

Supplementary Information

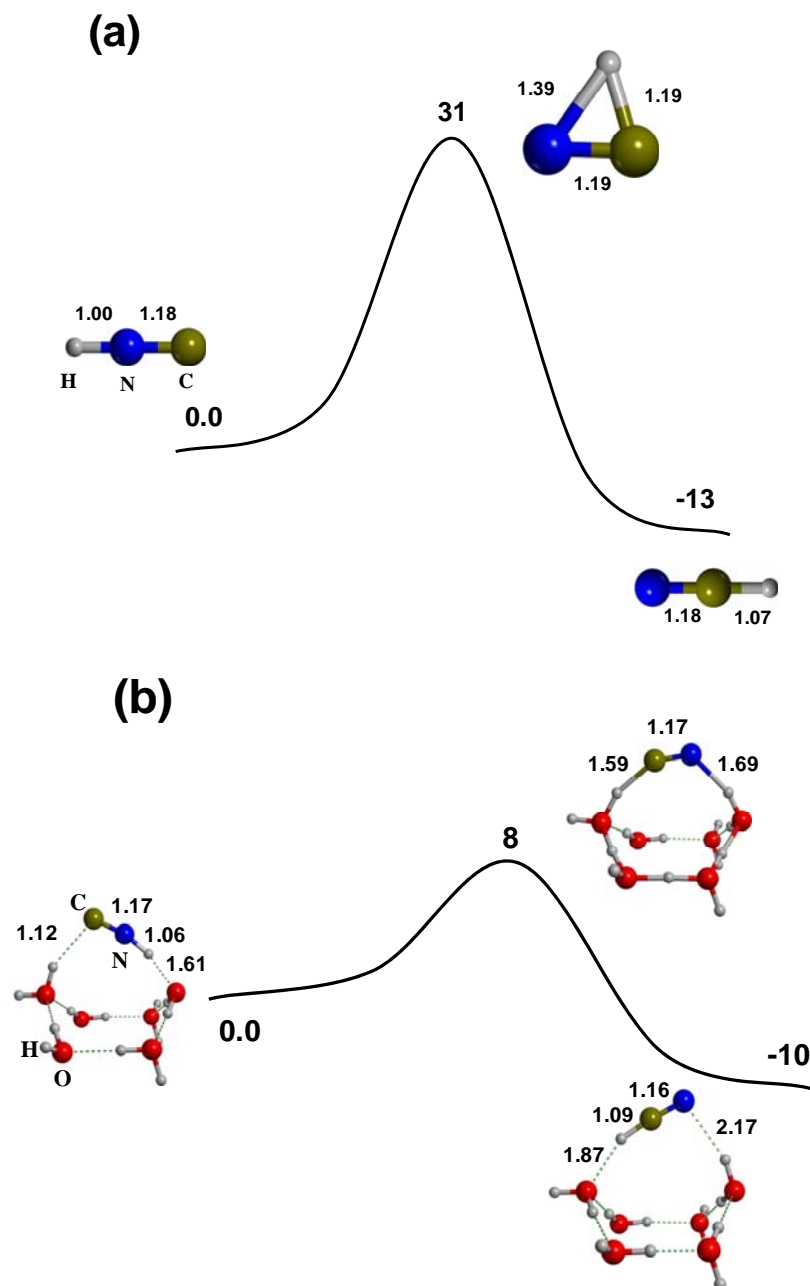
Deep-space glycine formation via Strecker-type reactions activated by ice water dust mantles. A computational approach.

