Formation of 3-Pyrolline in Interstellar Space: A Computational Study

A. Pandey,[1] A. Pathak,[2] and K. A. P. Singh[2]

[1]*Department of Physics, Institute of Science, Banaras Hindu University, Varanasi, India*

[2]*Department of Physics, Institute of Science, Banaras Hindu University, Varanasi, India*

Complex organic molecules (COMs) are thought to form on icy dust grains in the earliest phase of star formation. Interstellar detection of the straight-chain (n-propyl cyanide, n−C_3H_7CN) and branched-chain (i-propyl cyanide, i−C_3H_7CN) molecules toward the star-forming region, Sgr B2(N2) has attracted attention to study the formation mechanism of COMs [1]. The first detection of COM strongly hints the existence of other linear and ring-shaped molecules, which are prebiotic and building block of proteins.

Through computational methods, we suggest new possible formation and destruction pathways of branched aliphatic molecule to aromatic compounds in space. We computed binding energy, enthalpies of formation of several species. We also calculate the kinetic data of reactions and other spectroscopic information in order to understand the chemical evolution and formation of aromatic compounds to be present in the Interstellar medium (ISM).

References

[1] A. Belloche, R.T. Garrod, H.S.P. Müller, K.M. Menten,Sci. 345, 158 (2014)

[2] E.E. Etim, P. Gorai, Das. Ankan, E. Arunan, Eur. Phys. J. D (2017) 71: 86

[3] F. J. Lovas, J. M. Hollis, Anthony J. Remijan,P. R. Jewell,The Astrophysical Journal, 645: L137–L140, 2006 July 10

[4] J. Cernicharo1 , N. Marcelino, M. Agúndez , C. Bermúdez , C. Cabezas , B. Tercero , J. R.Pardo, A&A 642, L8 (2020)

[5] R. T. Garrod, A. Belloche, H. S. P. Müller, K. M. Menten , A&A 601, A48 (2017)