

Identification of $\text{HOC}\cdot\text{HC}(\text{O})\text{NH}_2$ intermediate in the reaction of H + glycolamide in solid *para*-hydrogen and its implications in astrochemistry

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Glycolamide [$\text{HOCH}_2\text{C}(\text{O})\text{NH}_2$], 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 $\text{HOCH}_2\text{C}(\text{O})\text{NH}_2$ under interstellar conditions remains largely unexplored. In this study, we performed the reaction involving H atoms and $\text{HOCH}_2\text{C}(\text{O})\text{NH}_2$ in solid *para*-hydrogen (*p*- H_2) at 3.2 K. The utilization of *p*- H_2 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 $\text{HOCH}_2\text{C}(\text{O})\text{NH}_2/p$ - H_2 and Cl_2 was photolyzed at 365 nm to generate Cl atoms; subsequent IR irradiation for promoting the reaction $\text{Cl} + \text{H}_2$ ($\nu=1$) \rightarrow $\text{HCl} + \text{H}$ generated H atoms which can tunnel through the *p*- H_2 matrix via quantum tunnelling. Among three different hydrogen-containing moieties of $\text{HOCH}_2\text{C}(\text{O})\text{NH}_2$, we exclusively observed H abstraction on the - CH_2 moiety, resulting in the formation of 2-amino-1-hydroxy-2-oxoethyl radical [$\text{HOC}\cdot\text{HC}(\text{O})\text{NH}_2$]. We successfully characterized the formation of both *Cis-cis* (*Cc*-) and *Trans-trans* (*Tt*-) conformers of $\text{HOC}\cdot\text{HC}(\text{O})\text{NH}_2$ from the reactions H + *Cc*- and *Tt*- $\text{HOCH}_2\text{C}(\text{O})\text{NH}_2$, with the ratio of *Cc*:*Tt* of $\text{HOCH}_2\text{C}(\text{O})\text{NH}_2$ 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*- $\text{HOCH}_2\text{C}(\text{O})\text{NH}_2$ revealed that H abstraction is the only feasible route for the H reaction on the CH_2 site, whereas H abstractions on OH and NH_2 sites are endothermic. In darkness, IR intensities of both conformers increased, indicating their formation via tunneling reactions. Although, H abstraction on the NH_2 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 $\text{NH}_2\text{C}\cdot\text{O}$, leading to the formation of malonamide, wherein the NH_2 moiety of $\text{HOCH}_2\text{C}(\text{O})\text{NH}_2$ 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 $\text{C}\cdot\text{H}_3$ and $\text{C}\cdot\text{H}_2\text{OH}$, respectively, in the dark regions of ISM.

