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Synthesis, Characterization and Antibacterial activities of Uracil and Uracil–Oxalate Complexes with Cr(III) and Fe(III)

Abstract- New complexes of the some trivalent transition metal ions of the uracil such as $[M(\text{Ura})_3\text{Cl}_3]$ and mixed ligand metal complexes with uracil and oxalic acid $[M(\text{Ura})_2(\text{OA})(\text{OH}_2)\text{Cl}]\cdot\text{H}_2\text{O}$ type, where (Ura)=Uracil, (OA= Oxalic acid dihydrate, ($M = \text{Cr}^{+3}$ and Fe^{+3}) were synthesized and characterized by the elemental analysis, FT-IR, electronic spectra, mass spectra and magnetic susceptibility as well as the conductivity measurements. Six-coordinated metal complexes were suggested for the isolated complexes of Cr^{+3} and Fe^{+3} with molecular formulas dependent on the nature of uracil and oxalic acid present. The proposed molecular structure for all complexes with their ions is octahedral geometries. The antibacterial efficiency was tested of metal salts, ligands and metal complexes to the pathogenic bacteria activity have been studied.

Keywords- Uracil, Oxalic acid dihydrate, Mixed ligand complexes, Elemental analysis, Spectral studies, Biological efficiency.

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1. Introduction

Coordination complexes are recognized by mixed ligands to play a significant role in biological systems [1-2]. 2,4(1H, 3H)- Pyrimidinedione commonly called through the trivial name Uracil (Ura) was known since 1900 while it was first secluded through hydrolysis of materials including RNA [3-4]. Other names of (Ura) is 2-Oxy - 4-Oxy pyrimidine or 2, 4 - dihydroxy pyrimidine or 2,4 pyrimidine diol, (Ura) structure is shown at Figure 1. (Ura) can as well link for a ribose sugar into composing the ribonucleoside uridine. When a phosphate concern for uridine, uridine 5'-monophosphate is created, nucleosides derived compose (Ura) are called uridine, pseudouridine, and uridine phosphate respectively [5-6]. Uracils have represented a category of compounds that consistently engage organic chemist, biochemists, medicinal chemists and photo biologists [7-10]. (Ura) was detected as RNA components, of which prepared through hydrolysis. Various (Ura) derivatives have been preceded like drugs, so, methylthiouracil [11], propylthiouracil are thyroid inhibitors [12], Uramustine (Uracil mustard) [13-14], Fluorouracil [15-16], and its masked compounds are anticancer agents. The latter interest at the preparation and structural realization from palladium(II) and platinum(II) compound for (Ura) can be referred into a part on the significance from these compounds like catalyst, anti-cancerous drugs, and biology effective compounds. Though many other transition metals are now very significance as

laboratory and industrial platinum and palladium catalysts are still being investigated largely in order that from their spread widely catalytic activity, their relatively inert properties, the anti-cancer activity and usual facial synthesis from their compounds [17-20]. Oxalic acid dihydrate (OA) depending on Figure 1. , the history from oxalates chemistry in long-term coordination and regeneration feature can be seen in recent years. The cause is the bis-chelating capacity from the oxalates at combination through current efforts in the preparation molecular based on materials through higher dimensions. Synthesis and properties from transitions metals compounds for carboxylates is widely studied [21-23]. Trivalent cations of Al(III) and Fe(III) shape strong coordination compounds through numerous chelating organic compounds [24] and it forms stabilize octahedral complexes for ligands like synthesis potassium trioxalato ferrate (III) [25] or chromate (III) [26] and numerous lanthanide – oxalate complexes have been notifying in the last years [27]. It was found that antimicrobial efficiency from several aliphatic carboxylic complexes is higher that the activity from the associated carboxylic acid for zinc (II) compounds [28].

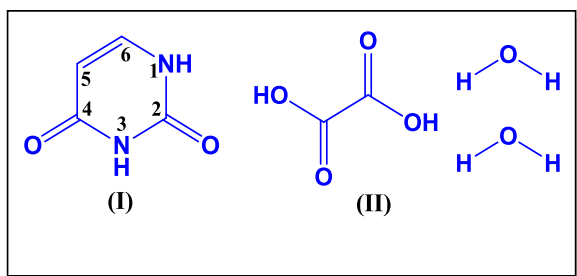


Figure 1: (I) Uracil and (II) Oxalic acid dihydrate

2. Materials and Experimental Procedure

I. Chemical

Uracil and oxalic acid dihydrate were purchased from (Merck and B.D.H.), metals chloride and solvents for (B.D.H., Riedel and Merck). Reagents were utilized without further refining.

II. Physical Mensuration

The measured molar conductance values (Λ_m) in DMF solution for compounds were measured in 25°C of 10^{-3} M solution at samples utilizing PW9527 Digital Conductivity Meter (Philips). The infrared (FT.IR) spectra were registered at 4000-400 cm^{-1} rang for ligands of metal complexes on a Shimadzu IR-470 Spectrophotometer employing KBr pellets. The electric spectra for the complexes in DMF solution (10^{-3}) were observed in 25°C at the 300-700nm rang through a Shimadzu-U.V-160.Altra

Violet-Visible-Spectrophotometer for $1.000 \pm 0.001 \text{cm}$ matched quartz cell. The content of C, H and N of the compounds were specified via the micro analytical unit for Eurverctor EA 3000A Elemental Analyzer. Whilst metal contents from the compounds were appointed through Atomic Absorption Technique (A.A) / Flame Emission Spectrophotometer employing AA-680 Shimadzu. Magnetic susceptibility mensuration was measured employing Bruker magnet BM6 instrument in 298 °K following Faradays the procedure. Melting points were determined through employing Stuart Scientific melting point apparatus. Mass spectra were registered via the 5975C VL MSD for Triple – Axis Detector by the analyzer Quadrupole at 230 °C.

