

Research Article

# Synthesis, Characterization, Antibacterial and theoretical Studies of New 1,1'-(1,4-phenylene)bis(N-(4H-1,2,4-triazol-4-yl)methanimine) With some transition metal ions

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## ABSTRACT

A new ligand 1,1'-(1,4-phenylene)bis(N-(4H-1,2,4-triazol-4-yl)methanimine) and its Co(III), Ni(II) and Cu(II) complexes were synthesized. The new ligand and its complexes have been characterized on the basis of their spectra of <sup>1</sup>H-NMR, IR, FTIR, as well as magnetic susceptibility, elemental analysis [CHN], atomic absorption and conductance measurements. The Gauss 09 program has been used for theoretical study of molecular properties by using B3LYP/6-31G\* level of theory. Hyperchem 8 has been used for theoretical accounts using PM3 method to study the electrostatic potential that provided good information about the complexity site. Of the results obtained we can suggest octahedral geometries for Co(III) and square planar geometry for Ni(II) and Cu(II). The ligand and its complex gave a good activity antibacterial.

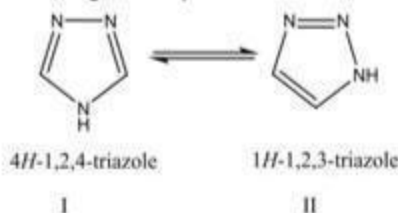
**Keywords:** ligand, complexes, characterization, triazole, antibacterial.

## INTRODUCTION

One of the most important groups in heterocyclic compounds is the five-membered ring, which contains one or more than one atom in the heteroatom system [1] such as triazoles which have three heteroatoms of nitrogen atoms in addition to carbon [2]. The nitrogen-containing heterocycles are commonly found in most of the therapeutic agents. With respect to position of the

nitrogen atoms, the triazole exists in two isomeric forms, the 1, 2, 4-triazole I and the 1, 2, 3-triazole II. Although, 1, 2, 4-triazoles I are considered to be pharmacologically more important isomer. In the last few decades, the chemistry of 1, 2, 4-triazoles and their fused heterocycles has got considerable attention due to their synthetic utility and broad-spectrum biological activity.

Fig. 1: Tautomeric forms of triazole



For example, a number of 1, 2, 4-triazole rings are found in a wide variety of pharmaceutical drugs including antimicrobial agents [3, 4], antibacterial [5], antifungal [6], antimycobacterial [7], anticancer [8], antiviral [9], antitubercular

[10], antimycotic activity [11], anticonvulsants [12], antimigraine agents, anti-inflammatory and analgesic [13], antinociceptive [14], antioxidant [15], anti-urease [16], CNS stimulants, antidepressant [17], anti-anxiety etc. properties