



Synthesis, characterization and molecular modeling of some transition metal complexes of Schiff base derived from 5-aminouracil and 2-benzoyl pyridine



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ABSTRACT

Multidentate Schiff base (H_2L) ligand results from condensation of 5-aminouracil and 2-benzoyl pyridine and its metal chloride (Mn(II), Co(II), Ni(II), Cu(II), Zn(II), Pd(II), Fe(III), Cr(III), Ru(III), Zr(IV) and Hf(IV)) complexes were prepared. The structural features of the ligand and its metal complexes were confirmed by elemental analyses, spectroscopic methods (IR, UV–Vis, 1H NMR, mass), magnetic moment measurements and thermal studies. The data refer to the ligand coordinates with metal ions in a neutral form and shows different modes of chelation toward the metal atom. All complexes have octahedral skeleton structure, tetrahedrally Mn(II), Ni(II), trigonalbipyramidal Co(II) and square planner Pd(II). Thermal decomposition of complexes as well as the interaction of different types of solvent of crystallization are assigned by thermogravimetric analysis. Molecular modeling of prepared complexes were investigated to study the expected anticancer activities of the prepared complexes. All metal complexes have no interaction except the complexes of Pd(II), Fe(III) and Mn(II).

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1. Introduction

Schiff base compounds exhibit broad biological activity due to their synthetic flexibility, selectivity and sensitivity toward the central metal atom, structural similarities with natural biological substances elucidating the mechanism of transformation and racemization reactions in biological system [1]. They are usable in catalyses, in medicine as antibiotics, anti-inflammatory agents, polymerization of olefins [2] additional to antimicrobial [3] and in industry as anticorrosion agents [4–6]. The Schiff base complexes are concerned to the study of the artificial metalloproteins and metalloenzymes [7–9].

Pyrimidine nucleus are central to the structure of nucleic acid in living cell. Pyrimidine derivatives have biological and therapeutic importance. They are also used as hypnotic drugs for nervous system [10]. Uracils are considered as very important class of pyrimidine derivatives. They exhibit significant pharmacological activity and have antitumor [11], antiallergic and antibacterial activity [12]. Fluorouracil and 5-cinnamoyl-6-aminouracil derivatives are extensively used as anticancer agents [13]. Aminouracil compounds

have a wide applications as starting materials for synthesis of many fused uracil compounds of biological significance. Also, they can be used as a coupling component in synthesized Schiff bases and dyes [13–15].

This work oriented to synthesize the Schiff (E)-5-((phenyl(pyridin-2-yl)methylene)amino) pyrimidine-2,4(1H, 3H)-dione ligand derived from condensation of 5-aminouracil and 2-benzoylpyridine. Also, complexes separated from the reaction of ligand and chlorid salts of Mn(II), Co(II), Ni(II), Cu(II), Zn(II), Pd(II), Fe(III), Cr(III), Ru(III), Zr(IV), Hf(IV) were prepared. All the obtained compounds are investigated by spectral method (IR, UV–vis, 1H NMR and mass spectra, magnetic, thermal and elemental analyses. The molecular modeling of complexes were constructed.

2. Experimental

2.1. Materials and methods

All chemicals were of analytical grade (BDH, Sigma or Aldrich) and were used as they had been received without further purification.

Elemental analyses (C and H) were performed on a Perkin Elmer-2400 elemental analyzer at Main Defense Chemical

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Table 1
Infrared spectral bands and their assignments for ligand.

Band	Assignment	Band	Assignment
3435 (m.b)	ν (OH) of H ₂ O in H.b.	1380 (m), 1315 (w),	ν (C–N) amide
3305 (m)	ν (NH)	1290 (w)	
3224 (sh), 3184 (w),	ν (NH) overtone	1241 (sh), 1221 (w),	CH (in plane bending phenyl ring)
3134 (sh)		1192 (sh), 1128 (s),	
		1090 (sh), 1050 (sh)	
3067 (w)	ν (CH) Ar	621 (s)	Pyridine ring bending in plane
3006 (w)	ν (CH) Py		
2929 (sh), 2863 (m)	ν (CH) (uracil)	980 (sh)	Pyridine ring breathing
1773 (sh), 1729 (w)	ν (C ₂ =O.....H)	935 (sh)	Ring vibration of uracil
1688 (s)	ν (C ₄ =O)	866 (sh), 824 (v.w.)	CH (out of plane deformation)
1610 (w)	ν (C=N) Schiff base	775 (m)	γ (NH) + CH (out of plane mono sub. ph. + 2-sub. py.)
1581 (w)	ν (C=C) + ν (C=N)Py	690 (w)	δ (N–C=O)
1536 (v.w)	ν (C=C) (Pheyl)	621 (s)	Py. ring bending in plane
		556 (m)	ν (C=O) (out plane)
1500 (m), 1445 (m)	δ (NH)	487 (s)	γ (C–C=O)
		411 (m)	ρ (NH) + py. ring bending out of plane

Abbreviations: v; very, s; strong, m; medium, w; weak, b; broad, sh; shoulder.

