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RESEARCH ARTICLE

Synthesis, Spectroscopic, and DFT Studies of Vanadium (III) Hydroxamate Complex with Potential Biological Applications

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ABSTRACT: A new vanadium (III) hydroxamate complex of composition V(4- $NO_2C_6H_4CH=CHCONHO)_3$ has been synthesized by reaction of VCl_3 with potassium salt of 4-nitrocinnamohydroxamate (4-$NO_2C_6H_4CH=CHCONHO$) in 1:3 molar ratio in dry methanol solvent. The newly synthesized complex is characterized by elemental analysis, molar conductivity, magnetic moment measurements and IR, UV-Vis spectral studies and mass spectrometry. DFT calculations were carried out by using Orca 4.2.1 program and the negative values of the energies of E_{HOMO} and E_{LUMO} for the V(III) complex confirm its stability. A distorted-octahedral geometry around vanadium center has been suggested for complex based upon physicochemical, spectroscopic and DFT studies, involving bonding through hydroxylamine and carbonyl oxygens (O O coordination). The cyclic voltammogram of the complex shows single anodic and cathodic peak. The TGA/DTA curve indicates the single step decomposion of complex. The biological potential of the ligand and complex have been tested by *in vitro* antimicrobial studies and cytotoxicity assay. Antimicrobial activity of complex has been found increased as compare to precursor and ligand. The results of cytotoxicity reveal the complex less toxic as compared to standard drug simvastatin.

Keywords: Vanadium (III) hydroxamate, Hydroxamic acid, DFT studies, Biological applications

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1. INTRODUCTION

Coordination complexes are of growing interest for inorganic chemists because of their different structural and electronic properties [1]. A variety of complexes have been reported in literature owing to their role in biological systems [2-4]. Furthermore, these synthesized complexes have been found with very effective therapeutic applications in pharmaceutical world [5, 6]. The vanadium complexes belong to the class having wide range of applications in diversified field [7-11]. Vanadium found in minerals and biological systems mostly in the form of vanadium (III), (IV) and (V) oxidation states. It is apparent from the scattered reports met in literature on vanadium (III) chemistry than vanadium (IV) and (V) oxidation states; synthesis of their complexes has been a subject of many experimental investigations. In general, the vanadium (III) complexes are prepared by reduction of higher oxidation states [12]. An interesting feature about vanadium(III) ion is to exhibit two different kind of six coordinated complexes i.e. pseudo-octahedral complexes $V(acac)_3$, where acac= anion of 2,4-pentanedione having trigonally distorted geometry and $VX_3(THF)_3$ (X = Cl, Br) having meridional geometries [13]. The vanadium (III) binding capabilities of some [O, O] or [N, O] donor biomolecules in solution have been reported [14]. The vanadium (III) and oxo vanadium (IV/V) complexes with amidate ligands exhibit immense applications, due to their interaction with body proteins [15]. Although vanadium (III) compounds are widely used in industry as polymerization catalysts and its biological relevance, the chemistry of vanadium (III) still remains scant. The therapeutic applications of vanadium (III) in biological system are limited because under physiological condition having pH > 3 it gets rapidly oxidized to vanadium (IV) and

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(V) [16].

Among organic ligands known to form metal complexes, hydroxamic acids (organic bioligands) are of great interest, known to possess immense pathological, toxicological and pharmacological importance [17]. The oxygen abstraction reactions of N-substituted hydroxamic acids with molybdenum (V) and vanadium (III) and -(IV) compounds have been reported [18]. The cobalt(III) complexes with tripodal tetradentate ligand tris (2-methylpyridyl)amine (tpa) with hydroxamate functionality (benzohydroxamate, propionohydroxamate and acetohydroxamate) have been reported to act as model of hypoxia activated prodrugs having low cathodic potential and hence find use in drug delivery [19]. Complex of composition [{Pt(R,R-chxn)}2(μ-bha)]$NO_3.2H_2O$ is known to display promising therapeutic potential against A2780 ovarian cancer cell-lines [20]. A series of hydroxamic acids viz. aceto-, propiono-, benzo-, and p-nitrobenzo) and their O-acetyl and O-benzoyl derivatives are known to display promising activity profile against *Salmonella typhimurium*. The acetylation of different hydroxamates (except p-nitrobenzohydroxamate) markedly enhances the toxic properties which is essential for cytotoxicity [21]. The drugs containing hydroxamate ligands can easily penetrate the biological membrane due to their lipophilicity [22, 23]. Although various vanadium complexes have been reported in literature but vanadium(III) complexes are very few, keeping in mind biological importance of both vanadium as well as hydroxamic acids, we, hereby synthesize a new vanadium(III) hydroxamate complex using VCl_3 as vanadium moiety and potassium-4-nitrocinnamo-hydroxamate as ligand.

2. EXPERIMENTAL DETAILS

2.1. Materials and Method

All reagents were of analytical grade and were further purified before use.

