



Geometrical structures, thermal properties and antimicrobial activity studies of azodye complexes



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ABSTRACT

A novel series of metal complexes with 4-(2,3-dimethyl-1-phenylpyrazol-5-one azo)-3-aminophenol ligand (HL) are prepared and characterized by elemental analyses, IR, UV–Visible spectra, ¹H NMR spectra, mass spectra, X-ray diffraction analysis, conductivity measurements and magnetic susceptibility measurements as well as thermal analysis. The IR spectrum revealed that the ligand (HL) coordinates as monobasic tridentate manner with ONO donor sites of nitrogen atom of azo group (—N=N), oxygen atom of the deprotonated phenolic —OH group and exocyclic carbonyl oxygen atom forming a five/six-membered chelate structures. The ¹H NMR spectra data indicated that the phenolic proton is also displaced during complexation. From the magnetic and spectral studies, it was obvious that the geometrical structures of these complexes are octahedral. The molecular structures of the ligand (HL) and its metal complexes are optimized theoretically and the quantum chemical parameters are calculated. The XRD patterns of the ligand (HL) and complex (3) are a mixture of crystalline and amorphous phases. The activation thermodynamic parameters, such as activation energy (E_a), enthalpy (ΔH^\ddagger), entropy (ΔS^\ddagger), and Gibbs free energy change of the decomposition (ΔG^\ddagger) are calculated using Coats–Redfern and Horowitz–Metzger methods. The ligand (HL) and its metal complexes are screened for their antimicrobial activity against, four bacteria (two Gram positive, i.e. *Bacillus subtilis*, *Streptococcus pneumoniae*, and two Gram negative, i.e. *Escherichia coli* and *Pseudomonas aeruginosa*) and two fungi species (*Aspergillus fumigatus* and *Candida albicans*). The obtained data implies that all the complexes have high antimicrobial activities toward *B. subtilis*, *S. pneumoniae*, *E. coli* and *A. fumigatus* than the ligand (HL). In addition to that, complexes (1), (3) and (5) showed antifungal effect against *C. albicans*.

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1. Introduction

Many authors reveal an excellent work devoted to the synthesis and characterization of azodyes as well as their metal complexes [1–4]. The variety of coordination modes of azodye of 3-aminophenol and/or pyrazolone were demonstrated in a number of complexes and their biological applications as well and potentiometric studies have been of considerable interest [5–7]. Many attempts were done to prepare symmetric/asymmetric polydentate ligands in order to achieve rare coordination number with divalent metal ions whose importance was mainly due to their ability to form metal chelates. Due to new interesting applications found in the field of pesticides and medicine, the metal complexes with bi/tridentate O, N/O, N, O types of alternative structures had attracted the attention of chemists [8]. Azo compounds are known to be involved in a number of biological reactions which based on heterocyclic amines have higher strength and give brighter dyeing than

those derived from aniline-based diazo components [9]. Furthermore, they were proved to have biological activity against bacteria and fungi organisms [10,11]. Azo derivatives containing antipyrine moiety have many advantages including color depending effect as an intrinsic property leading to better dye ability.

The data from our laboratory [1,12–14] have demonstrated that the bidentate azodye ligands play a key role in making new complexes with transition metal ions. However, little is known concerning the constitution of these complexes, as well as the chemistry involved in their preparation, or the structural and coordination in such complexes. El-Sonbati et al. [11,15] found that the stability of multiple hydrogen bonded ligands depends not only on the number of hydrogen bonds but also on the hydrogen bonding pattern.

This paper describes the characterization of 4-(2,3-dimethyl-1-phenylpyrazol-5-one azo)-3-aminophenol ligand (HL) and its metal complexes by elemental analyses, IR, ¹H NMR, UV–Vis spectra, X-ray diffractometer, magnetic moment, molar conductance, and thermal analysis. The antimicrobial activity of the ligand (HL) and its metal complexes are studied and comparison of the antimicrobial activity results of the ligand (HL) and its metal complexes with the standard antibacterial and

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antifungal drugs was carried out. The molecular structures of the investigated ligand (HL) and its metal complexes were studied and quantum chemical parameters were calculated. Moreover, the thermodynamic parameters are calculated and discussed.

