Abstract Submitted
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Aqueous Glycine Condensation Chemistry Under Extreme Conditions[1] NIR GOLDMAN, MATTHEW KROONBLAWD, Lawrence Livermore Natl Lab — We have performed high throughput quantum molecular dynamics simulations to determine the free energy surface for aqueous glycine condensation reactions from moderate to extreme temperatures similar to oceanic hydrothermal vents (1g/cc and temperatures ranging from 300 K to 1000 K). Our simulations identify significant changes in the free energy surface topology and subsequent chemical reactivity with increasing temperature. We predict that temperatures at 400 K and below glycine favor dipeptide formation whereas higher temperatures facilitate the reverse hydrolysis reaction, with solvated glycine molecules showing greater stability. This change in favorability is correlated with a shift in the location and characteristics of specific reaction bottlenecks or barriers. Simultaneously, we observe that relative free energy barriers (total energy plus entropic contributions) for both condensation and hydrolysis reactions generally decrease with increasing temperature. Our results indicate that relatively modest temperatures near 400 K may best facilitate formation of oligoglycine molecules in oceanic systems related to the synthesis of life-building compounds.

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