Study of formation processes of $C_2H_2N_2$ by quantum chemical calculation

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The amino acids that make proteins in organisms have left-handed enantiomers. This homochirality has also been detected in amino acids detected from meteorites, leading to discussions about the possibility that the origin of life on Earth may have originated in space. On the other hand, the origin of nucleobases which are important components of DNA, the blueprint for life on Earth, are not yet well understood. It is known that organisms can make nucleic acids from de novo synthesis by themselves. However, since nucleobases have also been detected in meteorites, it may be possible that some of the nucleobases of early life originated in space. Although the various laboratory experiments for the formation of nucleobases have been actively demonstrated on the surface of ice, in plasma discharges, and by the high energy particles by many researchers, how the nucleobases are formed is still an enigma. In the synthesizing process of one of the nucleobases, adenine $C_5H_5N_5$ with our plasma system the mass 54 corresponding to the same mass as $C_2H_2N_2$ is detected by a quadrupole mass spectrometer. This suggests that the formation of $C_5H_5N_5$ may be via $C_2H_2N_2$. Observations of E-HNCHCN have also been attempted toward Sgr B2 (N) by Zaleski et al. (2013). HNCHCN can be probably formed by polymerization of HCN, but the activation energy of the reaction is high, therefore this reaction is considered to be difficult to proceed at least in the gas phase in molecular cloud cores.

In this study, the possibility of the formation processes of E-HNCHCN and Z-HNCHCN other than the polymerization of HCN was examined by the quantum chemical calculation with the Hartree-Fock method. 6 -31 G (d, p) of the DZP basis was used as the basis function. As a result, it was found that, for example, NH_2CH_2CN is firstly formed from CH_3CN + NH and CH_2CN + NH_2 by the exothermic reactions and then E- and Z-HNCHCN are formed via a transition state with high activation energy, or via the intermediate molecule, NH_3CHCN and the some transition states with low activation energy. In this presentation, we will report the results of these analyses.

Keywords: Nucleobases, Interstellar medium, Plasma reaction, Quantum chemical calculation

