Contribution ID: **259** Contribution code: **S4 High Energy and Particle Physics** Type: **Oral Presentation**

A Computational Study of the Gas-Phase Formose-Like Reactions under the Interstellar-medium-like conditions

Friday 24 June 2022 13:30 (15 minutes)

Understanding the extraterrestrial origin of ribose, as one of the subunits of ribonucleic acid (RNA), is crucial to anticipating the formation of the building blocks of life under interstellar medium conditions. Under ordinary atmospheric conditions, the formation of sugar is suggested to occur through the formose reaction, where formaldehyde is solely used as the precursor in each of the iterative steps of the processes. On the other hand, sugar synthesis under interstellar medium conditions has evidently been shown to be significantly different from the terrestrial formose reactions due to the extremely low density of molecules and the very low temperature. In this study, we theoretically investigate the formose-like reactions for ribose formation catalyzed by a single proton through the mean of computer simulation based on first-principles density functional theory (DFT). The ribose formation reactions are modelled in the absence of solvation effects at absolute zero temperature to mimic the extremely low pressure and temperature found in interstellar molecular clouds. We observe that the presence of a proton gives rise to a more thermodynamically stable complex of the two reactive carbonyl compounds by bridging their oxygen atoms as required for the iterative formose reaction to proceed. In order to form a new carbon-carbon bond through an iterative process, only the region where the additional formaldehyde attaches to the existed protonated carbonyl compound is of great importance. Similar energy barriers for all the iterative steps during the ribose formation have been observed to be approximately 67 kcal/mol. Our findings show that a single proton can act as an efficient catalyst for the gas-phase ribose formation reactions. The results suggest that ribose formation can preferentially occur via the formose pathway in the presence of protons, which are presented in interstellar clouds.

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Session Classification: S4 High Energy and Particle Physics

Track Classification: High Energy and Particle Physics