

## Exploring Metal Ion Coordination and Ring Expansion Chemistry of Modified Purine Derivatives

Ilesha Avasthi<sup>1</sup>, Himanshu Mamtani<sup>1</sup>, Shruti Khanna<sup>1,4</sup>, Sandeep Verma<sup>1,2,3\*</sup>

<sup>1</sup>Department of Chemistry, Indian Institute of Technology Kanpur, Kanpur, Uttar Pradesh, India

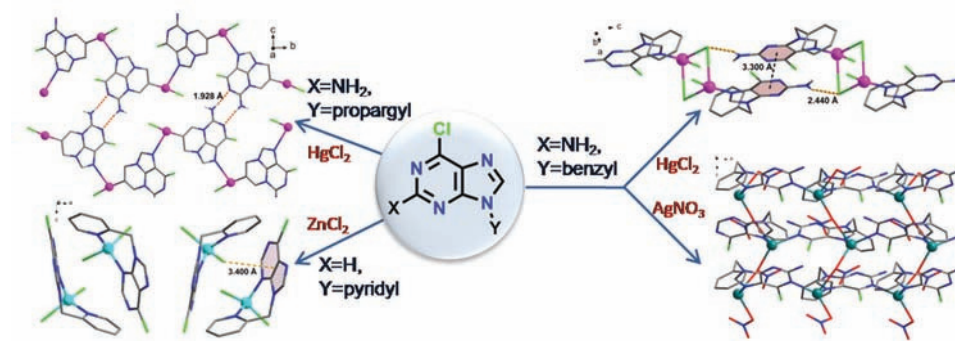
<sup>2</sup>Center for Environment Science and Engineering, Indian Institute of Technology Kanpur, Kanpur, Uttar Pradesh, India

<sup>3</sup>Center for Nanoscience and Soft Nanotechnology, Indian Institute of Technology Kanpur, Kanpur, Uttar Pradesh, India

<sup>4</sup>Department of Chemical Engineering, Indian Institute of Technology Delhi, Hauz Khas, New Delhi, India

(Dedicated to Prof. S.P. Singh on his 80<sup>th</sup> Birthday)

**ABSTRACT** Well-defined coordinating behavior and binding properties of nucleobases with metal ions result in intriguing supramolecular architectures and multidimensional useful coordination polymers. These naturally occurring heterocyclic moieties serve as a versatile tool for the development of interesting potential frameworks for desired applications. We present four complexes of transition metals (Hg, Ag, and Zn) derived from N9-modified 6-chloropurine and 2-amino-6-chloropurine. N9 derivatization involves exploring the influence of aliphatic, aromatic, and heteroaromatic substituents on the coordination behavior of the metals with purines. We also observed an interesting transformation where one complex supported Hg(II)-mediated cyclization followed by the formation of an organomercury adduct.



**KEY WORDS** 6-Chloropurine, Coordination behavior, Crystal, Stabilizing interactions, Metal-nucleobase.