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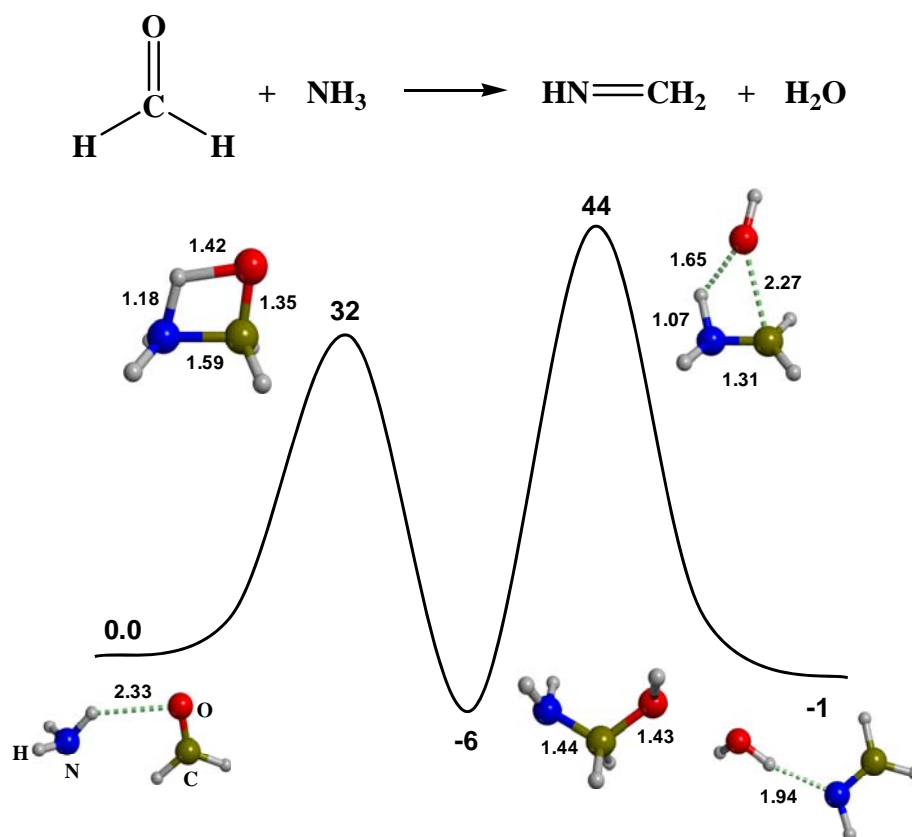


Figure S2. B3LYP/6-31+G(d,p) gas-phase ZPE-corrected profile of $\text{H}_2\text{C}=\text{O} + \text{NH}_3 \rightarrow \text{NH}=\text{CH}_2 + \text{H}_2\text{O}$ following the Strecker mechanism. Relative ZPE-corrected energies in kcal mol^{-1} , bond distances in \AA .

