Theoretical Study on the Isomerization and Detection of N_2H^+…OC Complex in Interstellar Clouds

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Abstract

In this study, we characterize N_2H^+…OC linear complex using Driven Molecular Dynamics (DMD) and Vibrational Self-Consistent Field Theory (VSCF) methods due to its relevance in astrochemistry. A central challenge is the detection of the molecular complex in interstellar media (ISM). Computational chemistry approaches can predict vibrational spectra, hence facilitate prediction of its existence and stability in the ISM. N_2H^+…OC involves the proton transfer process via hydrogen bonding interaction. Proton motion is highly anharmonic, therefore facing a significant challenge to characterize it accurately. Quantum mechanical variational methods are popular among many theoretical chemists for their efficiency producing accurate results. DMD simulations present an alternative route to predicting and assignment of infrared spectra. The N_2H^+…OC complex, is an important intermediate in the isomerization of COH^+ to HCO^+, with no published experimental results. We test the accuracy and performance of the MP2/aug-cc-pVDZ and CCSD(T) levels of theory by comparing theoretical and available experimental spectra for similar complex N_4H^+. We report strong evidence of a metastable alternative, distorted T-shaped structure along the isomerization pathway of N_2H^+…OC , that has never been reported before. Molecular vibration involving proton transfer along the molecular axis appears at ~1780 cm^{-1} predicted by both VSCF and DMD methods. This work provides an overview of IR spectra, line positions and mode assignment that allows experimentalist to quickly detect molecules. With limited published theoretical results and no direct experiment, the N_2H^+…OC complex remains an important target for theoretical and experimental chemists.