## Imidazole based ambiphilic ligands for anion sensing, metalation and photophysical properties

## S. Parveen, I. Avinash, G. Anantharaman

## Department of Chemistry, Indian Institute of Technology, Kanpur, Uttar Pradesh 208016,

garaman@iitk.ac.in, sabeeha@iitk.ac.in

Ambiphilic molecules such as phosphine-borane and amine-borane have drawn huge interest recently. Amine borane in particular, has been widely known to be efficient in sensing of hazardous anions such as fluoride and cyanide which can monitored using the fluorimetry. In addition, the coordination properties of P-/N- donor containing borane compounds with various coinage metals had a significant impact in their luminescence properties which can be utilized for various biological or electronic applications.<sup>1,2</sup>

Erstwhile, we have reported a series of backbone heteroatom-substituted imidazoles (SPh, PPh<sub>2</sub>, SiMe<sub>3</sub>, O<sub>2</sub>BPh, I, Br) as a precursors for the synthesis of functionalized NHC-metal complexes.<sup>3</sup> In this work, synthesis of ambiphilic ligand on metal halogen exchange with a Lewis acidic BMes<sub>2</sub> (Mes = mesityl) at the backbone of the imidazole was achieved.<sup>4</sup> Among them, two isomeric boron-phosphine functionalized imidazoles, monoboron-functionalized imidazoles, and its corresponding imidazolium salts were prepared and thoroughly characterized. Their solid-state structures reveal a dimeric B–N adduct that six-membered [C–B– N]2 ring, and a tetrameric B–N adduct that forms an interesting 16-membered macrocycle, among various other monomeric BMes<sub>2</sub>-substituted imidazoles. The fluoride sensing properties of the synthesised BMes<sub>2</sub>-containing imidazoles were studied using UV–vis and fluorescence spectroscopy.

The ideal separation provided by  $P^N$ -type ligand gives room for metal-metal interaction upon the coordination with coinage metals which in turn lead to bright luminescent. Here, the  $P^N$  type ligand synthesised was treated with CuX(X=Br,I) to give L<sub>2</sub>Cu<sub>4</sub>I<sub>4</sub>-type luminescent metal complexes. In addition, metalation of the  $P^N$  ligand with other coinage metal salts such as AgX (X=OTf, NO<sub>3</sub>), AuCl.SMe<sub>2</sub> was also tried. Upon crystalisation, their solid-state structures reveal the cleavage of C-5 BMes<sub>2</sub>



Figure 1. The chemical structure of various compounds synthesised, fluoride sensing and the metalation study of the P^N Ligand.

[1] Bouhadir, G. & Bourissou. D. (2016) Chem. Soc. Rev., 45, 1065.

- [2] (a) Ronga, M. K., Holtrop, F, Slootweg, J. C. & Lammert, K. (2019) Coord. Chem. Rev. 382 57. (b) Kumar, G. R. & Thilagar, P. (2016) Inorg. Chem. 55, 12220
- [3] (a) Karthik, V., Gupta, V., & Anantharaman, G. (2015) Organometallics 34, 3713 (b) Karthik, V., Gupta, V., & Anantharaman, G. (2014) Organometallics 33, 6218 (c) Karthik, V., Bhat, I.A. & Anantharaman, G. (2013) Organometallics, 32, 7006. (d) Gupta, V., Karthik, V. & Anantharaman. G. (2015) RSC Adv. 5, 87888. (e) Avinash, I., Gupta, V., Karthik, V. & G. Anantharaman, G. (2017) J. Organomet. Chem., 851, 104. (g) Avinash, I., Parveen, S. & Anantharaman, G. (2018) J. Indian Chem. Soc. 95, 713.
- [4] (a) Parveen ,S., Avinash, I., & Anantharaman, G. (2020) Inorg. Chem. 59, 5646. (b) Parveen ,S., Avinash, I., & Anantharaman, G. Manuscript under prepartion

## Keywords: Imidazole, ambiphilic; anion sensing; fluoride; luminescence

Authors thank Science and Engineering Research Board (SERB, India, No. SB/S1/IC-49/2012), for funding. Authors also thank IIT Kanpur (SP & IA) for the doctoral fellowship, and the infrastructural facilities.