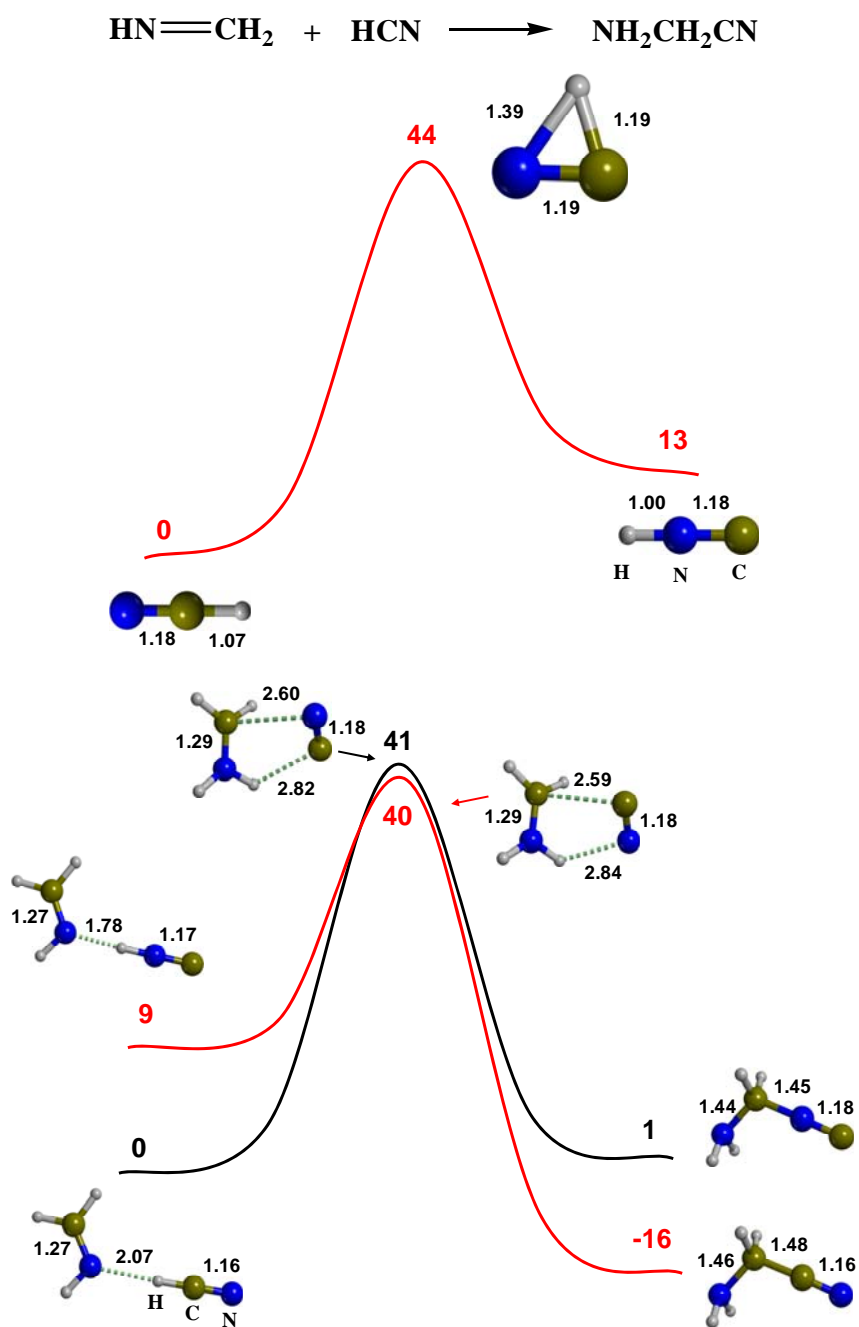


Figure S3. B3LYP/6-31+G(d,p) gas-phase ZPE-corrected profile of $\text{HCN} + \text{NH}=\text{CH}_2 \rightarrow \text{NH}_2\text{CH}_2\text{CN}$ following the Strecker mechanism. Relative ZPE-corrected energies in kcal mol⁻¹, bond distances in Å.