III. General Method for Synthesis of Metal Complexes

The following general procedure was adopted for the synthesis of the complexes:

A. *Uracil Solution*: Dissolve of (Ura) [0.112gm, 1mmol] in 5ml warm water and added [0.04gm, 1mmol] of the sodium hydroxide. B. *Sodium Oxalate Dihydrate Solution*: Dissolve of (OA) [0.126gm, 1mmol] in 5ml warm water and which was added [0.04gm, 1mmol] for the sodium hydroxide depending on the following Figure 2.

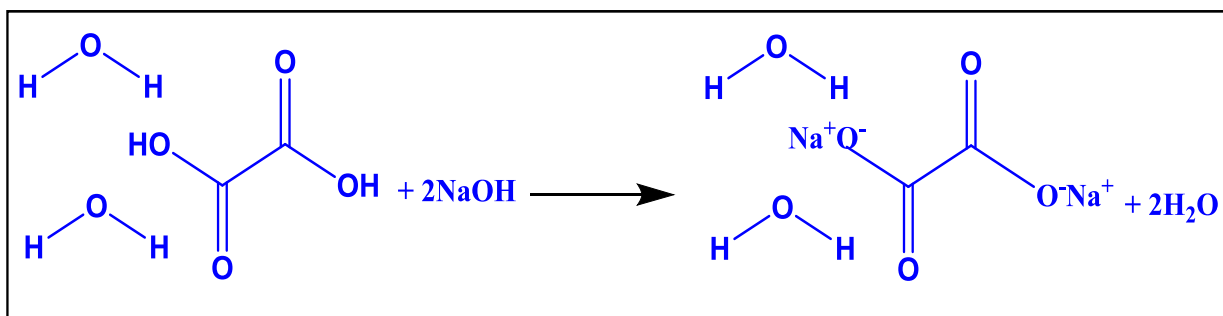


Figure 2: Sodium oxalate dehydrate

IV. Synthesis of the Metal Complexes

A. *Complexes of $[M(\text{Ura})_3\text{Cl}_3]$* : The compounds were prepared through the addition of the (Ura) solution to the warm stirred water solution for the respective metal (III) chloride of $\text{CrCl}_3 \cdot 6\text{H}_2\text{O}$ [0.267gm, 1mmol] and FeCl_3 [0.162gm, 1mmol], in the stoichiometric ratio metal:ligand (M:Ura), (1:3). The mixtures were heated at a water bath to reflux for a period of (30) hour with Cr^{+3} -complex and of the Fe^{+3} - complex for (40) hour at 70 °C. Metal complexes were crystalline residues observed. The precipitated complexes were thereafter filtrated off and washed for ether

followed through desiccation on room temperature and analyzed employing standard manners.

B. *Complexes of $[M(\text{Ura})_2(\text{OA})(\text{OH}_2)\text{Cl}] \cdot \text{H}_2\text{O}$* : Cr^{+3} and Fe^{+3} -complexes were prepared Conventionally by the reaction of oxalic acid hydrate solution and (Ura) solution into the warm stirred water solution of respective metal (III) chloride $\text{CrCl}_3 \cdot 6\text{H}_2\text{O}$ [0.267gm, 1mmol] and of FeCl_3 [0.162gm, 1mmol], in molar ratio 1:2:1 of ratio metal:ligand (M:Ura.:OA). The mixture was heated and refluxed with stirring for (60) hour of Cr^{+3} - complex and the Fe^{+3} - complex for (20)

hour at 70 °C. The colored precipitates were filtered, washed several times with ether followed by drying at room temperature and analyzed utilizing standard methods

V. Study of Biological Efficiency

The antibacterial efficacy into the metal salts, ligands and metal complexes was checked through agar well – diffusion manner [29]. The antibacterial efficacy to the metal salts, ligands, and the congruous complexes were examined with each other versus Gram-positive bacteria (G+ve), (*Staphylococcus aureus* and *Bacillus*) and Gram-negative bacteria(G-ve), (*E.Coli* and *Pseudomonas*) through nutritive agar well - diffusion manner. The solvent applied into work screen patterns and tropical were DMSO, the sample of 1 to 200 µg/ml was utilized. Antimicrobial efficacy to each compound was estimated through the well-diffusion manner. 1cm³ from a 24h broth culture including 10⁶ CFU/cm³ was set at sterilized Petri-dishes. Molten nutritive agar (15cm³) kept in ca. 45 °C was thereafter teeming at the Petri-dishes and pliable into stiffening. Thereafter punctures from 6mm punching diameter neatly utilizing a sterilized cork auger and these were perfectly padded for check solutions. Plates were brood until 24h in 37 °C.