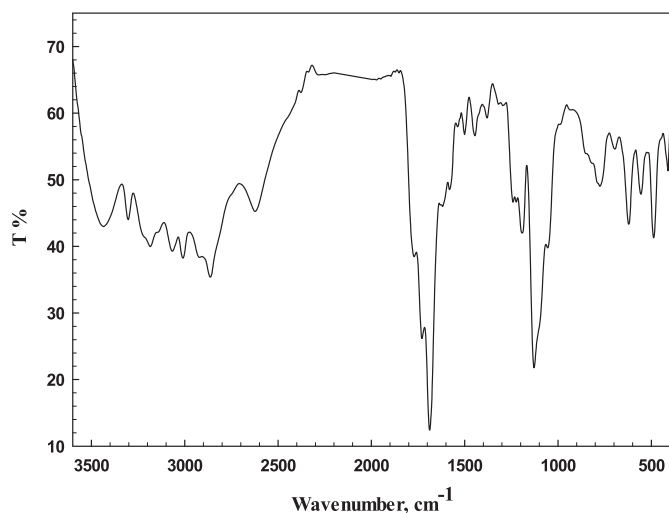


Fig. 1. IR spectrum of Schiff base ligand (H₂L).

Laboratory. Mn(II), Co(II), Ni(II), Cu(II), Zn(II), Fe(III) and Cr(III) ions of metal complexes were determined by complexometric titration [16]. While, Pd(II), Ru(III), Zr(IV) and Hf(IV) were obtained by gravimetric titration [16]. Also, chloride ions were estimated using Mohr's method [16]. Infrared spectra were registered on a Nicolet FT-IR spectrophotometer in the range 4000–400 cm⁻¹. The ¹H NMR spectra were recorded in DMSO-d⁶ on a Varian Gemini 200 NMR spectrophotometer at 300 MHz. The absorption electronic spectra were measured in nujol mulls using a Perkin Elmer Lambda 4B spectrophotometer. Molar conductivity measurements were made in DMSO solution (10⁻³ M) using a type CD6N Tacussel conductimeter. The thermal analysis (TG) was done by using a Shimadzu DAT/TG-50 thermal analyzer with a heating rate of 10 °C/min under N₂ atmosphere with a flowing rate of 20 mL/min from the room temperature up to 900 °C using platinum crucibles. Magnetic susceptibilities were measured at room temperature by a modified Gouy method using a Johnson Matthey magnetic susceptibility balance. Diamagnetic corrections were estimated using Pascal's constants [17]. The effective magnetic moments were calculated from the equation $\mu_{\text{eff}} = 2.84 (X_M^{\text{corr}} T)^{1/2}$, where X_M^{corr} is the molar magnetic susceptibility corrected for diamagnetism of all atoms in the compounds. Melting points were measured using Stuart melting point apparatus.

2.2. Preparation of ligand

The Schiff base ligand (**H₂L**) was prepared by refluxing an equimolar amount (1:1 M ratio) of 5-aminouracil (10 g, 0.01mol) with 2-benzoyl pyridine (14.41 g, 0.01mol) in ethanol, after 3 h a few drops of concentrated sulfuric acid were added to the reaction mixture. The precipitated product was filtered and washed several times with ethanol and dried in a vacuum desiccator over anhydrous CaCl₂ for one day, the reactions were monitored by TLC. The measured melting point of product is 207 °C.

2.3. Synthesis of Schiff base metal complexes

The metal complexes were prepared by adding 0.02 M of appropriate metal chloride salts of Mn(II), Co(II), Ni(II), Cu(II), Zn(II), Pd(II), Fe(III), Cr(III), Ru(III), Zr(IV) and Hf(IV) to 0.01 M of a suspended solution of ligand (**H₂L**) in 50 mL ethanol in (2 M:1 L) molar ratio. The reaction mixture was refluxed at 90 °C for 6 h in the presence of 1 ml of triethylamine. The obtained complexes were filtered off, washed several times with ethanol and dried in a vacuum desiccator over anhydrous CaCl₂ for one day. The measured melting points of all complexes are above 360 °C.

2.4. Molecular docking

Docking studies of the prepared complexes (1–10) were performed by Molsoft ICM 3.4-8C program.

2.4.1. Preparation of the target enzyme

Convert PDB file into an ICM object: The X-ray crystal structure of the enzyme with coumarin ligand DBC, 3,8-dibromo-7-hydroxy-4-methylchromen-2-one (PDB code: 2QC6), [18] was obtained from the protein data bank in PDB format. This conversion involves addition of hydrogen bonds, assignment of atom types, and charges from the residue templates. Click on MolMechanics/convert/protein, and then delete water molecules.

To perform ICM small molecule docking:

Setup Docking Project:

- (1) Set Project Name: Click on Docking/set project name, press OK.
- (2) Setup the Receptor: Click on Docking/Receptor setup, enter the receptor molecule in the receptor molecule data entry box (a*) will do, then click on "identify the binding sites" button to identify the potential ligand binding pockets, press

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