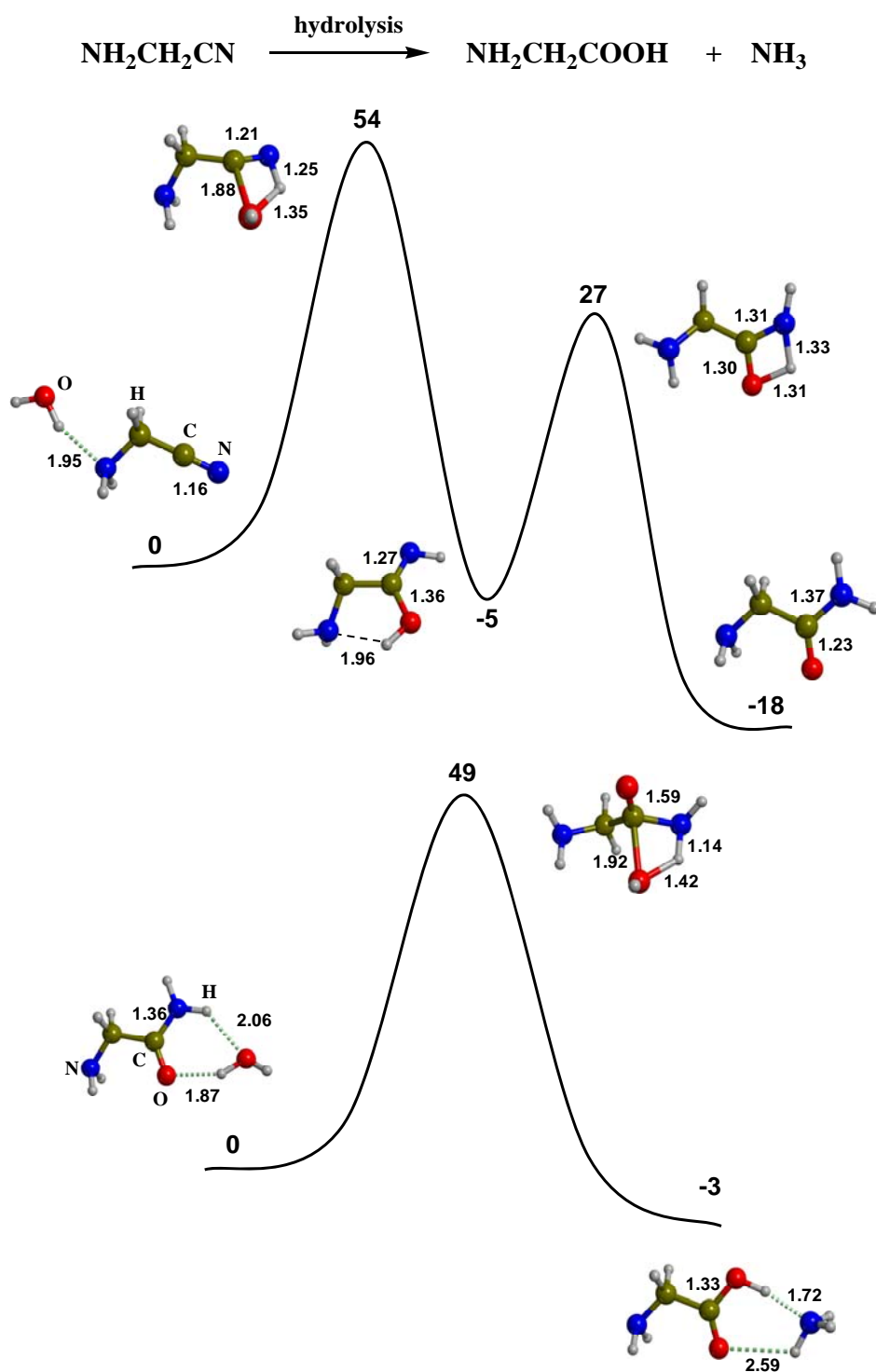


Figure S4. B3LYP/6-31+G(d,p) gas-phase ZPE-corrected profile of the hydrolysis of $\text{NH}_2\text{CH}_2\text{CN}$ to form glycine following the Strecker mechanism. Relative ZPE-corrected energies in kcal mol^{-1} , bond distances in \AA .

