

Students' Annual Seminar

Bis-*N*-Heterocyclic Olefins Derived Crystalline Dicationic Schlenk Hydrocarbon Diradicals

Priyanka Saha

The synthesis and successful isolation of diradicals are itself very challenging due to their limited stability and tedious synthetic process.^[1] The diradical character of such molecules can be tuned via different strategies. Among them, kinetic blocking at the reactive sites or changing the molecular framework have drawn attention. In the first part of the presentation I will talk about the importance of kinetic blocking in radicals/diradicals along with some of the recent results we obtained. In the second part, I will talk about the influence of changing molecular frameworks between diradical centres. Though the first ever non-Kekulé diradical (known as Schlenk diradical^[2]) with *m*-xylylene as a spacer, was synthesized by Schlenk in 1915, its chemistry is still unexplored. Diradicals having *m*-xylylene as a spacer are of great interest as they have a triplet ground state which lies below the lowest singlet state by 9.6 kcal/mol.^{[1],[3]} However, due to its higher reactivity its isolation becomes a challenging task.^[1] Different derivatives of *m*-xylylene have shown improved stability which can be useful in preparing numerous high spin diradicals.^[3] Here we report the synthesis, isolation and characterisation of Bis-*N*-Heterocyclic Olefins Derived Crystalline Dicationic Schlenk Hydrocarbon Diradicals involving *m*-xylylene as a spacer with/without methyl groups at 2, 4 position of the *m*-xylylene moiety.

References:

- [1] Hu *et al.* *Journal of Materials Chemistry C*, **2019**, 22, 6559-6563.
- [2] Schlenk *et al.* *Ber. Dtsch. Chem. Ges.* **1915**, 48, 661-669.
- [3] Rajca *et al.* *J. Am. Chem. Soc.* **2011**, 133, 4750-4753.

Monday, May 1st 2023

10:00 AM (Tea / Coffee 9.45 AM)

Seminar Hall, TIFR-H