Hydration and Association in Extraterrestrial Environments: Mapping Glycine Interactions in Ammonia-Water Mixtures

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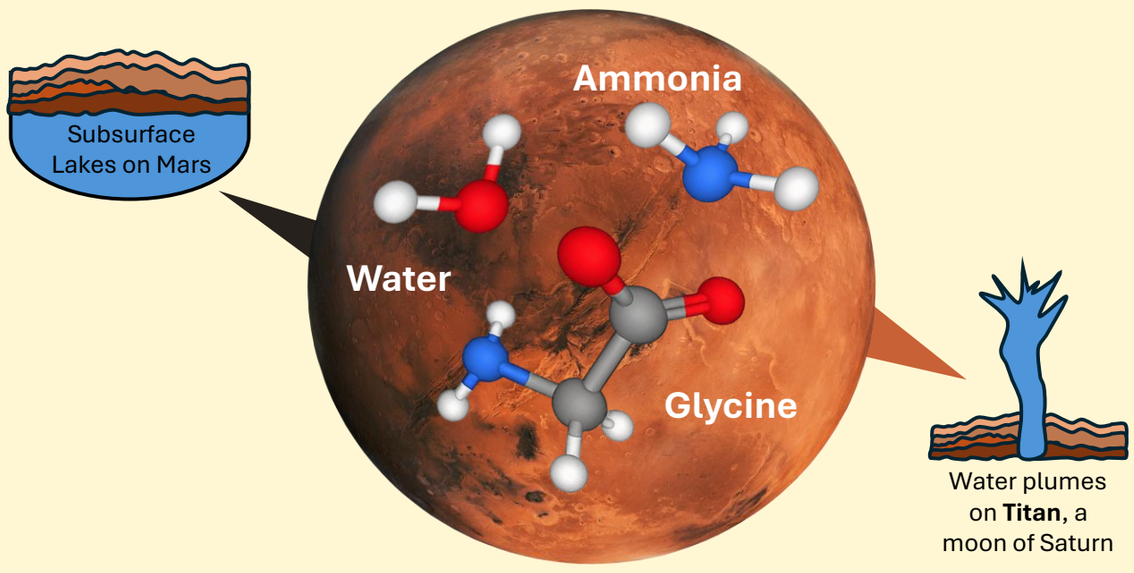
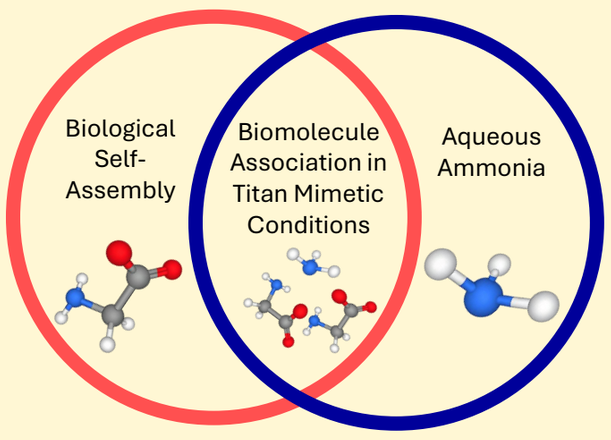
1. Big Picture

Ammonia–water mixtures exist in extraterrestrial environments. Can investigating amino acid assembly in ammonia-water shed light on the origins of complex life?



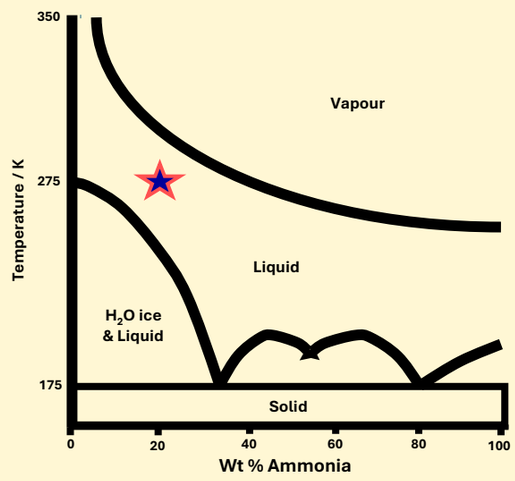
2. Background



As the simplest amino acid, glycine makes a good start point for investigating assembly under extreme conditions