2.2. Synthesis of vanadium (III) hydroxamate

The complex was synthesised by reaction of VCl_3 (0.24 g, 0.0015mol) in THF (5ml) with potassium 4-nitrocinnamohydroxamate (Figure 1) (1.13g, 0.0045 mol) in methanol (20mL) [24, 25].

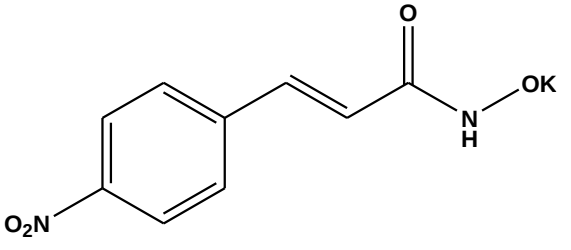
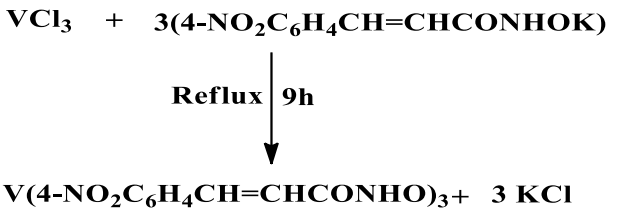


Fig. 1. Chemical structure of Potassium 4-nitrocinnamohydroxamate



Scheme 1. Synthesis of [V(4-NO_2-C_6H_4CH=CHCONHO)$_3$].

The reaction mixture was refluxed for 9 h under nitrogen atmosphere until color changes to dark green. Formation of white solid identified as KCl was observed during the course of the reaction. When no more separation of solid was observed, it was filtered off and the excess of solvent was removed by distillation. The concentrate was dried under vacuum by repeatedly washing with petroleum ether. The green colored solid thus obtained was recrystallized from methanol Yield: V(4-NO_2-C_6H_4CH=CHCONHO)$_3$ (88%) (Scheme 1); Analysis calculated for $C_{27}H_{21}N_6O_{12}V$, (%): C, 48.25; H, 3.15; N, 12.55, V, 7.65. Found: C, 48.21; H, 3.13; N, 12.50; V, 7.58; $\Lambda_m(PhNO_2)$ = 1.06 Scm^2mol^{-1}; μ_{eff} = 2.7 BM [26, 27] .

2.3. DFT Studies

To understand the electronic structures of the potassium 4-cinnamohydroxamate ligand and its V(III) complex, DFT calculations were carried out by using Orca 4.2.1 program package [28] using B3LYP/DeF2-SVP basis set [29, 30]. Optimized geometries and corresponding molecular orbitals energies for ligand and the complex were done using the Chemcraft [31] and Chimera [32] visualization program.

2.4. Biological activity test

2.4.1. Determination by two-fold serial dilution

The hydroxamate ligand, vanadium precursor and synthesized complex was tested in vitro for its biological activity against different selected fungi and bacteria by a reported minimum inhibitory concentration (MIC) method [33, 34] at different concentrations in DMSO (1mg mL^{-1}). All the samples were tested three times. All test cultures were streaked on soya bean casein agar (SCDA) and incubated overnight at 37°C. The MIC assay was performed in a 96-well μL plate. For MIC assay of each drug, a row of 12 wells was used out of which last two wells were taken as control. Each of the ten wells received 100μL of the Muller-Hinton broth, except the first well that received 200 μL of broth containing 500 μg mL^{-1} concentration of the test drug. From the first well (containing test drug), 100 μL broth was withdrawn with a sterile tip and added to the 100 μL of the broth in the second well and contents were mixed four times. Then 100 μL was withdrawn from second well and was added to the third well. In this way a range of two-fold serial

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dilutions were prepared (500-0.98 μgmL^{-1}) in DMSO. The broth in each well was mixed with 2µL of the bacterial culture and then contents were mixed properly. The plate was incubated at 35ºC thereafter and observation for growth of bacteria was recorded after 24h. The results were compared with standard antibacterial and antifungal drugs viz tetracycline hydrochloride and fluconazole respectively (treated control).

2.4.2. Cell culture

Human Cervix Carcinoma (HeLa) cells were trypsinized from a confluent monolayer culture obtained in a 25 cm^2 canted neck flask. The confluent monolayer of the cells was washed twice with phosphate-buffer saline (PBS), pH 7.2 followed by with exposure to Trypsin-EDTA (100 mg % EDTA and 125 mg % Trypsin 1:250; Sigma Chemical Co St Louis, USA) disaggregating solution for two minutes. The disaggregating solution was completely removed by decantation and the enzyme solution treated flask was incubated at 37ºC for three minutes. The disaggregated cells were re-suspended in appropriate volume of Dulbecco's modified Eagels's medium (DMEM) supplemented with fetal calf serum (FCS) (10%, v/V) and adjusted to a cell density of 4×10^3 cells/mL.

