ACCURATE SPECTROSCOPIC PARAMETERS FOR SMALL HYDROCARBON SPECIES CRITICAL TO DIFFUSE MOLECULAR CLOUDS

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The growth of molecular complexity in diffuse molecular clouds poses an important and interesting puzzle in astrophysics. The molecular inventory known to us currently comprises simple hydrides and small hydrocarbon species (containing up to 3 carbon atoms) on the one hand, and a very large molecule — the fullerene cation C_{60}^+ — on the other. The chemical and physical relationship between the two ends of this dichotomy remains poorly understood, and the species that are intermediate in size have not yet been found, due to the lack of deep astronomical, theoretical, and laboratory searches.

Recently, we have begun a dedicated observing campaign with the 100-m Green Bank Telescope (Abstract 4275) that aims to systematically explore the growth of chemical complexity in diffuse clouds. Some of our key findings include strong absorption by C_3H^+, and perhaps more excitingly, C_4H, which to our knowledge is the largest carbon chain radical detected so far in the diffuse gas. Understanding the presence of these species in the harsh environment of the diffuse gas requires accurate theoretical predictions of the structures and energetics of key reactive intermediates involved in their production. In this talk, I will discuss our efforts to perform high accuracy quantum chemical calculations of several small hydrocarbon species, both as to constrain the relative energetics as well as high precision predictions of spectroscopic parameters to guide laboratory and astronomical searches.