Amino acid assembly is a potential indicator of prebiotic chemistry and linked to the Origin of Life

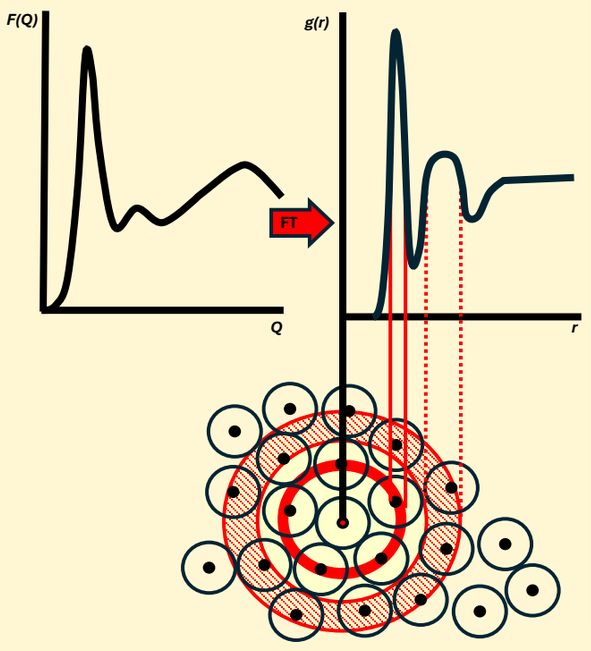
Near eutectic 20.5 wt.% ammonia was used to mimic aqueous environments on Titan



3. Methodology

Neutron Data

Total neutron scattering to probe how atoms arrange and interact in complex materials



Simulation Based Refinement

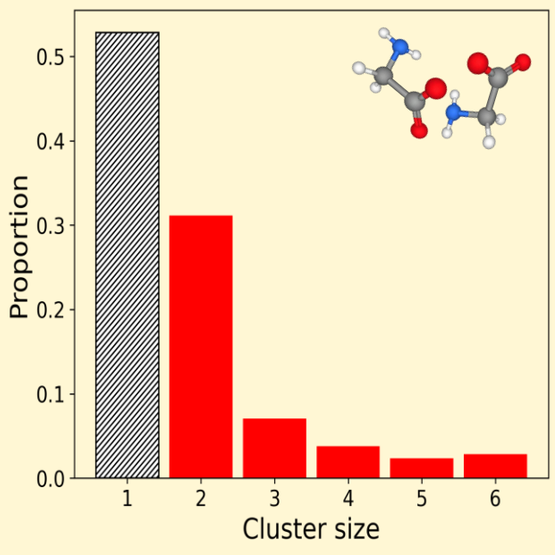
Atomistic Simulation
Run atomistic simulation using reference potentials

Compare to Data
Compare to multiple datasets for the system using isotopic substitution

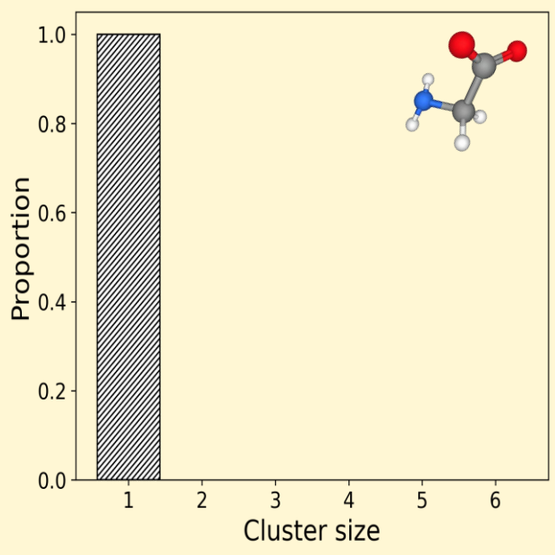
Add an Empirical Potential
Based on mismatch between simulated and experimental data

