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Stepwise Microsolvation Study of Prebiotic Aminoacetonitrile by Rotational Spectroscopy: NH2CH2CN–(H2O)n (n = 1–5, 7)

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Aminoacetonitrile (NH2CH2CN, AAN) is a prebiotically relevant molecule that can hydrolyze to form glycine,the simplest amino acid. It has been detected in interstellar space and in Titan's atmosphere—an analog of early Earth—where gas-phase microsolvation likely played a critical role, as many prebiotic reactions are believed to have occurred in the gas phase. In this study, we investigate the microsolvation of AAN by one to seven water molecules under isolated gas-phase conditions using broadband rotational spectroscopy in the 2–8 GHz and 8–12 GHz frequency ranges. Hydrates of AAN containing one to five and seven water molecules were experimentally identified, while the assignment of the six-water complex was unsuccessful due to its low dipole moment (strongest μa = 0.5 D).

As protonation at either the –NH2 or –CN group is a necessary step in AAN hydrolysis [1], we employed Local Energy Decomposition and N-body analysis [2] to probe site-specific interactions between water molecules and these two functional groups. In parallel, quadrupole coupling constants within the quadrupole principal axes system were employed to semi-experimentally assess the evolving ionic character (ic) of both functional groups. This combined approach reveals how site-selective ionization tendencies develop during stepwise microsolvation. Our results reveal detailed hydrogen-bonding topologies, cooperative interactions, and the evolution of ionic character at each site, providing deeper insight into the chemical behavior of AAN in gas-phase environments.

Keywords

This abstract is submitted for....

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