Abstract Submitted
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Complex prebiotic chemistry within a simple impacting icy mixture[1] NIR GOLDMAN, Lawrence Livermore National Laboratory — We present results of prebiotic molecule synthesis in shock compressed mixtures of simple ices from quantum molecular dynamics (MD) simulations. Given the likelihood of a CO_2-rich primitive atmosphere, it is possible that impact processes of comets or other icy bodies were partially responsible for the creation of prebiotic chemical compounds on early Earth. We have conducted simulations of the chemical reactivity within an oxidized astrophysical icy mixture to close to equilibrium using a density functional tight binding (DFTB) approach. We observe that moderate shock pressures and temperatures (35 GPa and 2800 K) produce a number of functionalized polycyclic aromatic hydrocarbons (PAHs), which remain intact upon expansion and cooling to lower conditions. At higher shock pressures and temperatures (48-62 GPa, 3700-4700 K), we observe the synthesis of a variety of short-lived, exotic C—C and C—N bonded oligomers which decompose upon expansion and cooling to form precursors to amino acids and other prebiotic compounds, such as long chain alkanes, HCN, CH_4 and formaldehyde. Our results provide a mechanism for shock synthesis of prebiotic molecules at realistic impact conditions that is independent of external features such as the presence of a catalyst, illuminating UV radiation, or pre-existing conditions on a planet.

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