4. Biomolecular Assembly

Aqueous Glycine

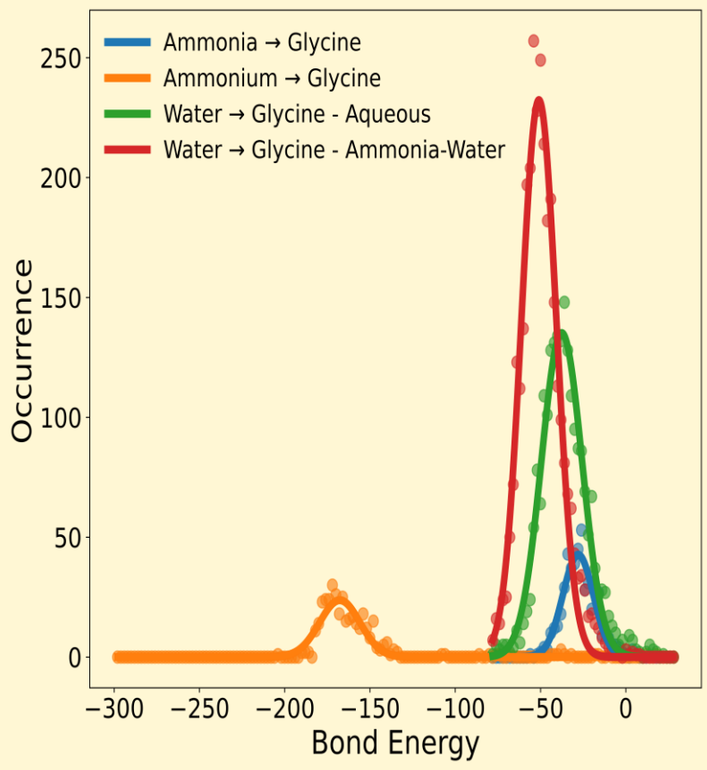


Glycine in Ammonia-Water



No evidence for glycine association in aqueous ammonia solution

5. Bond Enthalpies

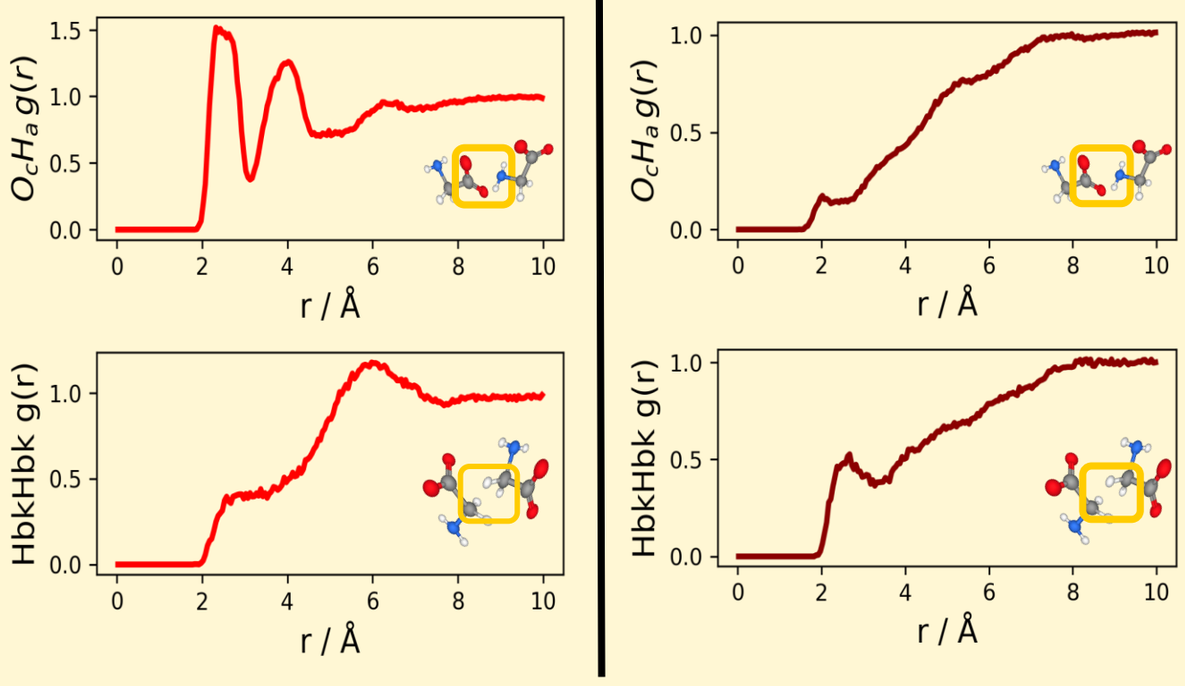


Bond enthalpies quantify strengths, reveal stability and driving forces in solvation, helping explain structural changes observed

