CALIFORNIA STATE SCIENCE FAIR
2013 PROJECT SUMMARY

Name(s)

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Project Number

S0604

Project Title

A Computational Investigation of the Structures, Energies, and Formation Pathways of Interstellar Anions

Abstract

Objectives/Goals

About 130 neutral and about a dozen positively-charged molecules have been discovered in space (the most abundant of which include H3+, CO+, N2H+, CH5+, etc). However, only recently did National radio Astronomy Observatory (NRAO) discover the butetraynyl (C4H-), hexatetraynyl (C6H-), and octatetraynyl (C8H-) anions in interstellar space. The presence of these molecules has been paradoxical to astronomers because it has long been thought that large negatively charged molecules would not be able to exist in the interstellar space. To explore this novel area of astrochemistry, we aimed to study the structures, energies, and formation pathways of these carbon chain anions in order to develop a deeper understanding of astrochemical processes.

Methods/Materials

In this study, we use computational techniques using density functional theory. All geometry geometry optimizations were performed at the B3LYP DFT level with the 6-31G* and the 6-311+G** basis sets. Optimization of minima and transition structures (states) was performed within the Gaussian 09 environment. We ran Intrinsic reaction coordinate (IRC) analyses on the transition states of the minimum-energy pathways to investigate formation and isomerization pathways. All of the relative energies were corrected using a zero point vibrational energy correction.

Results

First, we were successful in optimizing the structures of a number of nonlinear isomers of carbon chain anions, contradicting previous assumptions that C4H-, C6H-, and C8H- exist exclusively as linear molecules. Second, our computations posit that these isomers occupy energetic minima of reasonable electronic energy compared to the linear isomers, thus confirming that these nonlinear isomers may exist in appreciable quantities in interstellar space. And finally, our IRC computations enable us to account for the isomerization between the linear and 3-membered-ring conformations of the C4H- isomers.

Conclusions/Discussion

These results posit the existence of complex carbon chain isomers, especially ring and branched chains that are reminiscent of biologically relevant molecules such as amino acids and nucleotides. Consequently, our study challenges current assumptions regarding astrochemistry and fundamentally argues that the composition of interstellar space is much more complex than ever before imagined.

Summary Statement

We computationally studied the structures, energies, and formation pathways of interstellar carbon chain anions.

Help Received

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