



Bivalent metal complexes of a novel Schiff base of vitamin B6: green synthesis, characterization, DFT studies, AIM analysis and antibacterial studies

Mehrdad Aleshahidi¹ · Mostafa Gholizadeh¹ · Seyed Mohammad Seyed¹

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Abstract

Herein, a new pyridoxal Schiff base (**HL**) and its Mn(II), Cu(II) and Zn(II) complexes have been synthesized, where the used amine in Schiff base formation was 4-aminopyridine. All of the investigated compounds have been synthesized in methanol as well as two choline chloride deep eutectic solvents. The synthesized compounds have been characterized by using IR, NMR, Mass and UV–Vis spectroscopic methods. Also, the optimized geometries, the tautomerism, assignment of the NMR chemical shifts and IR bands as well as exploring the frontier orbitals of the synthesized species have been calculated using the Density Functional Theory (DFT) approaches. Methanol solution of the **HL** Schiff base involves its Enol tautomer. The deprotonated **L⁻** species acts as an anionic-bidentate ligand in structure of the synthesized [**ML₂**] complexes. The calculated IR wavenumbers and NMR chemical shifts are good in consistent with the corresponding experimental values, confirming validity of the optimized geometries for the investigated compounds. The covalent level and strength of the coordinative bonds as well as the intramolecular H-bonds have been examined using the Atoms In Molecules (AIM) analysis. Complexation to metal ions increased antibacterial activity of the **HL** Schiff base, where the Mn(II) complex showed a considerable antibacterial activity.

Keywords Schiff base · Pyridoxal · Deep eutectic solvent · DFT · Antibacterial activity

✉ Mostafa Gholizadeh
m_gholizadeh@um.ac.ir

¹ Department of Chemistry, Faculty of Science, Ferdowsi University of Mashhad, Mashhad, Iran

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