Water–glycine interactions weaken (−51 → −38 kJ/mol)

Ammonium forms very strong but scarce interactions with glycine (−168 kJ/mol)

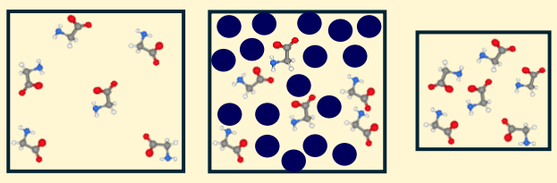
Ammonia forms weak but plentiful interactions (−28 kJ/mol|)



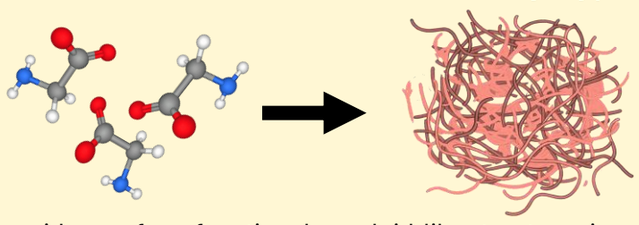
Glycine association occurs through hydrophilic interactions

6. Conclusions & Outlook

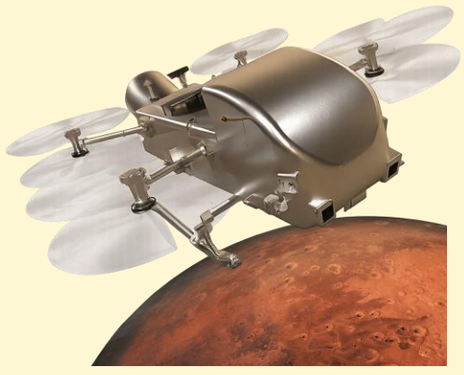
The data suggests that ammonia-rich environments alone are insufficient to support prebiotic self-assembly



Functional Abiotic Metabolite Assembly Hypothesis



Amino acids may form functional, amyloid-like structures in prebiotic environments, providing a bridge between prebiotic chemistry and the emergence of compartmentalised, catalytic, life-like systems



NASA Dragonfly will land on Titan in 2034, investigating prebiotic chemistry and habitability. Can we narrow down possible locations for biomolecular assembly?

References: 1. Orosei R, Lauro SE, Pettinelli E, Cicchetti A, Coradini M, Cosciotti B, et al. Radar evidence of subglacial liquid water on Mars. Science. 2018;361(6401):490-3. Taubner, R. S., Leitner, J. J., Firneis, M. G. & Hitzenberger, R. Modelling the Interior Structure of Enceladus Based on the 2014's Cassini Gravity Data. *Orig. Life Evol. Biosph.* **46**, 283–288 (2016). **2.** Laurent H, Soper A, Dougan L. Biomolecular self-assembly under extreme Martian mimetic conditions. Molecular Physics. 2019;117(22):3398-407, Nasralla M, Laurent H, Alderman OLG, Dougan L. Solution structure of Titan-relevant aqueous ammonia by neutron diffraction. Communications Chemistry. 2025;8(1):227. Kargel, J. S. Ammonia-water volcanism on icy satellites: Phase relations at 1 atmosphere. *Icarus* **100**, 556–574 (1992). **3.** Youngs T. Dissolve: next generation software for the interrogation of total scattering data by empirical potential generation. Molecular Physics. 2019;117(22):3464-77. **6.** Chakraborty, P., et al. (2026). "Functional Abiotic Metabolite Assembly: Hypothesis for the Early Events in the Origin of Life." ChemRxiv **2026(0212).** Lorenz, R. D., et al. (2021). "Selection and Characteristics of the Dragonfly Landing Site near Selk Crater, Titan." The Planetary Science Journal 2(1): 24. NASA (2026). "Dragonfly - Future Mission." 2026, from https://science.nasa.gov/mission/dragonfly/

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