Tata Institute of Fundamental Research
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Webinar

Synthesis and Characterization of Rationally Designed Carbene-Based Kekulé and non-Kekulé Diradicals

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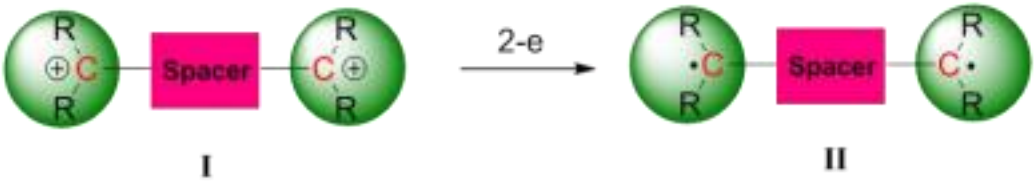
In recent years the synthesis of molecules with having multiple centers of carbon radical is considerably increased for the design of high-spin organic ferromagnetic materials and their potential applications in several fields of modern chemical physics, e.g., in singlet fission, molecular electronics, nonlinear optics, and dihydrogen activation.[1]

We have developed a general synthetic methodology [2] for the synthesis of various carbenes such as cyclic(alkyl)(amino)carbene,[3] acyclic diaminocarbene,[4] diamido carbene, and acyclic(aryl)(amino)carbene-based Kekulé and non-Kekulé diradicals **(II)** from corresponding dications **(I)** without using corresponding carbenes as a precursor. The cyclic(alkyl)(amino)carbene analogue of the Thiele hydrocarbon displays a closed-shell singlet ground state (Kekulé diradical) while the Schlenk hydrocarbon shows two unpaired electrons (non-Kekulé diradical) and undergoes an intermolecular double head-to-tail dimerization. We have also developed a synthetic methodology for anionic boron- and carbon-based heteronuclear diradicals. The incorporation of an electron-deficient heteroatom (boron) leads to open-shell singlets in the ground state and thermally accessible excited triplet states.



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Reference:

1. See selected review: a) M. Abe, *Chem. Rev.* **2013**, *113*, 7011−7088; b) T. Stuyver, B. Chen, T. Zeng, P. Geerlings, F. D. Proft, R. Hoffmann, *Chem. Rev.* **2019**, *119*, 11291−11351.
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11:00 AM