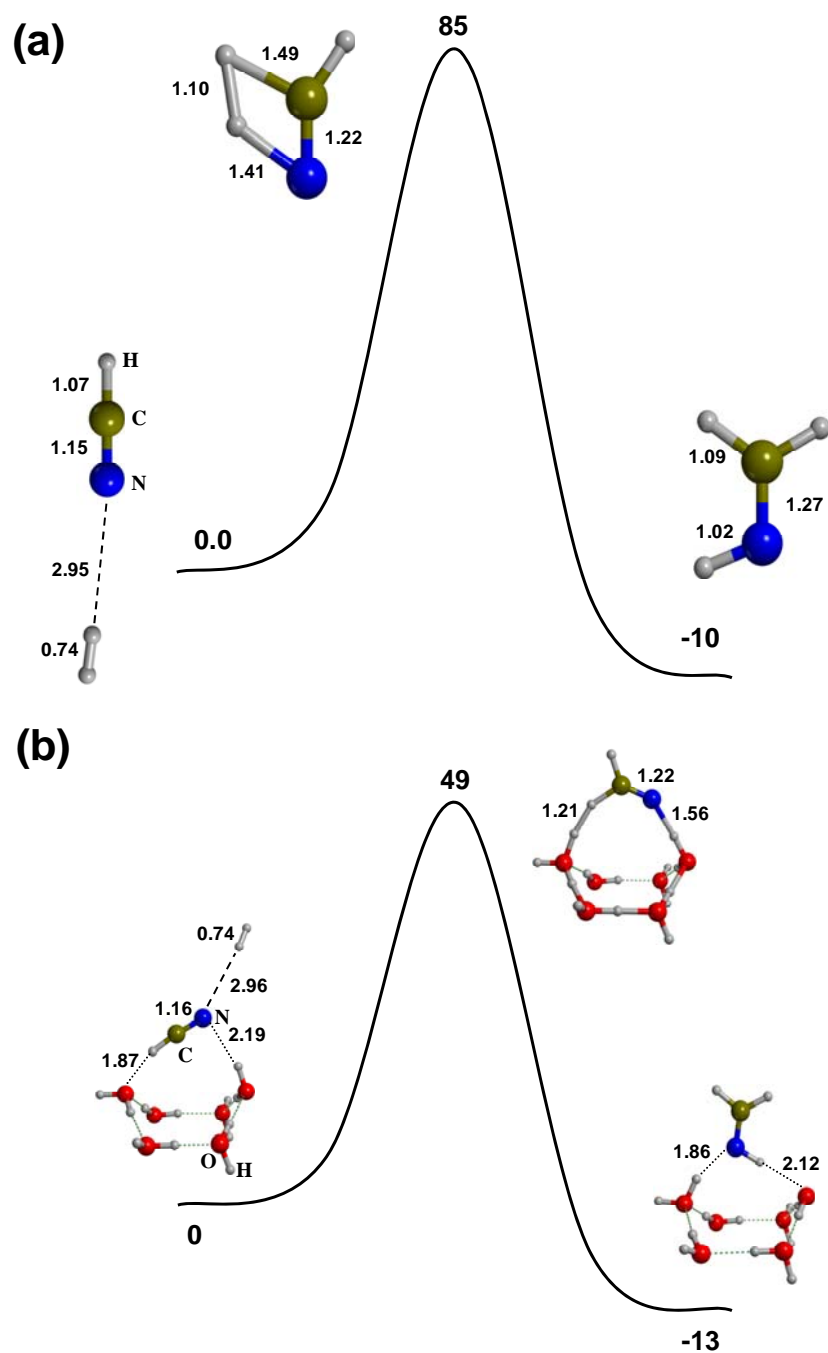


Figure S5. B3LYP/6-31+G(d,p) ZPE-corrected profile for the $\text{H}_2 + \text{HCN} \rightarrow \text{NH}=\text{CH}_2$ reaction: (a) in gas-phase, (b) at the H_2O -ice surface. Relative ZPE-corrected energies in kcal mol⁻¹, bond distances in Å.

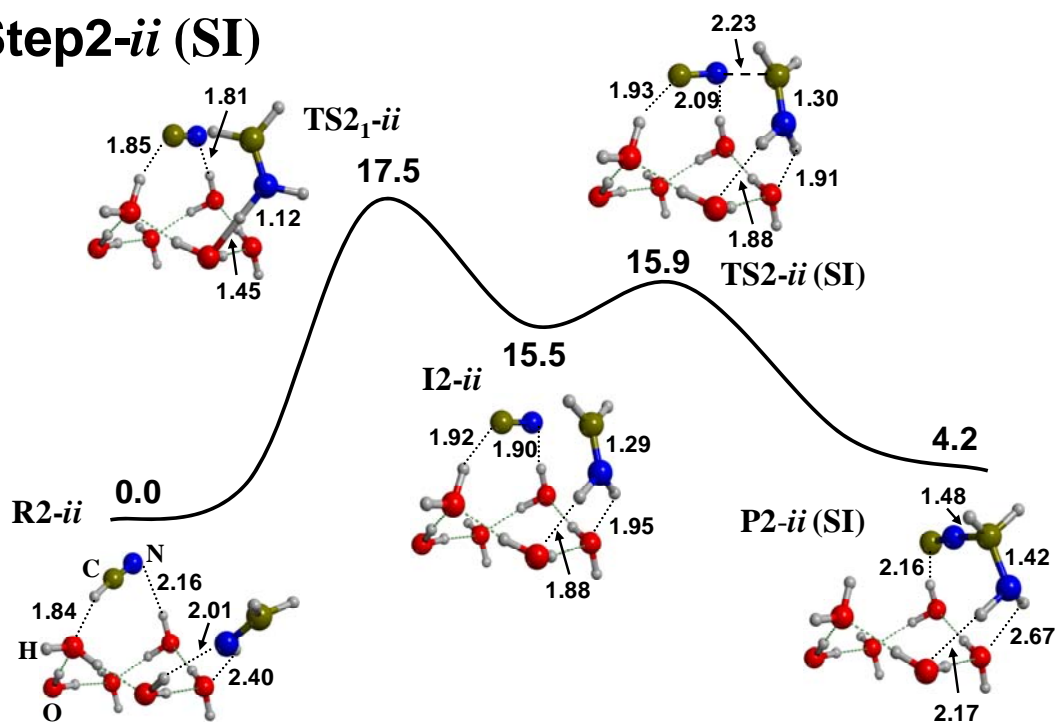
Step2-ii (SI)

