**Supporting Information**

Prebiotic Peptide Formation in Gas-Phase Atmospheric Nanoclusters of Water: From Glycine to Diglycine to Triglycine

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Section 1: Figures of Minimum Energy Clusters

Section 2: Energy Tables

Section 3: Optimized Geometries

Section 4: Derivation of Complete Basis Set Limit Extrapolation Formulas

**Section 1: Figures of Minimum Energy Structures**

The figures of all transition state structures, reactants, reactant clusters, products, and product clusters are present within the folder titled “SI Figures”.

**Section 2: Energetics of Structures**

The electronic energies, G correction values, and DLPNO-CCSD(T) electronic energies with the cc-pVnZ basis sets (n=D,T,Q) of all structures are present in excel files under the folder titled “Energy Tables”. The structures are organized based on the naming convention of the T.S. structures within the paper, with individual sheets inside the excel files containing different conformations.

**Section 3: Optimized Geometries**

The ωB97X-D coordinate files of all structures are presented as .xyz files within the folder titled “xyz files”.

**Section 4: Derivation of Complete Basis Set Limit Extrapolation Formulas**

The CBS extrapolation formulas are shown in the word document titled “CBS Extrapolation Formulas”.