23.02.2020

Dear Prof. XXX

We wish to submit the manuscript titled “Ab Initio Molecular Dynamics Reveals Formation Path of Benzonitrile and Other Molecules in Conditions Relevant to the Interstellar Medium.”

In the above manuscript, we wish to contribute to understanding a long-standing scientific puzzle, namely the formation of aromatic molecules in the interstellar medium (ISM). While the presence of aromatic molecules in the ISM is well established, their astronomical detection is extremely challenging. Only recently, benzonitrile molecule was detected in Taurus Molecular Cloud using its hyperfine spectra. (Science, 2018. **359**(6372))

Although benzonitrile has been observed – the molecular mechanism for its formation is still unknown.

In the manuscript, we show by means of quantum chemistry and *ab-inito* molecular dynamics that upon ionization of van der Waals clusters containing acetylene and cyanoacetylene — some of the building blocks found in Taurus Molecular Cloud-1 — the formation of benzonitrile cation emerges naturally. Based on the *ab-inito* molecular dynamics, we can study the potential energy surface that leads to its formation.

Moreover, our result shows that benzonitrile is only one of the molecules forms upon ionization of the cluster. A large variety of molecules are being formed, and we predict other aromatic molecules' formation. We anticipte that these predictions will help guide astronomers in the future search for additional aromatic molecules in the ISM

We believe that the result presented in this manuscript will interest scientists from several scientific fields, such as chemistry, astronomy and astrobiology, and hope you will find it suitable for publication in PNAS.

Best regards,

Dr. Tamar Stein

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