Supplementary Information

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

Albert Rimola,¹ Mariona Sodupe,²* and Piero Ugliengo¹*

¹Dipartimento di Chimica IFM, NIS Centre of Excellence and INSTM (Materials and Technology National Consortium), UdR torino, Università di Torino, Via P. Giuria 7, 10125 Torino, Italy.

²Departament de Química, Universitat Autònoma de Barcelona, Bellaterra 08193, Spain.

*Corresponding authors. E-mails: piero.ugliengo@unito.it; mariona@klingon.uab.es
Figure S1. B3LYP/6-31+G(d,p) isomerization reaction of CNH → HCN: (a) in gas-phase, (b) at the H₂O-ice surface. Relative ZPE-corrected energies in kcal mol⁻¹, bond distances in Å.
Figure S2. B3LYP/6-31+G(d,p) gas-phase ZPE-corrected profile of $\text{H}_2\text{C}=\text{O} + \text{NH}_3 \rightarrow \text{HN}≡\text{CH}_2 + \text{H}_2\text{O}$ following the Strecker mechanism. Relative ZPE-corrected energies in kcal mol$^{-1}$, bond distances in Å.
**Figure S3.** B3LYP/6-31+G(d,p) gas-phase ZPE-corrected profile of HCN + NH=CH$_2$ $\rightarrow$ NH$_2$CH$_2$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 NH₂CH₂CN to form glycine following the Strecker mechanism. Relative ZPE-corrected energies in kcal mol⁻¹, bond distances in Å.
Figure S5. B3LYP/6-31+G(d,p) ZPE-corrected profile for the H₂ + HCN → NH-CH₂ reaction: (a) in gas-phase, (b) at the H₂O-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 NH=CH₂ + HCN → NHCH₂NC reaction at the H₂O-ice surface. Relative ZPE-corrected energies in kcal mol⁻¹, bond distances in Å.
Figure S7. B3LYP/6-31+G(d,p) ZPE-corrected profile for the NH$_2$CH$_2$CONH$_2$ + H$_2$O $\rightarrow$ NH$_2$CH$_2$COOH + NH$_3$ assisted by the H$_2$O-ice surface. Relative ZPE-corrected energies in kcal mol$^{-1}$, bond distances in Å.