Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad – 500 046

Seminar

Diboron-Centred Diradicaloids, 1,1-Dehydration of Secondary Alcohols, and N-m-Terphenyl Substituted Cyclic (Alkyl)(Amino) Carbenes

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Open shell singlet molecules in general are known for its various photo-physical properties and its subsequent applications in modern-chemical physics.[1] In particular, the open-shell compounds such as diradicaloids involving electron-deficient boron are strikingly different, however their development is in early stage.[2] On the other hand, cyclic(alkyl)(amino)carbenes (CAACs) play an important role for the isolation of extremely reactive compounds in recent time[3] as well as it is known to exhibit transition metal like reactivity.[4] However, to our surprise there was no report of CAAC involving N-m-terphenyl substituent. We have developed a modular methodology for the synthesis of dianionic as well as neutral diboron-centered diradicaloids.[5] At the same time, we have disclosed the 1,1-dehydration of secondary alcohols to the synthesis of CAACs[6] and introduced N-m-terphenyl substituents for the synthesis of CAACs, which exhibit intramolecular aromatic C-H and C-C activation.

References

[1] Selected references are: (a) *Yang et al. J. Am. Chem. Soc.* ***2020***, *142*, 4329–4340. (b) *Reus et al. J. Am. Chem. Soc.* ***2013***, *135*, 12892–12907. (c) Kushida et al. J. Am. Chem. Soc. **2017**, *139*, 14336–14339.
[2] Selected references are: (a) *Scheschkewitz et al. Science* **2002**, *295*, 1880–1881. (b) Grützmacher *et al. Angew. Chem., Int. Ed.* ***2002***, *41*, 4006–4011. (c) Abe, *et al. Chem. Rev.* ***2013***, *113*, 7011–7088.
[3] Das *et al. J. Am. Chem. Soc.* ***2024***, *146*, 9004–9011.
[4] Selected references are: (a) Hopkinson *et al. Nature* ***2014***, *510*, 485–496. (b) Bellotti *et al. Nat Rev Chem.* ***2021***, *5*, 711–725. (c) Kundu *et al. Chem. Sci.*, ***2019***, *10*, 4727–4741.
[5] Lavallo *et al. Angew. Chem. Int. Ed.* ***2005***, *44*, 5705–5709.
[6] Das *et al. Angew. Chem. Int. Ed.* ***2022***, *61*, e202202637.

Friday, Jan 31st 2025

11:30 Hrs (Tea / Coffee 11:15 Hrs)

Auditorium, TIFRH