

## THEORETICAL STUDIES OF THE EXTRATERRESTRIAL CHEMISTRY OF BIOGENIC ELEMENTS AND COMPOUNDS

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Organic compounds, molecules related to those in living systems, are found in many different extraterrestrial environments. Including among these is interstellar space where over 70 molecules have been discovered. The study of organic astrochemistry is important to exobiology both because it demonstrates the ubiquity of processes which led to life on Earth and because the dust clouds where molecules are found are analogs of the solar nebula from which the Earth formed. In the long chain of events leading from the Big Bang, and a universe composed of atomic hydrogen and helium, to the emergence of life on Earth, molecular interstellar clouds are an early link, the most primitive objects which display any significant organic chemistry. One such cloud was the direct precursor to the solar system and to all objects which it contains.

Theoretical methods are ideally suited to studying interstellar cloud chemistry. They have been applied to determine spectroscopic constants of candidate interstellar molecules, mechanisms of ion-molecule reactions, and composition of dust grains. Accurate predictions of rotational constants and dipole moments of long-chain carbon molecules  $\text{HC}_{13}\text{N}$ ,  $\text{HC}_{15}\text{N}$ , and  $\text{C}_5\text{O}$  have been made to aid determining the size limit of gas-phase interstellar molecules. Models of gas-phase interstellar chemistry use reaction rate constants measured at room temperature and extrapolated to interstellar temperatures. The temperature dependence of  $\text{NH}_3^+ + \text{H}_2 \rightarrow \text{NH}_4^+ + \text{H}$  is anomalous, however, with a minimum rate at about 100K, casting doubt on the extrapolation procedures. The temperature dependence has now been explained.