COMPUTATIONAL SPECTROSCOPIC SIGNATURES OF PROTEINOGENIC GLUTAMIC ACID AND ITS ISOMERIC SPECIES OF ASTROPHYSICAL IMPORTANCE

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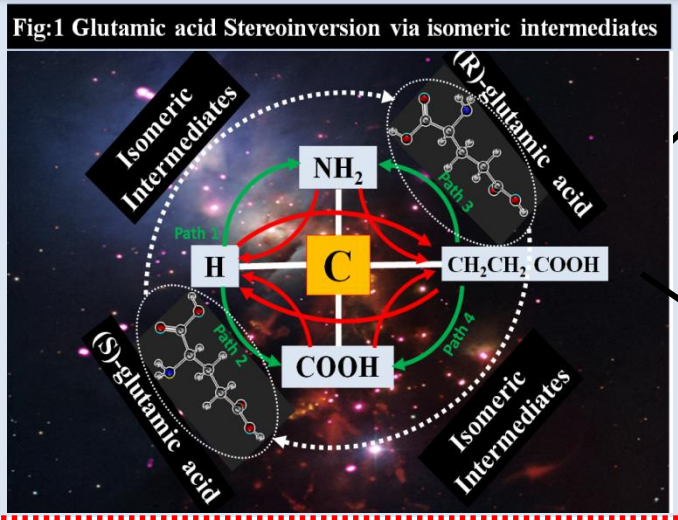
Fig:1 Glutamic acid Stereoinversion via isomeric intermediates



Rotational Spectroscopy

Rotational Parameters

A_e, B_e & C_e

A_0, B_0 & C_0

χ_{aa} χ_{bb} & χ_{cc}

μ_a, μ_b & μ_c

Δ_J, Δ_K, Δ_{JK}, δ_J & δ_K

Vibrational Spectroscopy

Fundamental vibrations

ν_{anharm} : anharmonic frequency

I_{anharm} : anharmonic intensity

Quartic and cubic force fields

second order vibrational perturbation theory **(VPT2)**

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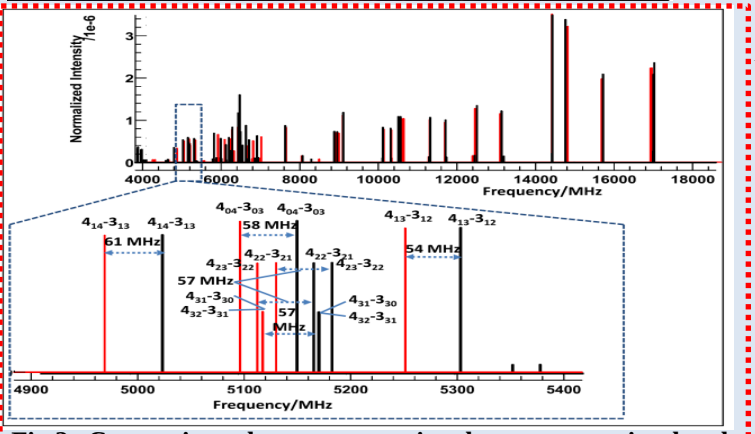

Fig.2 Comparison between rotational spectrum simulated through experimental parameters (depicted with red lines), and computed parameters.

Gas-phase rotational constants from Fourier transform laser-ablation microwave experiment (Literature)

Compared

Computed rotational constants for global minimum conformer of Glutamic acid

MP2/ 6-311++G(d,p)

This work provides valuable spectroscopic data for any endeavour (telescopically or laboratory based experiment) towards the detection of proteinogenic Glutamic acid and isomeric species of diverse chemistry related to its stereoinversion in outer space.

Computed Vibrational bands

Compared

Gas-Phase experimental vibrational spectra (Literature)

B3LYP-D3(BJ)/SNSD

Potential Energy Distribution (PED) Analysis of fundamental vibrational bands for all the isomeric species using VEDA

Scaling of Rotational Constants for all the isomeric species

Rotational Line Database generated for all the isomeric species using PGOPHER