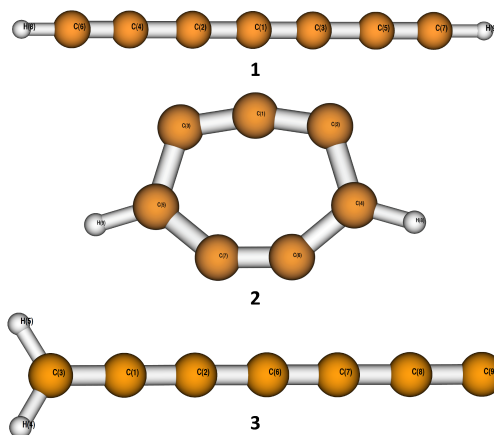


MOLECULES IN LABORATORY AND IN INTERSTELLAR SPACE? ^a

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 C_7H_2 isomers, which are yet to be identified in space. Although more than 100's of isomers are possible for C_7H_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**.



^aTHIS WORK IS SUPPORTED BY A RESEARCH GRANT (YSS/2015/00099) FROM SERB, DST, GOVERNMENT OF INDIA.

^bApponi, A. P.; McCarthy, M. C.; Gottlieb, C. A.; Thaddeus, P. Laboratory Detection of Four New Cumulene Carbenes: H_2C_7 , H_2C_8 , H_2C_9 , and D_2C_{10} . *Astrophys. J.* 2000, 530, 357-361.

^cBall, C. D.; McCarthy, M. C.; Thaddeus, P. Cavity Ringdown Spectroscopy of the Linear Carbon Chains HC_7H , HC_9H , $HC_{11}H$, and $HC_{13}H$. *J. Chem. Phys.* 2000, 112, 10149-10155.

^dDua, S.; Blanksby, S. J.; Bowie, J. H. Formation of Neutral C_7H_2 Isomers from Four Isomeric C_7H_2 Radical Anion Precursors in the Gas Phase. *J. Phys. Chem. A*, 2000, 104, 77-85.

^eThimmakondur, V. S. The equilibrium geometries of heptatriynylidene, cyclohepta-1,2,3,4-tetraen-6-yne, and heptahexaenylidene. *Comput. Theoret. Chem.* 2016, 1079, 1-10.