

## Abstract

A new class of pyrrole-based dialdehyde, *N,N*-bis( $\alpha$ -formylpyrrolyl- $\alpha$ -methyl)-*N*-methylamine, was synthesized in good yields by the Mannich reaction of pyrrole-2-carbaldehyde. The Schiff base condensations of the dialdehyde with diamines afforded several [2+2] macrocycles and [3+2] macrobicycles which were characterized by both spectroscopic and X-ray diffraction methods. In addition, the anion binding properties of the saturated Schiff base macrocycles were studied in solution by NMR titration methods which are supported by their solid state structures.

The Schiff base condensations of the dialdehyde with monoamines afforded open-chain Schiff bases of the type,  $\text{MeN}(\text{CH}_2\text{-}\alpha\text{-C}_4\text{H}_3\text{N-}\alpha\text{-CH=NAr})_2$ . The coordination chemistry of the open-chain Schiff base was studied in details. It afforded different types of Li, Ni(II), Pd(II), and Cu(II) metal complexes which are neutral, cationic and zwitterionic complexes and their structures were determined by single crystal X-ray diffraction analysis. In addition, a few Cu(II) complexes of the dialdehyde and their mixed ligand complexes with 2,2'-bipyridine, phenanthroline and neocuproine were synthesized and structurally characterized. Interestingly, two of the Pd(II) complexes were found to be excellent catalysts for Suzuki cross coupling reactions in water with low catalyst loadings (0.005 to 1 mol% ), in which the products are possibly formed via a mechanism without involving Pd(0) complex.

The Mannich reaction of pyrrole-2-carbaldehyde with piperazine afforded two new dialdehydes differed by the linked atoms which are the pyrrolic N and its  $\alpha$ -C. The Schiff base condensation reactions with diamine and monoamine gave the corresponding macrobicycles and open-chain molecules. The treatment of the open-chain Schiff base with copper carboxylates gave the corresponding dinuclear copper(II) carboxylate complex which are also structurally characterized.

**Keywords:** Schiff Base, Anion Binding, Macrocycles, Macrobicycles, Open-Chain Molecule, Pyrrole-based, Piperazine-based, Amine-Azafulvene, Tautamer, Coordination Chemistry, Mononuclear, Dinuclear, Pentacoordinate, Cationic, Zwitterionic, Variable temperature, Suzuki coupling, Heck reaction, Reduction, Heteroleptic, Mixed Ligand Complex, H-bonding, and Magnetic moment.