3. Results and Discussion

Stable complexes were isolated in all cases because of metal analysis, spectroscopic data, such as (FT.IR, U.V.and mass) spectra, molar conductance and magnetic susceptibility studies. The public formulation to the complexes can be described accordingly: $M(Ura)_3Cl_3$ and $[M(Ura)_2(OA)(OH_2)Cl].H_2O$ (M=Cr⁺³ and Fe⁺³) in both complexes. The analytical datum with each other for several physical characteristics of the complexes are a bridged at Table 1. [Cr⁺³ and Fe⁺³ – (Ura) complexes] and [Cr⁺³ and Fe⁺³ – (Ura) (OA) complexes] are colored. The compounds are insoluble in water and wide spread organic solvents, but soluble at DMF and DMSO. The molar conductance values about the complexes at DMF in 10⁻³M concentration and the type for non- electrolyte into each compound could be specified [30].

I. FT-IR Spectra

The FT-IR spectrum of the (Ura) and (OA) ligands and the prepared [Cr⁺³ and Fe⁺³- (Ura) and –(Ura)(OA) complexes] have been compared and the datum was Table 2 as well draw the complexes for $Cr(Ura)_3Cl_3$ and

$[Fe(Ura)_2(OA)(OH_2)Cl].H_2O$ according to Figure 3 and 4 .

Broad band that appears at the 3109cm⁻¹ into the free (Ura) ligand and (3101-3112) cm⁻¹ regions to the Cr⁺³ and Fe⁺³-(Ura) and -(Ura)(OA) complexes referred into the –NH stretching vibration. The FT.IR spectrum at (OA) displayed a broad band at 3433cm⁻¹, that was shown into the stretching vibration at U(OH) for H₂O molecular [31]. The appearance of another package broad in the 3412cm⁻¹ and 3437cm⁻¹ regions in the Cr⁺³ and Fe⁺³-(Ura)(OA) complexes are attributed to the OH stretching vibration of hydrated and coordinated H₂O molecules [32] and hydrogen bonds on the type N – H --- O [33]. Moreover, the occurrence for a strong band at the 860cm⁻¹ and 856 cm⁻¹ at the IR spectrum for the complexes, that is attribute into the OH rocking vibration, confirms the existence concerning coordinated water [34]. The absorption frequencies to the metal (III) compounds with (Ura) and (OA) were likened into that for the free (Ura) ligand on the area between (1800 – 1300) cm⁻¹ where the CO and NH frequency of (Ura) is located [35]. The bending vibrations of δNH₍₁₎ and δNH₍₃₎ at 1508 cm⁻¹ and 1419 cm⁻¹ of free (Ura) and on the complexes stay nearly steady both in density and location at 1508cm⁻¹ and (1417-1419) cm⁻¹ respectively. The ν(C₍₂₎=O)band at 1735 cm⁻¹ and 1716 cm⁻¹ in (Ura), that two bands showed, but on the complexes exhibited one band with complexes at (1739- 1700) cm⁻¹ and (1716-1665)cm⁻¹, Wherever shift at one on the packages for evidenced the second package happened. The ν(C₍₄₎=O) band at 1670 cm⁻¹ and 1643 cm⁻¹ in free (Ura) ligand, the small change at the band location for the 4-keto group to the (Ura) complexes and -(Ura)(OA) complexes at (1670-1640)cm⁻¹areas. In addition to FT-IR spectrum display strong proof support the participation of the carboxylic group (COO⁻) on coordination, at comparing with free ligand (OA), a band noticed at 1697 cm⁻¹ due into ν(COO⁻)_{e_{asy}} and the band at 1438cm⁻¹ into the spectrum for (OA), that was appeared into the U(COO⁻)_{sy}. On (OA) spectrum, it was shifted into lower wave number on spectra for mixed ligand compounds with Cr⁺³ and Fe⁺³-(Ura) (OA) complexes, representing coordination for a carboxylic group with metal ions through the oxygen atom, that provides the monotonicity of carboxylate group [36].

These observations were further refined through the occurrence of U(M-O) [37]. The presence of feature bands into the metal – oxygen with 2-keto group of the (Ura) at the (432-435) cm⁻¹ into metal (III) complexes [38].

Table 1: The physical properties of complexes

| Compound | M.W t. | Color | MM. P.* /Dec .** °C | Elemental Analysis | | | | | | | | Molar conductivity Λ_m .cm ² .M ⁻¹ 10 ⁻³ M in DMF | |
|---|-----------|--------------------|---------------------------------|--------------------|----------|-----------|----------|-----------|----------|-----------|-----------|---|-------|
| | | | | %C | | %H | | %N | | %Metal | | | |
| | | | | Cal c. | Fo u. | Cal c. | Fo u. | Cal c. | Fo u. | Ca lc. | Fou. . | | |
| Ura | 112.09 | White | 335 | - | - | - | - | - | - | - | - | - | 17.94 |
| OA | 126.07 | White | (101-102) | - | - | - | - | - | - | - | - | - | 14.37 |
| Cr(Ura) ₃ Cl ₃ | 496 | Dark - Green | >250 Dec. | 29.06 | 28.86 | 2.44 | 2.60 | 16.95 | 17.08 | 10.48 | 8.48 | 30.00 | |
| Fe(Ura) ₃ Cl ₃ | 500 | Brown- Radish | >250 Dec. | 28.83 | 26.28 | 2.42 | 3.08 | 16.81 | 15.18 | 11.32 | 8.95 | 10.18 | |
| [Cr(Ura) ₂ (OA) ₂ (OH ₂ Cl)]H ₂ O | 436 | Green | >250 Dec. | 27.55 | 26.27 | 2.77 | 4.25 | 12.85 | 14.94 | 11.93 | 10.43 | 29.50 | |
| [Fe(Ura) ₂ (OA) ₂ (OH ₂ Cl)]H ₂ O | 439 | Brown | >250 Dec. | 27.36 | 29.21 | 2.76 | 4.23 | 12.76 | 14.58 | 12.87 | 10.35 | 28.77 | |

