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Some Unusual, Astronomically Significant Organic Molecules

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Abstract

To date, astronomical surveys have confirmed the existence of over 120 molecules from a variety of extraterrestrial sources. The diversity of the molecular content of circumstellar and interstellar space can only be surmised, and there is continuing debate over the processes by which molecules are formed within these extreme environments. In this thesis we describe experimental and theoretical studies on a number of unusual organic molecules that may have tangible existences in the rarefied environments of space, or in the upper atmosphere of Earth. Stable, neutral precursors of the molecular systems investigated in this work have been generated experimentally via unequivocal pathways by the application of conventional condensed phase synthetic techniques. The molecules, once prepared, were then probed by mass spectrometry. These investigations were supported by computer-based quantum chemical calculations, by which further understanding can be gained about the structures and energetics of the systems under investigation.

Accordingly, various covalently bound, anionic and neutral oxocarbon species, C_nO_m (n = 2, m = 3, 4) were formed and studied. These systems are particularly pertinent to atmospheric chemistry. Additionally, two analogous C_3HX (X = O, S) heterocumulenic systems were investigated. Some isomers of either system, when energised, were shown to undergo gas-phase rearrangement processes.