

HOW NUCLEOBASES FORMED IN ASTEROIDS AND COMETS: SIMULATING 15 CANDIDATE REACTION PATHWAYS. Ben K. D. Pearce¹ and Ralph E. Pudritz², ¹University of British Columbia, Department of Physics & Astronomy, 6224 Agricultural Rd, Vancouver, BC, ²Origins Institute, McMaster University, 1280 Main St, Hamilton, ON

Introduction: After the late heavy bombardment on the early Earth [1], the rate of meteorite and comet impacts dropped low enough for the planet to cool and sustain liquid water. At that time, it is conceivable that meteorites, comets and interplanetary dust particles could have delivered a variety of important biomolecules, including the nucleobases that would then polymerize to form the first chains of RNA and DNA.

This theory of the planetesimal (asteroidal) and cometary origin of the primeval Earth nucleobases is substantiated by the guanine, adenine and uracil found in several carbonaceous meteorites on Earth [2-10]. These nucleobases are thought to be extraterrestrial in origin, though it is currently unknown which reaction is responsible for their synthesis within the parent bodies.

As part of a long term project to understand the formation of biomolecules and their delivery to forming planets, Cobb & Pudritz [11] first collated and displayed the abundances of amino acids in carbonaceous chondrites. Theoretical work on the origin of amino acids by means of aqueous Strecker reactions occurring in planetesimals was then carried out and compared with the meteoritic record [12].

In the current work, we extend the approach to nucleobases by first presenting the available data on nucleobase abundances within meteorites. We then perform an extensive survey of all of the published chemical methods that have been employed or suggested as pathways for the abiotic formation of nucleobases. This survey is presented as a starting point in order to understand the reaction pathway(s) that could occur within planetesimals. The comprehensive list is reduced by disregarding reactions that are unlikely to occur within planetesimals. A final list of 15 candidate nucleobase reaction pathways within planetesimals is then proposed. These reactions are separated into three types: Fischer-Tropsch, non-catalytic and catalytic.

In the second stage of our work, we use equilibrium chemistry software to model the synthesis of these 15 candidate reactions within a planetesimal environment. Given initial reactant concentrations, this software calculates the resultant molecular abundances that minimizes of Gibbs free energy of the system for a given temperature and pressure. These reactions are run in groups (by type), and individually, to understand

how abundantly they can synthesize while competing and not competing with other reactions.

Results and Discussion: Preliminary results show that Fischer-Tropsch synthesis (for guanine, adenine and cytosine) is the most prolific nucleobase synthesis reaction when reactions are run individually, followed by non-catalytic (usually HCN-based) reactions. Catalytic reactions (starting with neat formamide as the sole reactant) are modeled using the Gibbs free energies of amide due to lack of formamide Gibbs data. These simulations produce no nucleobases.

Simulation of the deamination of cytosine into uracil in an aqueous solution (releasing ammonia in the process) is found to be extremely effective at equilibrium. Simulations of the sole thymine candidate reaction were found to be unproductive until temperatures above 200°C when competing with the synthesis of glycine, and until temperatures above 100°C when competing with the non-catalytic synthesis of the other 4 nucleobases. Since thymine has a half-life of < 100 years at 100°C, and a half-life of < 17 hours at 200°C [13] these simulations suggest that thymine is unlikely to be very productive in planetesimals with any interior temperature.

Therefore these simulations give an excellent explanation of the lack of cytosine and thymine found in meteorites.

Simulations are still currently being run to better understand which reactions are most likely producing the meteoritic nucleobases.

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