Figure S6. B3LYP/6-31+G(d,p) ZPE-corrected profile for the $\text{NH}=\text{CH}_2 + \text{HCN} \rightarrow \text{NHCH}_2\text{NC}$ reaction at the H_2O -ice surface. Relative ZPE-corrected energies in kcal mol⁻¹, bond distances in Å.

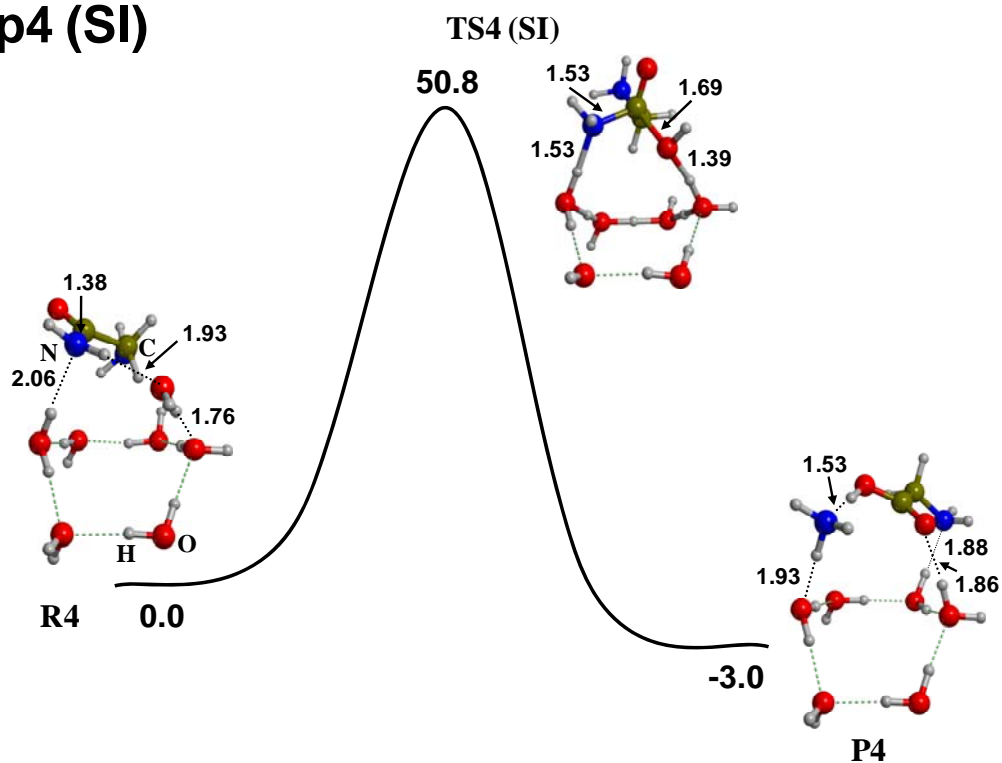
Step4 (SI)

Figure S7. B3LYP/6-31+G(d,p) ZPE-corrected profile for the $\text{NH}_2\text{CH}_2\text{CONH}_2 + \text{H}_2\text{O} \rightarrow \text{NH}_2\text{CH}_2\text{COOH} + \text{NH}_3$ assisted by the H_2O -ice surface. Relative ZPE-corrected energies in kcal mol⁻¹, bond distances in Å.