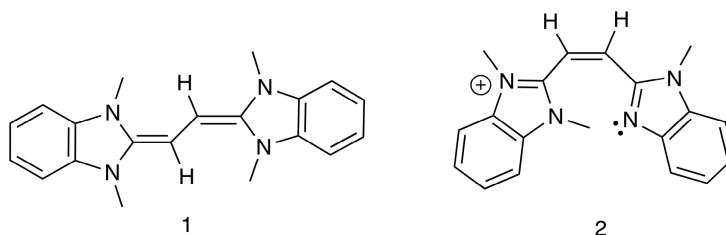


Theoretical Insights to Coordination Chemistry of Carbon: Novel Bonding and New Organic Chemistry

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Consideration of coordination chemistry of carbon, whereby carbon acts as a Lewis acidic centre stabilized by donor ligands, has led to an emerging new field of organic chemistry. Here we report outcomes from theoretical and experimental studies, employing N-heterocyclic carbene (NHC) and cyclic alkyl-amino carbene (CAAC) ligands, to stabilize various C₂ containing fragments [1]. We have discovered a form of ligand-stabilized acetylene (1) [2], featuring a formal double bond that is weaker than a typical C-C single bond [1], and the first example of a diorganoalkene that prefers to adopt a cis- configuration (2) [3-4]. The electronic structure of these systems has been investigated with MO, NBO, QTAIM, I-SAPT, and EDA analyses, to provide an understanding of electronic structure, bonding, and non-covalent interactions. The focus of this presentation will be on the electronic structure and bonding description of these novel species.



References

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