MOLECULES IN LABORATORY AND IN INTERSTELLAR SPACE? 

VENKATESAN S. THIMMAKONDU, Department of Chemistry, Birla Institute of Technology and Science, Pilani, K K Birla Goa Campus, Goa, Goa, India.

In this talk, the quantum chemistry of astronomically relevant molecules will be outlined with an emphasis on the structures and energetics of \( \text{C}_7\text{H}_2 \) isomers, which are yet to be identified in space. Although more than 100’s of isomers are possible for \( \text{C}_7\text{H}_2 \), to date only 6 isomers had been identified in the laboratory.\(^b\),\(^c\),\(^d\) The equilibrium geometries of heptatriynylidene (1), cyclohepta-1,2,3,4-tetraen-6-yne (2), and heptahexaenylidene (3), which we had investigated theoretically will be discussed briefly.\(^e\) While 1 and 3 are observed in the laboratory, 2 is a hypothetical molecule. The theoretical data may be useful for the laboratory detection of 2 and astronomical detection of 2 and 3.

\(^a\)This work is supported by a research grant (YSS/2015/00099) from SERB, DST, Government of India.
\(^b\)Apponi, A. P.; McCarthy, M. C.; Gottlieb, C. A.; Thaddeus, P. Laboratory Detection of Four New Cumulene Carbenes: \( \text{H}_2\text{C}_7, \text{H}_2\text{C}_8, \text{H}_2\text{C}_9 \), and \( \text{D}_2\text{C}_{10}, \text{Astrophys. J.} \ 2000, 530, 357-361. \)
\(^c\)Ball, C. D; McCarthy, M. C.; Thaddeus, P. Cavity Ringdown Spectroscopy of the Linear Carbon Chains \( \text{HC}_7\text{H}, \text{HC}_9\text{H}, \text{HC}_11\text{H}, \) and \( \text{HC}_{13}\text{H}. \text{J. Chem. Phys.} \ 2000, 112, 10149-10155. \)
\(^d\)Dua, S.; Blanksby, S. J.; Bowie, J. H. Formation of Neutral \( \text{C}_7\text{H}_2 \) Isomers from Four Isomeric \( \text{C}_7\text{H}_2 \) Radical Anion Precursors in the Gas Phase. \text{J. Phys. Chem. A.} \ 2000, 104, 77-85.
\(^e\)Thimmakondu, V. S. The equilibrium geometries of heptatriynylidene, cyclohepta-1,2,3,4-tetraen-6-yne, and heptahexaenylidene, \text{Comput. Theoret. Chem.} \ 2016, 1079, 1-10.