PRODUCTION OF C_α-ALANYL RADICAL AND VINYLAMINE IN THE REACTION H + α-ALANINE IN SOLID *p*-H_2 AND ITS IMPLICATIONS IN ASTROCHEMISTRY

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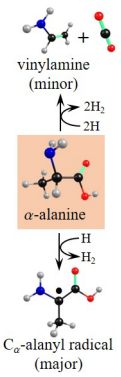

Amino acids, key building blocks of protein, gained enormous attention in interstellar chemistry because they were detected in comets and meteorites; these observations provided strong evidence for the cosmic origin of amino acids on Earth. However, detailed investigations regarding their formation and reactivities with interstellar relevant species under cosmic-like conditions are scarce. We utilized the characteristics of *para*-hydrogen (*p*-H_2), which served as a quantum-solid matrix host and a medium for efficient hydrogen-atom reaction, to investigate the reaction between α-alanine [$H_2NCH(CH_3)C(O)OH$] and H atoms at 3.2 K. To produce H atoms, we performed UV photolysis at 365 nm on a matrix co-deposited with a mixture of $H_2NCH(CH_3)C(O)OH$/*p*-H_2 and Cl_2 to produce Cl atoms, followed by infrared irradiation to promote the Cl + H_2 (ν = 1) $\rightarrow$ H + HCl reaction. Among four different hydrogen-containing moieties of $H_2NCH(CH_3)C(O)OH$, H abstraction on the -CH moiety to produce C_α-alanyl radical [$H_2N \bullet C(CH_3)C(O)OH$] from the conformer with the least energy is the most favorable. This radical plays a vital role in the asymmetric synthesis of complex organic molecules. In parallel, possibly H abstraction on both -C(O)OH and CH_3 moieties led to the fragmentation to produce vinylamine ($NH_2CH = CH_2$) and CO_2 through the second-most favorable channel. Recently, vinylamine has been detected in the interstellar medium.[a] These assignments were supported by isotopic substitution experiments and a comparison of experimental results with vibrational wavenumbers of possible products predicted with the B3LYP/aug-cc-pVTZ method.

[a] S. Zeng et al. Astrophys. J. Lett. 2021, 921, L27.