23.02.2020

Dear Prof. XXX,

We are writing to submit the manuscript entitled “Ab Initio Molecular Dynamics Reveals Formation Path of Benzonitrile and Other Molecules in Conditions Relevant to the Interstellar Medium” for consideration for publication in PNAS.

In this paper, we seek 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, the benzonitrile molecule was detected in Taurus Molecular Cloud-1 using its hyperfine spectra (*Science*, 2018. **359**(6372)).

Although the presence of 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 initio molecular dynamics, that upon ionization of van der Waals clusters containing acetylene and cyanoacetylene — some of the building blocks found in the Taurus Molecular Cloud-1 — the formation of benzonitrile cations occurs naturally. Applying ab initio 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 that form upon ionization of the cluster. A large variety of other molecules are also formed, and we predict other aromatic molecule formation. We anticipate that these predictions will help guide astronomers in searching for additional aromatic molecules in the ISM

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

Sincerely,

Dr. Tamar Stein

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