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Computational Study of Glycine and its Radical Cation and Contributions to the Interstellar Chemistry

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Abstract: Glycine is mostly present in interstellar medium (ISM) in solid phase, covered by a ice mantle. But, subjected to some high energy phenomena of the hostile ISM, glycine can undergo to gas phase.[1] This hypothesis is corroborated since the fragments associated to this amino acid decomposition are frequently encountered in space, even though molecule itself is hardly found in gas phase.[2] This work aims to the understanding of the chemical behavior of glycine in the ISM. Specifically, a kinetic study of glycine decomposition is undergone in order to bring some answers to its formation and decomposition channels and to the possibility of its survival in the ISM, in its way to Earth. All calculations including geometry optimizations, vibrational frequencies and reaction paths, have been performed at the B3LYP/6-311++G(2d,2p) level and additional single point calculations at the CCSD(T)/6-311++G(2d,2p)//B3LYP/6-311++G(2d,2p) level have been performed in order to improve the electronic energies. A detailed study of the structures and reactivity of glycine as an isolated system is performed. Moreover, considering that glycine can also be ionized due to the impact with high-energy photons and particles, similar work has been performed for the radical cation. A conformational analysis of glycine in its neutral and radical cations forms reveals a spectrum of eight and four conformers of glycine and glycine radical cation, respectively. The conformers were characterized according to the dihedral angles and this nomenclature scheme of the conformers is suggested. The population analysis suggests that the lowest energy conformer prevails over all other conformers (~100% to 75%, neutral form, from 50 to 300 K and ~100% to 95%, radical cation form, from 50 to 300K). An interconversion scheme was proposed and rate coefficients were calculated. The calculated ionization energy, 9.0 eV, is in very good agreement with the experimental determinations (8.8 – 9.3 eV). Saddle points have been located for the deamination and decarboxylation reaction of the neutral form and decarboxylation of the radical cation and reaction paths have been calculated adopting the IRC algorithm. Dissociation reactions have also been explored using modified Morse Potentials. Among dissociations and decomposition reactions, the deamination reaction is the dominant channel for the neutral form, with a barrier height of 44.76 kcal/mol and the dissociation that leads to HOCO and $(CH_2NH_2)^+$ products was the most favored radical cation unimolecular reaction, with a dissociation limit of 53.04 kcal/mol. In this work, it was proposed that high energy phenomena can make solid phase glycine undergo to gas phase glycine in neutral and cation radical form, in

fundamental state and neutral form in excited state. With the data reported in this work and a possible study of glycine in excited state, we can finally understand the role of glycine in the ISM and the possible paths leading to its formation and decomposition in primitive Earth.

Key-words: amino acids, astrochemistry, chemical kinetics, glycine, B3LYP, DFT
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