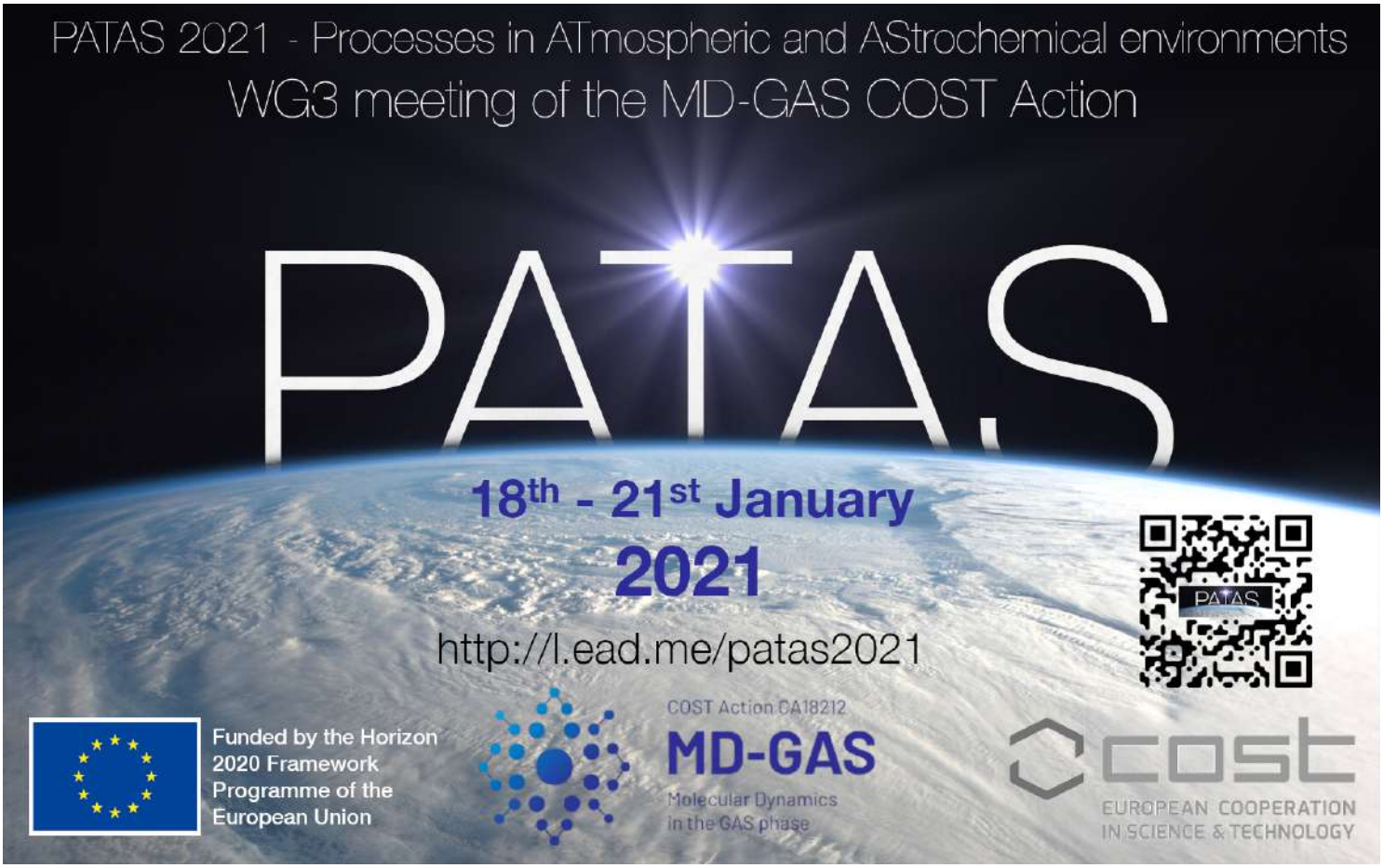
Book of abstracts
PATAS 2021



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MASS SPECTROMETRY AND INFRARED STUDIES ON DIPEPTIDES REVEAL AN EFFECTIVE (AND NON-CHEMICALLY ACTIVATED) CYCLISATION MECHANISM IN ABIOTIC CONDITIONS

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The linear (ℓ-) and cyclic (c-) dipeptides, being the simplest prototype peptides, are the building blocks of proteins and enzymes, and determine their structures and functions. Moreover dipeptides may have played a key role in the origin of life [1,2]. Among the several processes leading to the structural rearrangement of dipeptides from the ℓ- to the c- structure, the role of the temperature is the least investigated and characterized. Nevertheless, it may be crucial in the astrochemical harsh environment as well as in the sublimation used in the laboratory to produce effusive molecular beams for photoemission (PES and XPS) and mass spectrometry (MS) measurements [3,4]. In this work we combine gas-phase studies of ℓ- and c-dipeptides by means of Time-Of-Flight Mass Spectrometry (TOF-MS) with Thermogravimetric Analysis (TGA), Infrared and Raman spectroscopies in condensed phase to investigate temperature induced peptide bond formation and disruption. Theoretical calculations have been implemented to simulate the IR spectra of ℓ- and c- dipeptides, which were used to predict and identify the vibrational frequencies that witness changes in the chemical structure of the sample. The experimental results and theoretical predictions provided evidences that, at least in some ℓ-dipeptides, an irreversible cyclisation mechanism driven by temperature does happen in the condensed phase under UHV conditions. This mechanism does not require the presence of activating agents, chemical precursor or liquid water. Thus, it may occur spontaneously over the different periods of time and physico-chemical conditions experienced by comets and carbonaceous chondrites [5,6]. The process proves to be a "clever" reaction cycle from ℓ- to c-structure that preserves the aminoacid sequence for further peptide evolution.

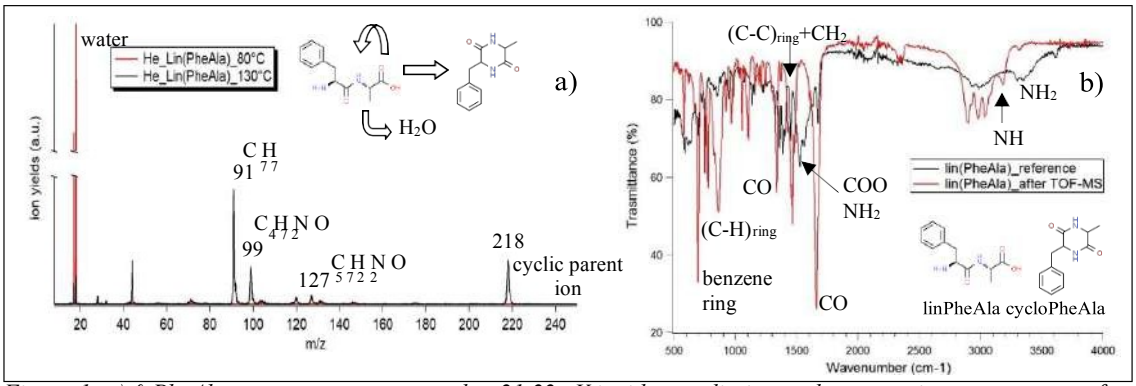

Figure 1: a) ℓ-PheAla mass spectra measured at 21.22 eV incident radiation and evaporation temperature of 80°C (red line) and 130°C (black line). b) Comparison between IR spectra at room temperature (RT) performed on the pristine ℓ-PheAla (black line) and on the sample residual in the crucible used for MS experiments, after sublimation at 130°C for 24 h (red line).

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References

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