29/10/2021

Dear Editorial Committee,

We are writing to submit the manuscript titled “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. My PhD graduation date is 06/2013.

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

The manuscript shows using quantum chemistry and ab initio molecular dynamics that HNC-to-HCN occurs extensively in the HNC cluster after ionization. The extensive isomerization contrasts with results in ionized HCN clusters, where HCN-to-HNC isomerization is only observed at large clusters (larger than pentamer). 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 route for diaminonitrile, a known precursor of amino acids and nucleobases, to form.

We believe that the results presented in this manuscript will be of interest to the scientific community in several fields, such as chemistry, astronomy and astrobiology, and we hope that you will find it suitable for publication in 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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