

Synthesis and Crystal Structures of a New μ -Bis(tetradentate) Schiff Base Ligand and its Mononuclear Iron(III) Complex: Iron(III) Induced Imidazolidine Ring Hydrolysis of Binucleating Schiff Base Ligand

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The μ -bis(tetradentate) ligand, [C₂₇H₂₆Cl₃N₄O₄], H₃L', 1,3-bis[N-(5-chloro-2-hydroxybenzylidene)-2-aminoethyl]-2-(5-chloro-2-hydroxyphenyl)imidazolidine and its mononuclear iron(III) complex, [Fe(L)](ClO₄), L = N, N'-bis(5-chloro-2-hydroxybenzylidene)-triethylenetetramine have been synthesized and their crystal structures determined. Minimum energy conformations of the ligand were calculated (MOPAC, AM1) as a function of two torsion angles and the results compared with optimized crystal structure. The ligand (H₃L') reacts with Fe(ClO₄)₂ · 6H₂O in aqueous methanol to form the mononuclear [Fe(L)](ClO₄) complex with the imidazolidine ring cleaved by hydrolysis. The complex has an N₄O₂ donor atom set forming a distorted octahedral coordination geometry around the metal atom as established from a crystal structure determination. The terminal oxygen donor atoms occupy *cis* positions, and the remaining four nitrogen atoms (two *cis* amine and two *trans* imine) complete the coordination sphere.

Key words: Schiff Base, Iron Complex, Imidazolidine Ring, Crystal Structure, Conformational Analyses