

Structural Diversity of Mercury (II) Complexes Derived from Substituted Pyrazoles

Indranil Chakraborty, Shambhu Kandel and Raphael G. Raptis*

*Department of Chemistry and Biochemistry
Florida International University, Miami, FL 33199*

This work stemmed from our interest in suitable pyrazole-based extractants for removal of both organic and inorganic mercury from low-level nuclear waste (LLW) at the Savannah River Site (SRS). In our exploration we have examined reactions of several substituted pyrazoles with Hg(II) salts, such as HgCl₂ and Hg(CH₃COO)₂. In general, pyrazole derived complexes are quite stable and the 3-, 4-, and 5-positions on this heterocyclic ligand offers the amenability for functionalization with different groups, which dictates the structural diversity and properties of the resulting complexes. Herein we describe the synthesis and crystal structures of Hg(II) pyrazole/pyrazolato complexes prepared under acidic or basic conditions. Due to the varying steric and electronic properties of the pyrazoles employed here, dinuclear and polymeric Hg(II) complexes have been isolated: [Hg₂Cl₂(3,5-Me₂-4-NO₂-pz)₃] (1), [Hg(μ-Cl)Cl(4-I-pzH)]_n (2), [Hg(μ-Cl)₂(4-I-pzH)]_n (3), [Hg₂(CH₃COO)Cl₂(3-NO₂-pz)]_n (4), [HgCl(μ-4-NO₂-3,5-Me₂-pz)]_n (5), [Hg(CH₂COCH₃)(4-NO₂-bis(2,4-dinitrophenyl)pz)]_n (6), [HgCl(2,4,6-Et₃-1,3,5-tris(4-Ph-pz)]_n (7). In these complexes, all possible coordination numbers (from CN = 2 - 6) around Hg (II) centers have been encountered.