Table 2: FT-IR spectral data for ligands and complexes

| Compound | $\nu(\text{OH})_{\text{H}_2\text{O}}$ | $\nu(\text{NH})$ | $\nu(\text{CH})$ | $\nu(\text{C}_2=\text{O})$ | $\nu(\text{C}_4=\text{O})$ | $\delta\text{NH}_{(1)}$ | $\delta\text{NH}_{(3)}$ | $\nu_{\text{as}}(\text{CO} + \text{O})$ $\nu_{\text{s}}(\text{CO} - \text{O})$ | $\nu(\text{M} - \text{O})$ |
|--|---------------------------------------|------------------|------------------|----------------------------|----------------------------|-------------------------|-------------------------|---|----------------------------|
| (Ura) | - | 3109w | 3039w 2985w | 1735w 1716w | 1670w 1643w | 1508s | 1419s | - | - |
| (OA) | 3433br. | - | - | - | - | - | - | 1697br. 1438sho | - |
| Cr(Ura) ₃ Cl ₃ | - | 3103w | 3026w 2937w | 1735w 1665w | 1670s 1647w | 1508s | 1417s | 1665w 1390sho | 43s |
| Fe(Ura) ₃ Cl ₃ | - | 3101w | 3039w 2985w | 1700w 1716s | 1670w 1647w | 1508s | 1419s | 1670w 1388sho | 43s |
| [Cr(Ura) ₂ (OA) ₂ (OH ₂ Cl)].H ₂ O | 3412br. | 3112w | 3013w 2987w | 1734w 1665w | 1670w 1643w | 1508s | 1417s | 1665w 1390sho | 49w 43s 5w |
| [Fe(Ura) ₂ (OA) ₂ (OH ₂ Cl)].H ₂ O | 3437br. | 3111w | 2987w 2937w | 1739w 1665w | 1670w 1643w | 1508s | 1419s | 1665w 1392sho | 52w 43s 5w |

s = sharp, br. = broad, w = weak, sho = shoulder

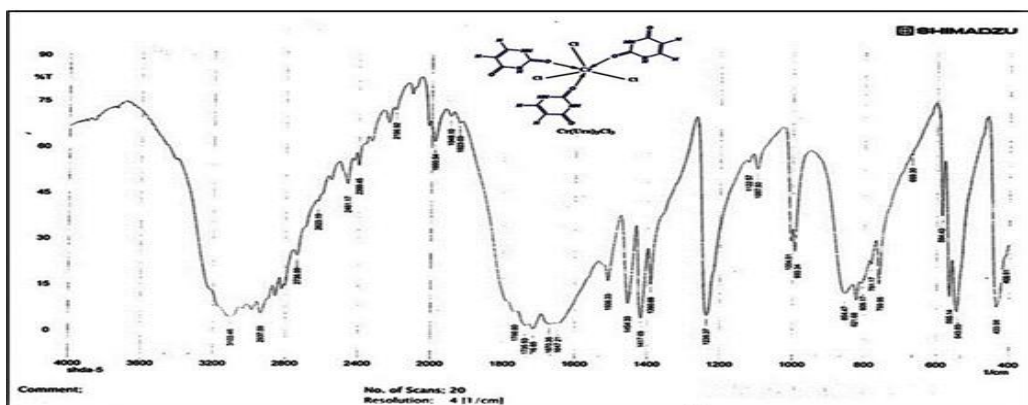


Figure 3: FT-IR spectrum of $\text{Cr}(\text{Ura})_3\text{Cl}_3$ complex

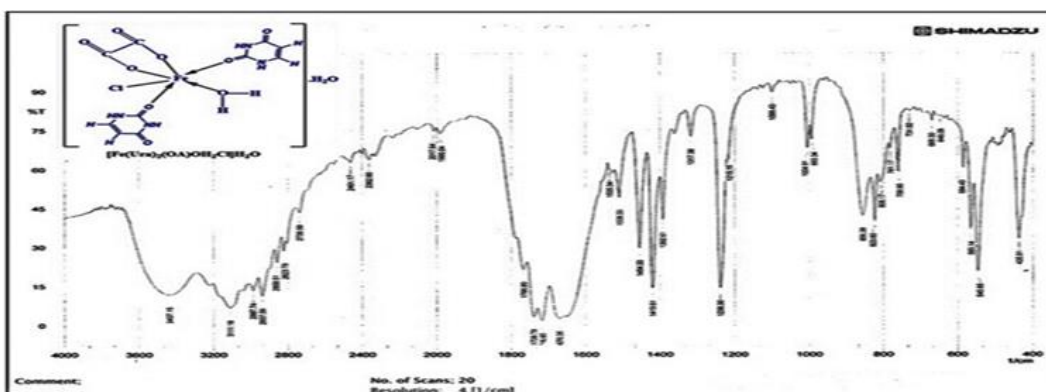


Figure 4: FT-IR spectrum of $[\text{Fe}(\text{Ura})_2(\text{OA})\text{OH}_2\text{Cl}]\cdot\text{H}_2\text{O}$ complex

