2nd Iranian Student Chemistry Conference
University of Guilan, Rasht, 6-8 Oct. 2015

# The First Coordination Polymers with an $[O]_2[N]P(S)$—Hg Segment

**Elham Torabi Farkhani[a], Mehrdad Pourayoubi[a]*, Pavel V. Andreev[b], Ekaterina S. Shegravina[c]**

[a]*Department of Chemistry, Faculty of Sciences, Ferdowsi University of Mashhad, Mashhad, Iran*
[b]*Department of Physics, N. I. Lobachevsky State University of Nizhni Novgorod, pr.Gagarina, 23-3, Nizhni Novgorod, Russia*
[c]*Department of Chemistry, UNN Lobachevsky State University of Nizhny Novgorod, Gagarin avenue, 23, Nizhni Novgorod, Russia*
*torabielham2010@gmail.com*
*pourayoubi@um.ac.ir*

**Abstract**:

During the last two decades, design and synthesis of novel coordination polymers are attracting more attention[1]. In addition, the coordination chemistry of bidentate ligands has been studied for over thirty years[2]. The bidentate ligands with phosphoryl and thiophosphoryl groups have been used as effective coordinating agents in the different metal chemistry.

In this work two new mercury (II) coordination polymers with thiophosphoryl ligands $\{[C_2H_5O]_2P(S)\}_2X$, X = $NC_4H_8N$ & $NHC_6H_4NH$ are studied:$\{Hg(Cl)(\mu\text{-}Cl)_2Hg(Cl)[(S)P(OC_2H_5)_2NC_4H_8NP(OC_2H_5)_2(S)\}_n$ (1) and $\{Hg(Cl)(\mu\text{-}Cl)_2Hg(Cl)[(S)P(OC_2H_5)_2NHC_6H_4NHP(OC_2H_5)_2(S)\}_n$ (2). The coordination polymers 1 and 2 are the first structural studies of the mercury coordination polymers with the ligands containing an $[O]_2P(S)[N]$ segment. Indeed, any structure with an $[O]_2[N]P(S)$—Hg segment was not found in the Cambridge Structural Database (CSD, version 5.35, updated in February 2014)[3].

In both complexes 1 and 2, the two Hg centers are within an $[S][Cl]Hg(\mu\text{-}Cl)_2Hg[Cl][S]$ segment with a distorted tetrahedral environment for each Hg center. In each structure, the asymmetric unit is composed of half of the monomer related to the other half by a $C_2$ rotation axis. On the other hand, in complex 1 the $NC_4H_8N$ part adopts a nearly chair conformation and the two P═S groups [bonded to nitrogen atoms] bond vectors in opposite side with respect to each other. In complex 2, the $NHC_6H_4NH$ part is nearly planar considering the heavy atoms and the P═S groups bonded to the nitrogen atoms of the noted part adopt an *anti*-conformation with respect to each other.

In both structures, the weak intermolecular C—H…Cl and C—H…S interactions are observed. The spectroscopic features of ligands and complexes are investigated.

**Keywords:** Thiophosphoryl, Mercury(II), Crystal structure, Coordination polymer

## References

[1] O. V. Moroz, V. A. Trush, I. S. Konovalova, O. V. Shishkin, Y. S. Moroz, S. Demeshko, V. M. Amirkhanov, *Polyhedron* **2009**, *28*, 1331.

[2] J. R. Dilworth, N. Wheatley, *Coordinat. Chem. Rev.* **2000,** *199*, 89.

[3] C. R. Groom, F. H. Allen, *Angew. Chem. Int. Ed.* **2014**, *53*, 662.