

Reactions of Nitrogen-Containing Carbanions in the Gas Phase

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A fundamental goal of astrobiology is to discover the origin of life in the universe. An intimate knowledge of the chemical reactions taking place in the interstellar medium (ISM) may contribute more pieces to this complex puzzle. Reactions involving organic molecules are especially important to astrobiology. Several carbon- and nitrogen-containing anions (CN^- , C_3N^- , and C_5N^-) have been spectroscopically detected in the ISM, and this study focuses on the gas phase reactivity of these and related anions with the most abundant atomic interstellar species, hydrogen atom. The tandem flowing afterglow-selected ion flow tube (FA-SIFT)¹ was used to experimentally determine the rate constants and products of these reactions. C_nN^- ($n = 1-6$), C_nN_2^- ($n = 1, 3, 4, 5$), and C_nN_3^- ($n = 2, 4$) were formed by discharge from a graphite rod in the presence of N_2 , and were thermalized in helium buffer gas. Reagent ions were then mass-selected using a quadrupole mass filter before entering the reaction flow tube. Hydrogen atoms were formed by the thermal dissociation of H_2 , and subsequently introduced into the flow tube. A second quadrupole mass filter coupled to an electron multiplier was used to detect the reaction products, and the observed reaction efficiencies are reported in the attached figure. Theoretical calculations at the B3LYP/aug-cc-pVTZ level of theory were conducted to further understand the mechanisms of these reactions. In future studies, these anion species will be studied in the context of their reactivity with nitrogen and oxygen atoms. Overall, an exploration of interstellar reactions is integral to answering one of the principal questions raised by astrobiology: the origin of life in the universe.

References

- (1) Van Doren, J. M.; Barlow, S. E.; DePuy, C. H.; Bierbaum, V. M. *Int. J. Mass Spectrom.* **1987**, 81, 85-100.