II. UV Visible Spectra and Magnetic Moments

The UV-Vis spectrum datum to the free ligands (Ura and OA) and complexes were registered at DMSO as point out at Table (3) and (ligands and two complexes) by Figure (5). The UV-Vis spectrum of free (Ura) ligand at 272nm and 349nm assigned to $(\pi-\pi^*)$ and $(n-\pi^*)$ transition of the carbonyl groups respectively [39], while the (OA) ligand shows a peak in 264nm was referred to $(\pi-\pi^*)$ electronic transition [40]

Octahedral Cr^{+3} - complexes are foreseeable to display three spin allowed d-d transitions, in both the Cr^{+3} - complexes at that study only three bands are observed in $\text{Cr}(\text{Ura})$ complex at (271, 305 and 724) nm. The electronic spectrum gave absorption peak at 271nm related for ligand field (L.F), at 305nm related to charge transfer (MLCT). Another peak at 724nm due to $4A_2g(F) \rightarrow 4T_1g(F)$.

The electronic spectrum for $\text{Cr}(\text{Ura})(\text{OA})$ complex offered peaks at 268 nm due into (L.F), and at 394nm, 726 nm and 971 nm that may be display into the $4A_2g \rightarrow 4T_1g(p)$ (U3), $4A_2g \rightarrow 4T_1g$ (U2) and $4A_2g \rightarrow 4T_2g(F)$ (U1) spin allowed d-d transition, respectively [41].

The $\text{Cr}^{+3}(\text{Ura})$ and $\text{Cr}^{+3}(\text{Ura})(\text{OA})$ complexes show μ_{eff} values 3.94 B.M and 3.88B.M., Corresponding to three unpaired electrons, which

suggests a high spin octahedral stereochemistry [42]. The electronic spectra of $\text{Fe}^{+3}(\text{Ura})$ and $\text{Fe}^{+3}(\text{Ura})(\text{OA})$ complexes at 271nm and (273nm and 368nm) due to (L.F) and (MLCT) respectively, and other peaks 421nm and 530nm were assigned to electronic transition type ${}^6A_1g(F) \rightarrow {}^4T_2g(G)$ and ${}^6A_1g \rightarrow {}^4T_1g(G)$ respectively, which obscures the low-intensity d-d absorption bands. The magnetic moment value of both complexes was found μ_{eff} values 5.31 B.M. and 5.72B.M., which was very close to the value of octahedral spatial structure of high spin state [43].

III. Mass spectra for the Complexes

The mass spectra for $\text{Cr}(\text{Ura})_3\text{Cl}_3$ complex of Figure 6, $\text{Fe}(\text{Ura})_3\text{Cl}_3$ complex of Figure 7, $[\text{Cr}(\text{Ura})_2(\text{OA})\text{OH}_2\text{Cl}]\cdot\text{H}_2\text{O}$ complex Figure 8, and $[\text{Fe}(\text{Ura})_2(\text{OA})\text{OH}_2\text{Cl}]\cdot\text{H}_2\text{O}$ complex Figure 9., showed peaks assigned to molecular ions m/z at 496, 500 and 436 and 439 M^+ , respectively.

The pattern of fragmentation complexes does show loss one water molecule, in each of Cr^{+3} and $\text{Fe}^{+3}(\text{Ura})(\text{OA})$ complexes.

The fragmentation patterns of the studies for Cr^{+3} , and Fe^{+3} complexes, respectively, obtained from the mass spectra are given in table 4.

Table 3: Electronic spectra of the studied complexes and two ligands

| Compounds | $\lambda(\text{nm})$ | $\nu(\text{cm}^{-1})$ Wave Number | Assignment of the Transition | μ_{eff} (B.M.) | Suggested Structure |
|---|----------------------|--------------------------------------|---|------------------------------|------------------------|
| (Ura) | 240 | 41666.6 | | $(\pi-\pi^*)$ | - |
| | 349 | 28653.3 | | $(n-\pi^*)$ | |
| (OA) | 264 | 37878.8 | | $(\pi-\pi^*)$ | - |
| $\text{Cr}(\text{Ura})_3\text{Cl}_3$ | 271 | 36900.3 | L.F. | 3.94 | Oh. |
| | 305 | 32786.9 | MLCT | | |
| | 724 | 13812.2 | ${}^4\text{A}_{2g}(\text{F}) \rightarrow {}^4\text{T}_{1g}(\text{F})$ | | |
| $\text{Fe}(\text{Ura})_3\text{Cl}_3$ | 271 | 36900.3 | L.F. | 5.31 | Oh. |
| | 421 | 23752.9 | ${}^6\text{A}_{1g}(\text{F}) \rightarrow {}^4\text{T}_{2g}(\text{G})$ | | |
| $[\text{Cr}(\text{Ura})_2(\text{OA})(\text{O} \text{H}_2)\text{Cl}]\cdot\text{H}_2\text{O}$ | 268 | 37313.4 | L.F. | 3.88 | Oh. |
| | 394 | 25380.2 | ${}^4\text{A}_{2g} \rightarrow {}^4\text{T}_{1g}(\text{P})$ | | |
| | 726 | 13774.1 | ${}^4\text{A}_{2g} \rightarrow {}^4\text{T}_{1g}(\text{F})$ | | |
| | 971 | 10298.7 | ${}^4\text{A}_{2g} \rightarrow {}^4\text{T}_{2g}(\text{F})$ | | |
| $[\text{Fe}(\text{Ura})_2(\text{OA})(\text{O} \text{H}_2)\text{Cl}]\cdot\text{H}_2\text{O}$ | 273 | 36630.0 | L.F. | 5.72 | Oh. |
| | 347 | 28818.4 | MLCT | | |
| | 421 | 23752.9 | ${}^6\text{A}_{1g} \rightarrow {}^4\text{T}_{2g}(\text{G})$ | | |
| | 530 | 18867.9 | ${}^6\text{A}_{1g} \rightarrow {}^4\text{T}_{1g}(\text{G})$ | | |

