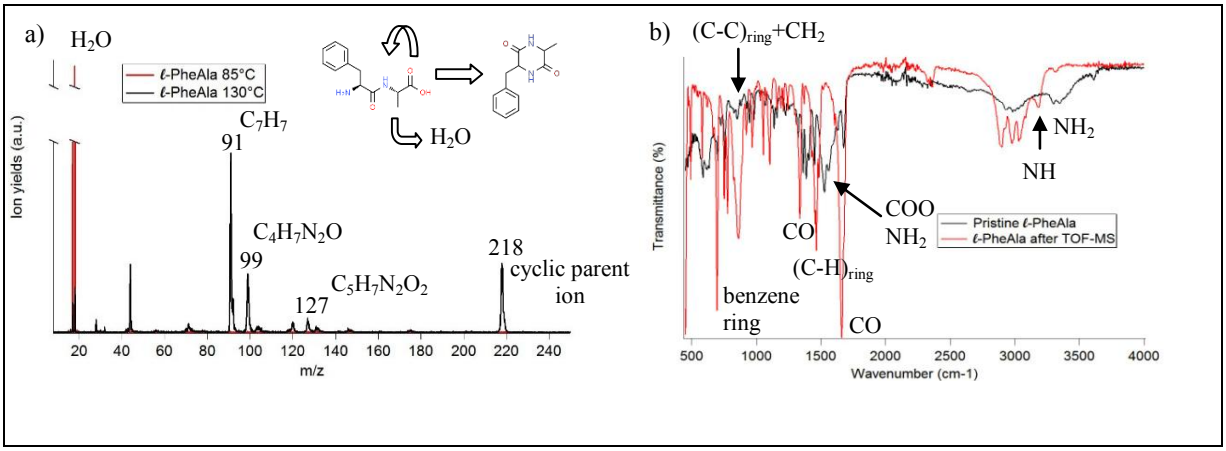

***Figure 1**: a) ℓ-PheAla mass spectra at 85 °C (red line) and after the sublimation at 130 °C (black line) measured at 21.22 eV incident radiation. b) Comparison between IR spectra measured at room temperature (RT) on pristine ℓ-PheAla (black curve) and on the sample residual in the crucible used for MS experiments (red curve), after sublimation at 130 °C for 24 h.*

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