2. Experimental

2.1. Preparation of the ligand (HL)

The ligand (HL) was prepared as described previously [5,7] by coupling an equimolar amount of 1-phenyl-2,3-dimethyl-4-aminopyrazol-5-one and 3-aminophenol as shown in Fig. 1. In a typical preparation, 25 ml of distilled water containing 0.01 mol hydrochloric acid was added to 1-phenyl-2,3-dimethyl-4-aminopyrazol-5-one (0.01 mol). To the resulting stirred and cooled (0 °C) mixture, a solution

of 0.01 mol sodium nitrite in 20 ml of water was added dropwise. The formed diazonium chloride was consecutively coupled with an alkaline solution of 0.01 mol 3-aminophenol, in 10 ml of pyridine. Immediately, the deep purple precipitate formed was filtered through sintered glass crucible and washed several times by distilled water. The crude product was purified by recrystallization from hot ethanol (yield ~68%) then dried in a vacuum desiccator over anhydrous P₂O₅. The structure of the formed ligand (HL) was established by elemental analyses, IR and ¹H NMR spectroscopies.

2.2. Preparation of complexes

The metal complexes were prepared by the addition of hot solution (60 °C) of the appropriate metal chloride (0.664 mmol) in absolute ethanol (15 ml) to the hot solution (60 °C) of the organic ligand (0.3 g HL)

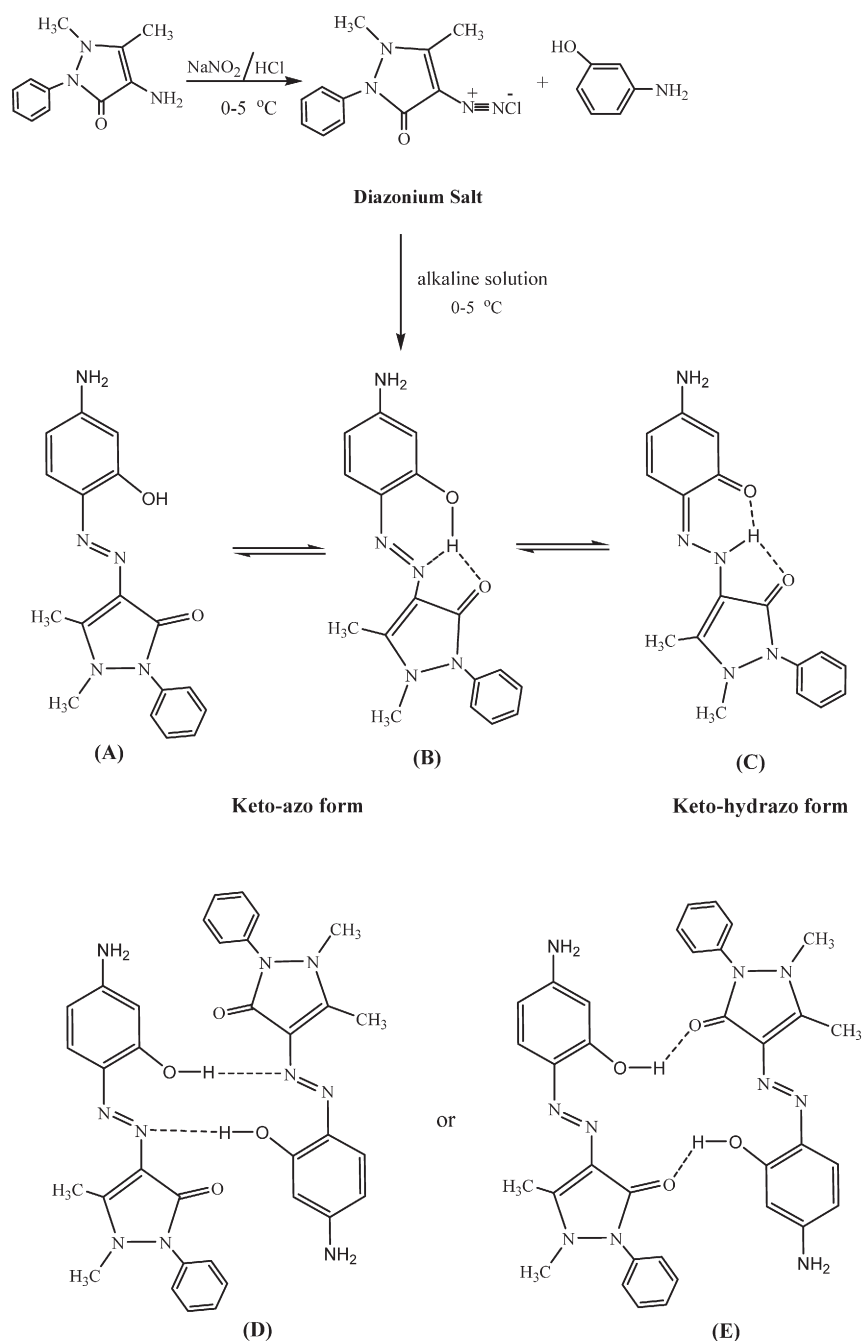


Fig. 1. The formation mechanism and tautomeric structures of the azo ligand (HL).

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