

ARTICLE / INVESTIGACIÓN

Synthesis, characterization, biological studies and DFT study of Schiff Bases and their complexes derived from aromatic diamine compounds with cobalt (II)

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Abstract: Based on vanillin and diamine compounds (ortho phenylene diamine; meta phenylene diamine; 3,4-diamine toluidine), derivation of two new Schiff base ligands (L^1 and L^2) was done, after which synthesis and treatment with $\text{Co}^{(II)}$ chloride was performed at a metal-to-ligand ratio of 1:1 to get two new complexes; i.e., $[\text{Co}(L^1)\text{Cl}_2]^+$ and $[\text{Co}(L^2)\text{Cl}_2]^+$. These complexes and ligands were characterized by employing NMR, IR, atomic absorption, UV-visible absorption, molecular weight determination, molar conductivity, and magnetic measurement techniques. As per IR data, the ligands were found to be bi-functional ligands that were linked to two isoquinoline nitrogen sites. It was suggested that these complexes were paramagnetic electrolyte compounds that possessed coordination number four. Screening of the ligands and metal complexes was done to assess the antimicrobial activities against gram-negative and gram-positive bacteria, which was found to show biological activity. Calculations using quantum chemistry were done to examine the molecule geometry. The investigation includes several quantum chemical characteristics derived from frontier molecular orbitals.

Key words: Schiff bases, transition metal complexes, vanillin, diamine aromatic compounds, antibacterial activity, DFT study.

Introduction

The general structure of Schiff bases includes $R-\text{C}(=\text{N}-\text{Ar})-\text{R}'$, where Ar and R represent the aromatic and aliphatic groups due to the condensation of primary amines with ketones or aldehydes. These can be characterized based on the ($\text{H}-\text{C}(=\text{N}-)$) group, which include biological characteristics like antimicrobial¹, antibacterial² and anticancer activities³. Schiff bases derived based on diamines and aldehydes have one of the most critical synthetic ligand systems for asymmetric catalysis. They are considered significant for a wide variety of progress metal catalysis responses, including epoxidation of olefins⁴, lactide polymerization⁵, and the opening of the asymmetric rings of epoxides⁶. The chelating Schiff base ligands derived based on different carbonyl compounds and diamines include a highly notable class of compounds with numerous applications in synthesis^{7,8}, catalytic^{9,10}, clinical¹¹, analytical¹², and biochemical¹³ processes. Previous studies have shown that enhancement of the coordinating potential of diamine compounds like meta phenylene diamine happens when they are combined with different carbonyl compounds. However, the literature at view did not show any studies or research work conducted regarding the transition metal complexes of Schiff bases that have been derived from vanillin and certain diamines. The current research focuses on preparing Schiff bases based on the condensation of vanillin along with certain aromatic diamines and synthesizing their complexes with cobalt (II) ions. These Schiff bases and complexes have been identified based on ^1H NMR, ^{13}C NMR, UV-visible and IR, and atomic absorption techniques. This focus also examined these complexes' conductivity, antibacterial activity, and magnetic characteristics. DFT calculations upheld

the research findings. The ground state characteristics of the ligand and its complexes were studied by DFT at the PBE0 YP/B31G(d,p) and PBE0 YP/B31GZP, respectively.

Materials and methods

Merck provided all the employed reagents, which have been used without purification. The melting point was determined based on a Thermo Fisher apparatus. An FTIR 8400 S Shimadzu spectrometer was employed to record the IR spectra in the 400–1000 cm^{-1} via KBr pellets. An NMR spectrophotometer (Bruker – 500 MHz) was used to record the ^1H NMR spectra of CDCl_3 , while a Jenway Comb conductivity meter was used to measure the conductance in DMF at room temperature. An SPV 705 (Germany) spectrophotometer was used to record the UV-visible spectra in THF. An atomic absorption apparatus (Analyst 200 Atomic Absorption Spectrometer) determined the metal-to-ligand molar ratio. The magnetic properties were measured at room temperature by employing $\text{Hg}[\text{Co}(\text{NCS})_4]$ as the calibrant based on the Gouy method.

Results

Synthesis of Schiff Base Ligands and L^1 and L^2

Vanillin (3.01 gm and 20 mmol) was mixed with diamine (10 mmol) in ethanol (50 mL), and a few drops of glacial acetic acid were added. Then reflux mixture for 14–20 hrs. According to the TGA examination, the starting materials

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