October 29, 2021

Dear Editorial Committee,

We are writing to submit our manuscript, “Isomerization of Hydrogen Cyanide and Hydrogen Isocyanide in a Cluster Environment: Quantum Chemical Study”, for consideration for publication in the Journal of Chemical Physics, Special Issue: JCP Emerging Investigators Collection. I am the primary author and completed my PhD in June 2013.

This paper aims to shed light on the chemistry and isomerization processes in ionized HNC clusters in conditions relevant to the interstellar medium (ISM), which are thus far not completely deciphered.

The manuscript shows that, using quantum chemistry and *ab-initio* molecular dynamics, HNC-to-HCN isomerization occurs extensively in the HNC cluster after ionization. This extensive isomerization contrasts with results from ionized HCN clusters, where HCN-to-HNC isomerization is only observed in large clusters (larger than pentamers). We analyze the energetics of the clusters in terms of the intermolecular hydrogen bonds and stability of the different isomers to explain the observed isomerization trends. Additionally, we suggest a barrierless formation route for diaminonitrile, a known precursor of amino acids and nucleobases.

We believe that the results presented in this manuscript will be of interest to the scientific community in several fields, including chemistry, astronomy, and astrobiology, and we hope that you will find it suitable for publication in the JCP Emerging Investigators Collection.

We confirm that this manuscript has not been previously published and is not currently under consideration by any other journal.

Sincerely,

Dr. Tamar Stein

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