Self-Assembly of Prebiotic Organic Materials from Impact Events of Amino Acid Solutions*.

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Abstract: Proteinogenic amino acids can be produced on or delivered to a planet via abiotic sources and were consequently likely present before the emergence of life on early Earth [1]. Aminoacids could have been delivered by exogenous sources, such as meteorites, comets, and interstellar dust partcles [2]. Dipeptides of proteinogenic amino acids have been produced in the laboratory in interstellar ice models [3]. Shock synthesis of amino acids has also been observed in both computational and experimental studies [4]. Shock compression in astrophysical ices can induce the formation of extended C-N bonded networks similar to peptide chains [5]. However, the role that these materials played in the in the emergence of life remains an open question, in part because little is known about the survivability and reactivity of astrophysical prebiotic compounds upon impact with a planetary surface. Potential life building synthesis derived from amino acids and peptide activating agents would depend heavily on their fate during extreme pressures and temperatures.

To this end, we have used quantum simulations to explore the role of extreme conditions in the emergence of organization of amino acids. Using a force matching semi-empirical quantum simulation method in development in our group [6], we have studied oblique impacts of aqueous glycine solutions at conditions of up to 40 GPa and 3000 K for approximate chemical equilibrium timescales. A parallel replica approach allowed us to probe systems sizes an order of magnitude larger than previously possible. We find that these elevated conditions induce the formation of glycine-oligomeric structures with a number of different chemical moieties such as hydroxyl and amine groups diffusing on and off the C-N backbones. The C-N backbones of these structures generally remain stable during cooling and expansion, yielding relatively large three-dimentsional molecules that contain a number of different functional groups and embedded bonded regions akin to proteinogenic amino acids (Figure 1). Our results help determine the role of comets and other celestial bodies in both the delivery and synthesis of polypeptides and homochirality to early Earth. This will help guide future experimentation by providing both a possible synthetic mechanism as well as a catalogue of possible chemical products to be investigated.

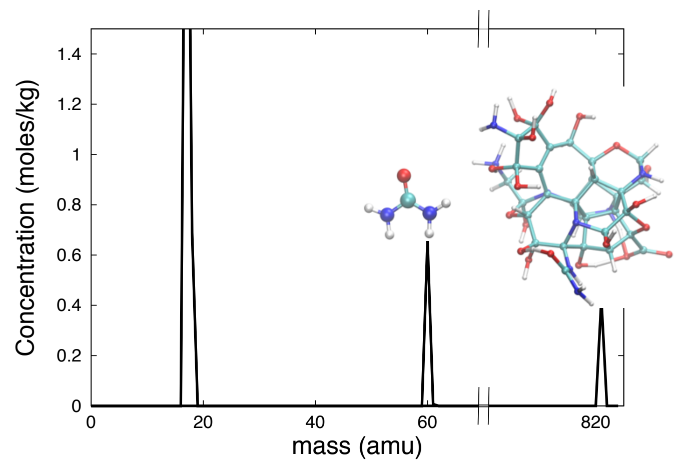

Figure 1: Simulated mass spectrum of recovery products after expansion and cooling from 40 GPa and 3000 K. Red atoms correspond to oxygen, white to hydrogen, teal to carbon, and dark blue to nitrogen. The peak at 17-18 amu corresponds to H_2O and NH_3. Urea was found in appreciable amounts at 60 amu, and a large 3D polypeptide-like structure was found at ~820 amu.

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