

Dynamics of autocatalytic reaction networks and the origin of life

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An important and open question in understanding the origin of life relates to the origin of self-assembling and self-sustaining organized structures. One of the puzzles is the origin of long molecules such as proteins and RNA molecules starting from much smaller precursors that were abundant on the prebiotic earth, and their buildup in sufficient concentrations to seed life. We use a mathematical model based on an artificial but prebiotically plausible chemistry to investigate how certain specific chemical species can be selected out of a large set of possible combinations. We start by considering a set of small molecules that represent simple molecular species that might have been abundantly present around a hydrothermal vent. We then construct a network of chemical reactions amongst these molecules and their reaction products. The chemical dynamics of the molecular populations is simulated as a set of coupled ordinary differential equations. We find that under certain circumstances, autocatalytic sets (ACSs) come to dominate the chemistry in that the concentrations of the molecules belonging to an ACS are much higher than the background. We describe a cascading mechanism by which large and improbable molecules are formed relatively easily in our system, thereby making more plausible the appearance of macromolecules like proteins, RNAs, etc., in pre-biotic settings.

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