**TIFR Centre for Interdisciplinary Sciences** 



## **Internal Seminar**

### Synthetic Strategy of N-Alkyl Substituted Cyclic Alkyl(Amino)Carbene

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Carbene derivatives have played significant role in stabilization of the active catalysts during the catalytic procedure.<sup>[1]</sup> Carbenes of the types Nheterocyclic carbenes (NHCs), Cyclic alkyl(amino)Carbenes (CAACs), Fischer carbenes not only exhibit different catalytic activity but also exhibit different reactivity due to their differences in  $\pi$ -acceptance and  $\sigma$ -donating properties.<sup>[2,3]</sup> The HOMO-LUMO energy gap of the CAACs are lower than that of the NHCs. Due to the low lying LUMO and high lying HOMO in CAACs compared to NHCs, the reactivity of the CAACs are higher than NHCs. However, reaction between NHC and protonated form of the CAAC ligands, i.e., aldiminium salts, leads to the formation of NHC-CAAC heterodimers.<sup>[4]</sup> The molecular structures of the N-tBu and N-iPr substituted aldiminium salts are shown in Figure 1. Although, the examples of N-aryl substituted CAACs containing compounds are large,<sup>[5]</sup> compounds containing N-alkyl substituted CAACs have not been reported. Herein, we have attempted to synthesize the N-alkyl substituted CAAC-NHC heterodimers, and also N-alkyl substituted CAAC containing lowvalent and low-coordinate compounds.





Figure 1: Molecular structure of N-tBu substituted aldiminium salt

#### **References:**

[1] W. A. Herrmann, Angew. Chem. Int. Ed.2002,41, 1290-1309.

[2] V. Lavallo, Y. Canac, C. Präsang, G. Bertrand, Angew. Chem. Int. Ed.2005, 44, 5705-5709.

[3] B. Rao, H. Tang, X. Zeng, L. Liu, M. Melaimi, G. Bertrand, Angew. Chem. Int. Ed.2015,54, 14915-14919.

[4] D. Munz, J. Chu, M. Melaimi, G. Bertrand, Angew. Chem. Int. Ed.2016,55, 12886-12890.

[5] M. Soleilhavoup, G Bertrand, Acc. Chem. Res.2015, 48, 256-266.

# Wednesday, Feb 8<sup>th</sup> 2017 10:30 AM (Tea/Coffee at 10:15 AM) Seminar Hall, TCIS