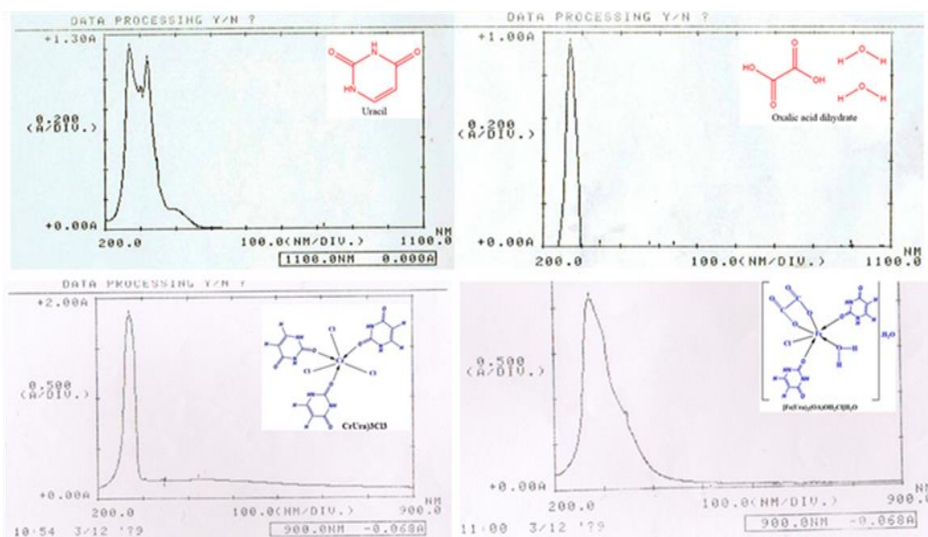


Figure 5: UV spectrum of ligands $\text{Cr}(\text{Ura})_3\text{Cl}_3$ and $[\text{Fe}(\text{Ura})_2(\text{OA})(\text{OH}_2)\text{Cl}]\cdot\text{H}_2\text{O}$ complex



Figure 6: Mass spectrum of $\text{Cr}(\text{Ura})_3\text{Cl}_3$ complex

Figure 8: Mass spectrum of $[\text{Cr}(\text{Ura})_2(\text{OA})(\text{OH}_2)\text{Cl}]\cdot\text{H}_2\text{O}$ complex

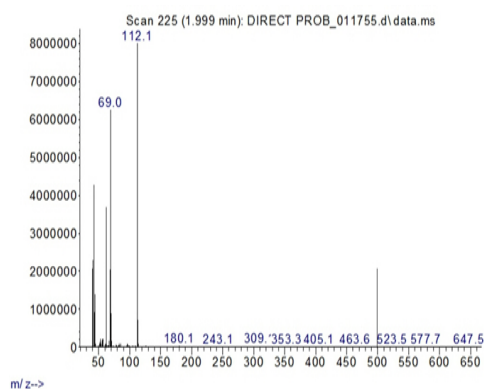


Figure 7: Mass spectrum of $\text{Fe}(\text{Ura})_3\text{Cl}_3$ complex

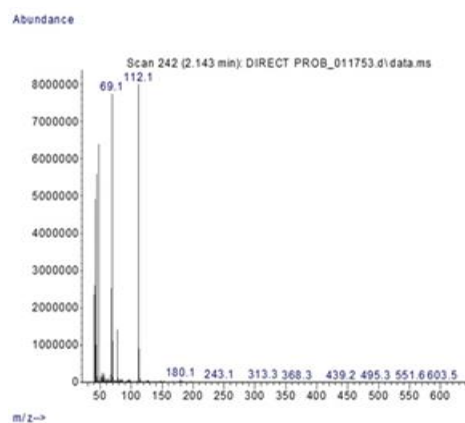


Figure 9: Mass spectrum of $[\text{Fe}(\text{Ura})_2(\text{OA})(\text{OH}_2\text{Cl})]\text{H}_2\text{O}$ complex

