Unsaturated Carbon Chains

The exploration of unsaturated carbon chains of varying lengths has been a primary focus of the group. The HC$_3$, HC)$_5$, and HC)$_7$ systems have been synthesized and characterized. They are believed to be important molecules in the Interstellar Medium (ISM). Further studies of the substituted RC$_4R$ are currently underway.

A diazo precursor for dimethylpropynylcarbene (1) has been synthesized and matrix isolated. Irradiation of diazo 3 under matrix-isolation conditions leads to triplet dimethylpropynylcarbene (2) which can undergo a hydrogen shift to methylacetylene (2). The photochemistry of the CH$_3$C=CH$_2$ system is still under investigation.

Carbonyl Diazide & Diazirinone

Our interest in prospective molecules to be found in the Interstellar Medium lead us to investigate the metastable molecule diazirinone (7), which can be thermolysed from the explosive carbonyl diazide (8). Under matrix-isolation conditions, carbonyl diazide (7) will photolysate to produce two isomers of CO$_2$ and N$_2$, but diazirinone (6) was not observed (Beekers, H. and coworkers Angew Chem. Int. Ed. 2011). Under thermolysis conditions, diazirinone was made from carbonyl diazide by the loss of two molecules of dinitrogen (Beekers, H. and coworkers Angew Chem. Int. Ed. 2011). Thus far, computational studies of the pathways below have not identified any viable pathway to diazinorim from carbonyl diazide. We hope that further computational studies will solve this puzzle and explain the lack of diazinorin formation.

Benzothiophene Carbones

Computational studies have been carried out on both the 2- and 3-substituted benzothiophene carbones and their possible rearrangement products at the B3LYP/6-31G* level of theory. From the DFT calculations, the 2-benzothiophene system, the following electronic structure (PES) was generated connecting the observed bicyclic product with both molecules of the carbene. Currently studies are underway to finish mapping the PES for the 3-substituted benzothiophene carbene.

Selected Recent Publications


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Funding