# A theoretical study of glycine formation reactions in interstellar medium

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Search for extraterrestrial prebiotic molecules has attracted attention in the fields of astrochemistry and astrobiology. Several amino acids were detected in meteorites, such as Murchison meteorite [1], and recently, glycine, the simplest amino acid, was found in comet 67P/Churyumov-Gerasimenko [2]. In addition, many laboratory experiments were carried out to suggest the plausible formation pathway of amino acids under possible astrophysical conditions. However, the reaction mechanism in interstellar medium has yet to be elucidated.

In the present study, two possible pathways for the formation of glycine are investigated by means of density functional theory (DFT). We analyzed reaction mechanisms via aminoacetonitrile, which is a possible prebiotic precursor of glycine and detected in an interstellar cloud. The first pathway is Strecker reaction, which generates glycine by hydrolyses of aminoacetonitrile. The second one is the formation of hydantoin (2,4-imidazolidinedione) by Bucherer-Bergs reaction and its hydrolysis to generates glycine. In order to examine the reactions on interstellar ices, which play important roles in astrochemistry, simple model systems containing an additional water molecule were also studied. The calculations were performed at DFT level of theory with B3LYP functional and 6-31G* basis set.

The energy profile of both reaction mechanisms showed that they require activation energies which are too high to overcome at low temperature in interstellar space. It is shown that addition of a catalytic water molecule lowers several reaction barriers, however, the highest activation energies are still high, i.e., 49 kcal/mol and 55 kcal/mol for the first and the second pathways, respectively. Thus, energy sources, such as collisional heat during planetary formation or UV light irradiation, are needed for these reactions to proceed.

References

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