Table 4: Mass spectra data of important mass peaks for complexes

| Complexes | Proposed structure | m/z |
|---|---|-----|
| $\text{Cr}(\text{C}_{12}\text{H}_{12}\text{N}_6\text{O}_6\text{Cl}_3)$ | $[\text{CrC}_{12}\text{H}_{11}\text{N}_6\text{O}_6\text{Cl}]^+$ | 423 |
| | $[\text{CrC}_{12}\text{H}_{11}\text{N}_5\text{O}_6]^+$ | 373 |
| | $[\text{C}_{12}\text{H}_9\text{N}_5\text{O}_4]^+$ | 287 |
| | $[\text{C}_{12}\text{H}_5\text{N}_4\text{O}_2]^+$ | 237 |
| | $[\text{C}_{11}\text{H}_4\text{N}_2\text{O}]^+$ | 180 |
| | $[\text{C}_8\text{H}_2\text{N}]^+$ | 112 |
| | $[\text{C}_5\text{H}_2]^+$ | 62 |
| $\text{Fe}(\text{C}_{12}\text{H}_{12}\text{N}_6\text{O}_6\text{Cl}_3)$ | $[\text{FeC}_{12}\text{H}_{11}\text{N}_6\text{O}_6\text{Cl}_2]^+$ | 463 |
| | $[\text{FeC}_{11}\text{H}_9\text{N}_4\text{O}_5\text{Cl}_2]^+$ | 405 |
| | $[\text{FeC}_{11}\text{H}_9\text{N}_4\text{O}_4\text{Cl}]^+$ | 353 |
| | $[\text{FeC}_{10}\text{H}_9\text{N}_4\text{O}_2\text{Cl}]^+$ | 309 |
| | $[\text{FeC}_9\text{H}_7\text{N}_4\text{O}]^+$ | 243 |
| | $[\text{FeC}_9\text{H}_2\text{N}]^+$ | 180 |
| | $[\text{C}_8\text{H}_2\text{N}]^+$ | 112 |
| $\text{Cr}(\text{C}_{10}\text{H}_{12}\text{N}_4\text{O}_{10}\text{Cl})$ | $[\text{CrC}_{10}\text{H}_6\text{N}_4\text{O}_{10}\text{Cl}]^+$ | 430 |
| | $[\text{CrC}_7\text{H}_6\text{N}_4\text{O}_8\text{Cl}]^+$ | 362 |
| | $[\text{CrC}_7\text{H}_6\text{N}_2\text{O}_6\text{Cl}]^+$ | 302 |
| | $[\text{CrC}_7\text{H}_6\text{NO}_4\text{Cl}]^+$ | 256 |
| | $[\text{CrC}_4\text{H}_2\text{NO}_4]^+$ | 180 |
| | $[\text{C}_4\text{H}_2\text{NO}_3]^+$ | 112 |
| | $[\text{C}_3\text{H}_2\text{O}_2]^+$ | 70 |
| $\text{Fe}(\text{C}_{10}\text{H}_{12}\text{N}_4\text{O}_{10}\text{Cl})$ | $[\text{CH}_2\text{O}_2]^+$ | 46 |
| | $[\text{FeC}_8\text{H}_{11}\text{N}_3\text{O}_8\text{Cl}]^+$ | 368 |
| | $[\text{FeC}_6\text{H}_{10}\text{N}_2\text{O}_7\text{Cl}]^+$ | 313 |
| | $[\text{FeC}_6\text{H}_8\text{N}_2\text{O}_5]^+$ | 243 |
| | $[\text{FeC}_2\text{H}_7\text{NO}_5]^+$ | 180 |
| | $[\text{CH}_7\text{NO}_5]^+$ | 112 |
| | $[\text{CH}_4\text{O}_4]^+$ | 79 |
| $[\text{CH}_2\text{O}_2]^+$ | 45 | |

Table 5: Showed the inhibition circle diameter in millimeter for the bacteria after 24h

| Compounds | <i>Bacillus</i> (G+ev) | <i>Staphylococcus aureus</i> (G+ev) | <i>Pseudomonas</i> (G-ev) | <i>E. Coli</i> (G-ev) |
|--|---------------------------|--|------------------------------|--------------------------|
| Control (DMSO) | 0 | 5 | 0 | 0 |
| CrCl ₃ .6H ₂ O | 9 | 12 | 13 | 15 |
| FeCl ₃ | 7 | 12 | 11 | 11 |
| Uracil | 15 | 0 | 20 | 18 |
| Oxalic acid dihydride | 0 | 0 | 11 | 13 |
| Cr(Ura) ₃ Cl ₃ | 0 | 0 | 13 | 14 |
| Fe(Ura) ₃ Cl ₃ | 0 | 0 | 0 | 12 |
| [Cr(Ura) ₂ (Ox)(OH ₂)Cl].H ₂ O | 12 | 9 | 0 | 20 |
| [Fe(Ura) ₂ (Ox)(OH ₂)Cl].H ₂ O | 0 | 0 | 11 | 17 |

IV. Biological Efficiency Study

The outcomes obtained to antibacterial check models studies through agar well – diffusion bioassay uncovered biological efficiency to the metal salts, ligands and metal complexes after 24h in Table 5 and Figure 10. In case of Cr⁺³ and Fe⁺³-(Ura) (OA) complexes, the antibacterial efficiency in *E.Coli* shows the higher inhibition area of 20 mm and 17mm is higher activity from ligands, metal salts and other complexes through comparing with Cr⁺³ and Fe⁺³-(Ura)(OA) complexes. In case (Ura)ligand shows the higher inhibition area of 20 mm and 15mm with *Pseudomonas* and *Bacillus* respectively, as compared to the ligands, metal salts and all complexes. While, in the CrCl₃.6H₂O and FeCl₃ the antibacterial activity in *Staphylococcus aureus* shows the higher inhibition area of 12mm is a higher activity of ligands, and all complexes

4. Conclusions

1. On this paper, we reported the synthesis, spectroscopic and structural study for complexes of Cr⁺³ and Fe⁺³ ions employing (Ura) as a primary ligand and (OA) as a secondary ligand.
2. It may be thus deduced that (Ura) is monodentate ligand into all the status tested coordinating during its carbonyl oxygen and (OA) acts as a bidentate ligand via coordinating by its –O- of –OH group and COO- group at FT.IR. Spectrum study.

