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Bivalent Transition Metal Complexes Of The 2-Oxo-N-(Pyridine-2-Yl)-2-(2-(1-(Pyridin-2-Yl) Ethylidene)Hydrazinyl) Acetamide: Spectroscopic Characterization, Dft, Potentiometric And Biological Studies

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ABSTRACT

Co(II), Hg(III), Cd(II) and Mn(II) complexes of the 2-oxo-N-(pyridine-2-yl)-2-(2-(1-(pyridin-2-yl)ethylidene)hydrazinyl)acetamide synthesized. The isolated compounds illustrated via altered spectroscopic techniques. Potentiometric studies of H_2L with Co(II) in DMSO performed. The antimicrobial and colorimetric assay for compounds that bind DNA achieved.

Keywords: *hydrazones, DFT, DNA, Potentiometry*

1. Experimental

2.1. Preparation of ligand and its metal complexes

The 2- oxo -N- (pyridine-2-yl) – 2 - (2-(1-(pyridin-2-yl) ethylidene) hydrazinyl) acetamide and its Co (II), Mn (II), Cd (II), Hg (II) were synthesized as shown in (Scheme 1).

1.1. Instrumentation

The equipment that used to illustrate the prepared compounds was showed in Scheme 2

1.2. Solutions

All the chemicals used were pure. The used glasses were soaked overnight in (K2Cr2O7 + concentrated H2SO4) mixture washed carefully with bi-distilled water and dried in an oven at 120 ºC.

1.3. Potentiometric measurement

The potentiometric titration was considered the most convenient technique for the determination of the protonation constants of H_2L as well as the stability constants of the Co(II) complex in solution. The experimental method consists of making pH metric titration of hydrogen ion concentration of solutions of the ligand in presence & in absence of the Co (II) ion. The potentiometric titrations were achieved at (298, 308 and 318°) K by using pH–meter HANNA 8519 apparatus. For

The DMOL3 software [16, 17] wasemployed to estimate the gathering calculations. The imitations of geometry optimization of ready solid compounds were accomplished by the intensity functional theory (DFT) *via* the GAUSSIAN 09 software. The DNP base sets were of analogous class to 6-31G Gaussian base sets [18]. The DNP base sets had higher accuracy than Gaussian base sets of the identical scope [19]. Atop base of the general gradient appro- ximation (GGA), the RPBE functional [20] was the maximum excellent exchange-correlation functional [21]. The geometric optimization was performed with no regularity restraint.

1.5. Biological activity

1.5.1. Antimicrobial activity

The minimum inhibitory concentration (MIC) measurement was performed by using disc diffusion method. The organizing discs containing (1.9 – 1000 µg/ml) of compound against gram-positive bacteria (*S. aureus*&*B. subtilis*), gram-negative bacteria (*E.coli*&*P. aeuroginosa*) andfungi (*C. albicans*&*A. flavus*). The microorganism suspensions at 10 CFU/ ml concentration exist immunized to the conforming wells;the plates exist carefully mixing the solution contents a magnetic stirrer was used during the titration process. The buffer solutions of (pH=4 & pH=9) was used to calibrate the pH-meter from time to time. The procedure of experimental included the pH-metric titrations of solution blends arraigns homogeneous NaOH solution ($8.5x10^{-3}$ M) free carbonate in 50% (v/v) DMSO-H_2O at constant ionic strength using KCl solution (1 M).

The solution mixtures were set as shown:

- 1.25 ml ($1.12 x10^{-2}$ M) HCl + 1.25 ml (1M) KCl + 12.5 ml DMSO +10 ml bidstilled H_2O.
- 1.25 ml ($1.12x10^{-2}$M) HCl + 1.25 ml (1M) KCl + 2.5 ml ($5x10^{-3}$M) H_2L + 10 ml DMSO + 10 ml bid stilled H_2O.
- 1.25 ml ($1.12x10^{-2}$M) HCl + 1.25 ml (1M) KCl + 2.5 ml ($5x10^{-3}$M) H_2L + 10 ml DMSO + 0.5 ml ($5x10^{-3}$ M) Co (II) + 9.5 ml bidistilled H_2O.
- The solution was stirred for about 2 min. after adding of each increment of the titrant, and the pH reading is then recorded.

1.4. Molecular modelling

like the percentage of the untreated standard [24].

incubated at 36 C for one day.Ampicillin was used as standard for bacteria while Colitrimazole as standard forfungi. At the end of the incubation epoch, the minimum inhibitory concentrations (MIC) values were recorded as the bottom concentration of the substance that had no visible turbidity. Controls experiments with DMSO and UN inoculated media exist run parallel to the test compounds under the same condition. [22, 23].

1.5.2. Colorimetric assay for compounds that bind DNA

- 100 ml of 0.05 MTris-HCl buffer (pH 7.5) containing 7.5 mm $MgSO_4$ and suspended (20mg)of DNA methyl green was prepared.The mixture was stirred at 37 °C for 24 h. The investigated samples (10,100, 1000 mg) dissolved in absolute ethanol in Ependoff, then adding 200µl of (DNA/methyl green) to all tube. Samples exist incubated in darkness by ambient temperature. After 24 h, the absorbance was
- estimated at 642.5-645 nm. The outcome data wereadapted for initial absorbance and controlled

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