

## عنوان مقاله:

Synthesis, characterization, theoretical calculation and antimicrobial properties of a new zinc chloride complex

## محل انتشار:

بیست و یکمین سمینار شیمی معدنی انجمن شیمی ایران (سال: 1398)

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## خلاصه مقاله:

Schiff bases derived from aromatic carbonyl compounds have been widely studied in connection3 with metalloprotein models and asymmetric catalysis, due to the versatility of their steric and electronic properties. Schiff bases and their biologically active complexes have been often used as chelating ligands in the coordination chemistry of transition metals as radiopharmaceuticals for cancer targeting, agrochemicals, as model systems for biological macromolecules, as catalysts and as dioxygen carriers. The phenyl derivatives of schiff bases are used as corrosion inhibitors. Schiff bases derived from aldehyde and diamines constitute one of the most relevant synthetic ligand systems with importance in asymmetric catalysis and they appear to be of importance for a broad range of transitionmetal catalyzed reactions including lactide polymerization, epoxidation of olefins, hydroxylation and asymmetric ring opening of epoxides. Schiff bases can be used to obtain optical materials and conducting polymers[1-3]. In this work, we present synthesis and characterization of a new zinc halide complexes with formula of ZnLCl2 in which L= a new ligand formed via condensation of bromobenzaldehyde and bis(2-aminoethyl)amine). The ligand and its complex were characterized by physical and spectral data. After characterization, the ligand and its complex have been subjected to biological standard tests for their antimicrobial activities. Finally, the compound structur was optimized and then some .structural parameters and vibrational frequencies were calculated at the B3LYP/LANL2DZ level of theory

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