3. The study of the spectrum of UV-visible spectra and magnetic moments, all complexes were high spin octahedral stereochemistry.

4. The fragmentation patterns of the studies for Cr⁺³ and Fe⁺² complexes suggested a molecular formula of these complexes was provided through resembling their molecular formula weights with m/z values. The Cr⁺³ and Fe⁺³ – (Ura) complexes show lose three of chlorine, means the present of three chlorine atoms in the field coordination. While in the case of Cr⁺³ and Fe⁺³ - (Ura)(OA) complexes, show lose one of chlorine and one of the water molecule, which those in the field of coordination with a water molecule remaining outside the field of coordination. The structural formula of these complexes was reached by studying these spectra. The structure in Figure 11 and Figure 12 is proposed for the Fe(Ura)₃Cl₃ complex and [Fe(Ura)₂(OA)OH₂Cl]H₂O complexes.

- 5. The current work deals for the antibacterial study of the of these reported compounds. The results of biological screening references compared with metal salt and ligands using four types of bacteria. The outcomes to the biological screening point out that at some complexes, as in case antibacterial efficiency in *E.Coli* for the Cr⁺³ and Fe⁺³-(Ura)(OA) complexes are more active than free ligands, increased efficiency to the complexes can be expounded on the basis for chelation theory [44].

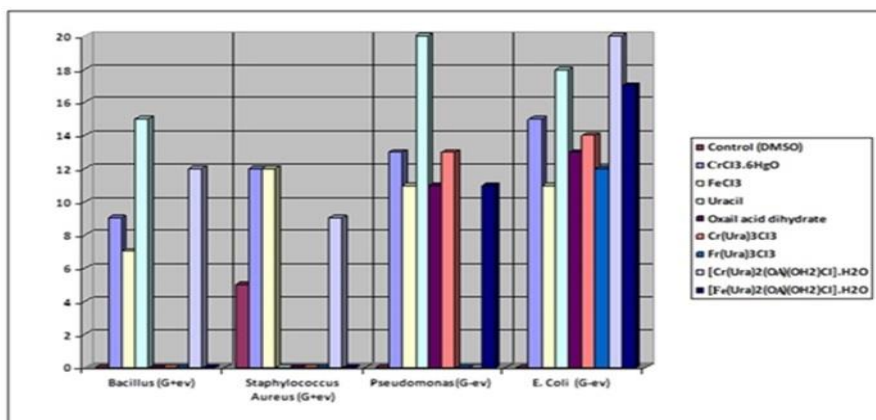


Figure 10: Shows the antibacterial efficiency for metal salts, ligands and complexes against bacteria (*E.coli*, *Pseudomonas*, *Streptococcus* and *Bacillus* pathogenic)

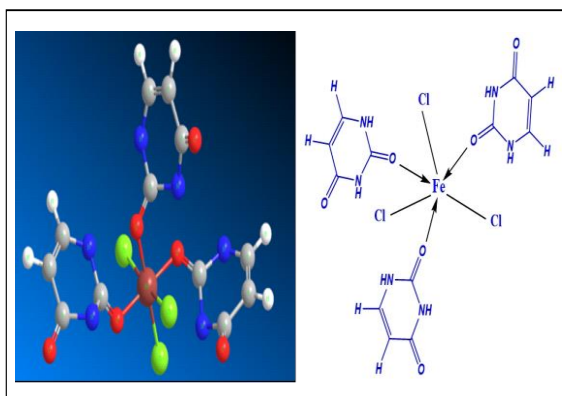


Figure 11: The structure proposed and 3D-geometrical structure of complexes $\text{Fe(Ura)}_3\text{Cl}_3$

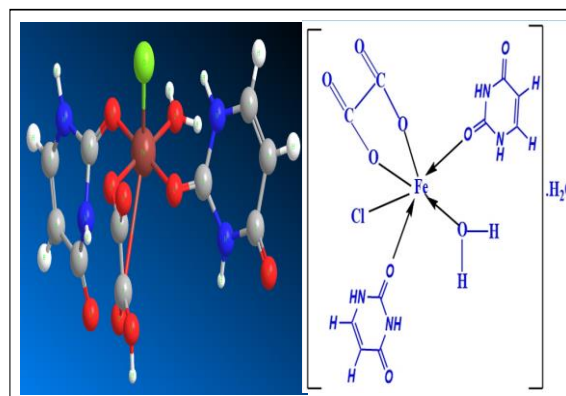


Figure 12: The structure proposed and 3D-geometrical structure of complexes $[\text{Fe(Ura)}_2(\text{OA})(\text{OH}_2).\text{Cl}].\text{H}_2\text{O}$

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