Identification of HOC*HC(O)NH₂ intermediate in the reaction of H + glycolamide in solid para-hydrogen and its implications in astrochemistry

Joshi, P.R., 1* Lee, Y.-P. 1, 2
*presenter  
1 e-mail - prasad.nctu@gmail.com, Department of Applied Chemistry and Institute of Molecular Science, National Yang Ming Chiao Tung University, Hsinchu 300093, Taiwan  
2 Center for Emergent Functional Matter Science, National Yang Ming Chiao Tung University, Hsinchu 300093, Taiwan

Glycolamide [HOCH₂C(O)NH₂], an isomer of glycine, has gained more attention in recent years because of its detection in the interstellar medium (ISM); the presence of inherent peptide bond [-NH-C(O)-] is fundamental to building block of proteins and pivotal to the origin of life. Despite of its importance in ISM, detailed investigations regarding the reactivity of HOCH₂C(O)NH₂ under interstellar conditions remains largely unexplored. In this study, we performed the reaction involving H atoms and HOCH₂C(O)NH₂ in solid para-hydrogen (p-H₂) at 3.2 K. The utilization of p-H₂ serves dual purposes; it acts as a quantum-solid matrix host and facilitates a medium for efficient hydrogen-atom reactions. To generate H atoms, the co-deposited mixture of HOCH₂C(O)NH₂/p-H₂ and Cl₂ was photolyzed at 365 nm to generate Cl atoms; subsequent IR irradiation for promoting the reaction Cl + H₂ (ν=1) → HCl + H generated H atoms which can tunnel through the p-H₂ matrix via quantum tunnelling. Among three different hydrogen-containing moieties of HOCH₂C(O)NH₂, we exclusively observed H abstraction on the -CH₂ moiety, resulting in the formation of 2-amino-1-hydroxy-2-oxoethyl radical [HOC*HC(O)NH₂]. We successfully characterized the formation of both Cis-cis (Cc)- and Trans-trans (Tt)-conformers of HOC*HC(O)NH₂ from the reactions H + Cc- and Tt-HOCH₂C(O)NH₂, with the ratio of Cc:Tt of HOCH₂C(O)NH₂ estimated to be 3:2 in the deposited matrix. The spectral identification of these radicals and their roles were not reported so far. These assignments agree satisfactorily with vibrational wavenumbers predicted with the B3LYP/aug-cc-pVTZ method. The PES of the reactions H + Cc/Tt- HOCH₂C(O)NH₂ revealed that H abstraction is the only feasible route for the H reaction on the CH₂ site, whereas H abstractions on OH and NH₂ sites are endothermic. In darkness, IR intensities of both conformers increased, indicating their formation via tunneling reactions. Although, H abstraction on the NH₂ moiety is essential for the protein synthesis through the elongation of peptide chain; this study suggests that the emergence of peptide linkage via observed radicals might be possible when the radicals further react with NH₂C*O, leading to the formation of malonamide, wherein the NH₂ moiety of HOCH₂C(O)NH₂ perhaps prefer N-terminal of the peptide linkage. In addition, these radicals could serve as potential precursors for the formation of higher-order amides bearing a chiral center, such as lactamide and glyceramide (glycerol amide) after their reactions with C*H₃ and C*H₂OH, respectively, in the dark regions of ISM.