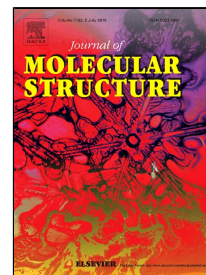


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Synthesis, Characterization, Molecular Modeling, Antioxidant and Microbial Properties of Some Titanium(IV) Complexes of Schiff Bases

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Abstract

The titanium(IV) complexes of Schiff bases derived from aroylhydrazine e.g. benzoylhydrazine, salicyloylhydrazine, nicotinic acid hydrazide with aldehyde or ketone are reported and characterized based on UV-vis spectroscopy, (Infra-red) IR spectra, ¹H NMR spectra, mass spectra, magnetic susceptibility and molar conductance measurements. Complexes are found to possess 1:2 (metal:ligand) stoichiometry. The prepared ligands were act as dibasic tridentate ligands. On the basis of experimental evidences octahedral geometry has been proposed for prepared complexes. Geometry was confirmed by the optimized structure obtained from computational study. The synthesized ligands, in comparison to their titanium(IV) complexes, were also screened for their microbial and antioxidant properties.

Keywords: Schiff bases, titanium(IV) complexes, aroylhydrazine, nicotinic acid hydrazide, dibasic tridentate ligands, computational study, octahedral geometry, anti-microbial and antioxidant properties.

1. Introduction

Schiff base ligands are considered as “privileged ligands” [1] because they are easily prepared by condensation between aldehydes and primary amines. The chemistry of transition metal complexes with Schiff bases has played an important role in the development of coordination chemistry as a whole. The field of Schiff base complexes is fast developing because of the wide variety of possible structures for the ligands, depending on the aldehyde and amines used. Many Schiff bases and their complexes have been widely studied because

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