2.4.3. In-Vitro Cytotoxicity Assay

In the selected wells of 96-wells tissue culture plate with marked column was added uniform volume of Hep2C cell suspension (200 µL/well). The columns were marked. The sterilized drug compound prepared in DMSO (0.1 M stock) was dispensed in each well of marked coloumn to achieve final concentration of 2, 4, 8, 20 and 28mM. After this the cells treated with drug compound under study were incubated in a CO_2 incubator with 95% humidity at temperature 37ºC for time period of 16-18 h. Each of the drug compound was tested quadruplicate at each concentrations and mean values were calculated after MTT assay (using 5mg mL^{-1} in PBS, 0.1 M pH 7.2 of MTT (1-(4,5-dimethyl-thiazol-2-yl)-3,5-diphenylformazan). DMSO solvent was used to prepare stock solution and also incubated alone to test its effect on viability of the proliferating cells cultured in vitro.

3. RESULTS AND DISCUSSION

3.1. Infrared Spectra

The IR spectra of vanadium precursor VCl_3, potassium hydroxamate and newly synthesized complex were compared. The free hydroxamate ligands absorb in range 1637 cm^{-1} and 1341 cm^{-1} region due to υ(C=O) and υ(C-N) mode respectively. The IR absorption spectra of VCl_3 is known to exhibit absorption bands at 528(w), 473(m), 416(m), 320(vs), 250(m), 205(w) cm^{-1} [35] (Figure 2). The absorption bands due to υ(C=O) mode in free ligand KHL has been observed at 1637 cm^{-1} (Figure 3). It exhibits a shift to lower wave number upon coordination by ketonic oxygen to metal and have been appeared sharp band at 1628 cm^{-1} in complex [36] (Figure 4).

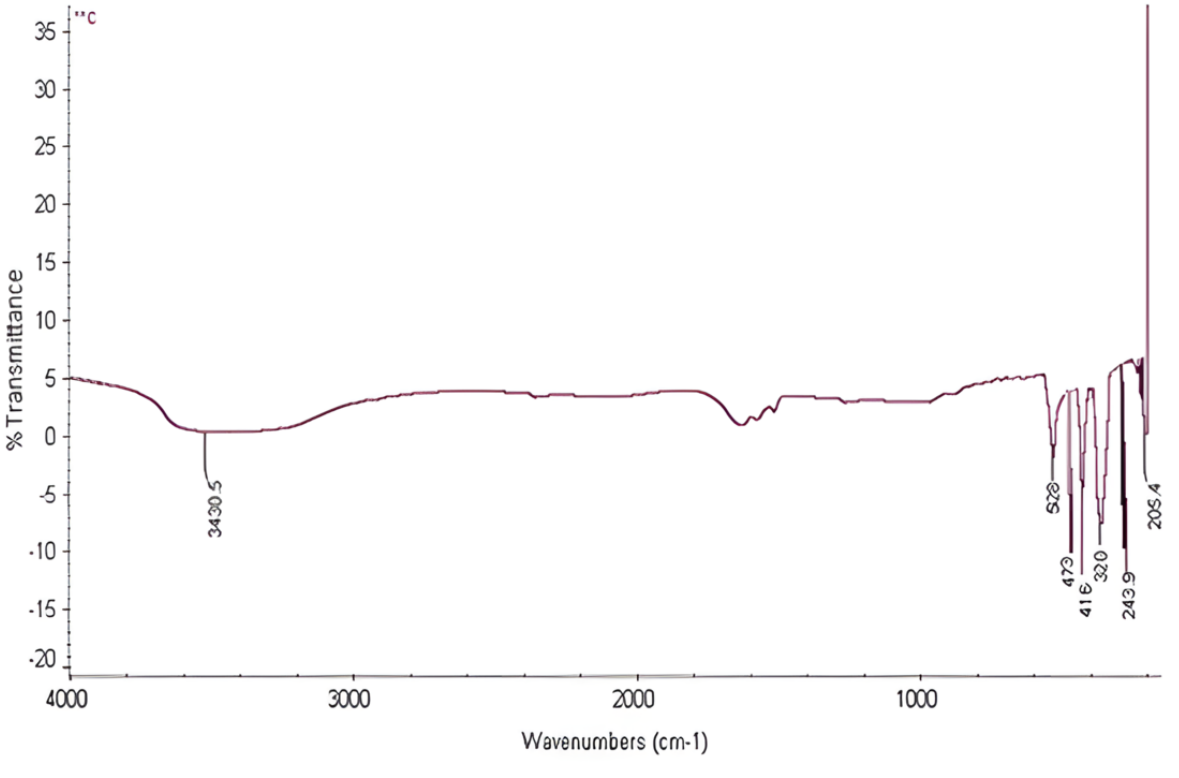

Fig. 2. IR spectrum of VCl_3.

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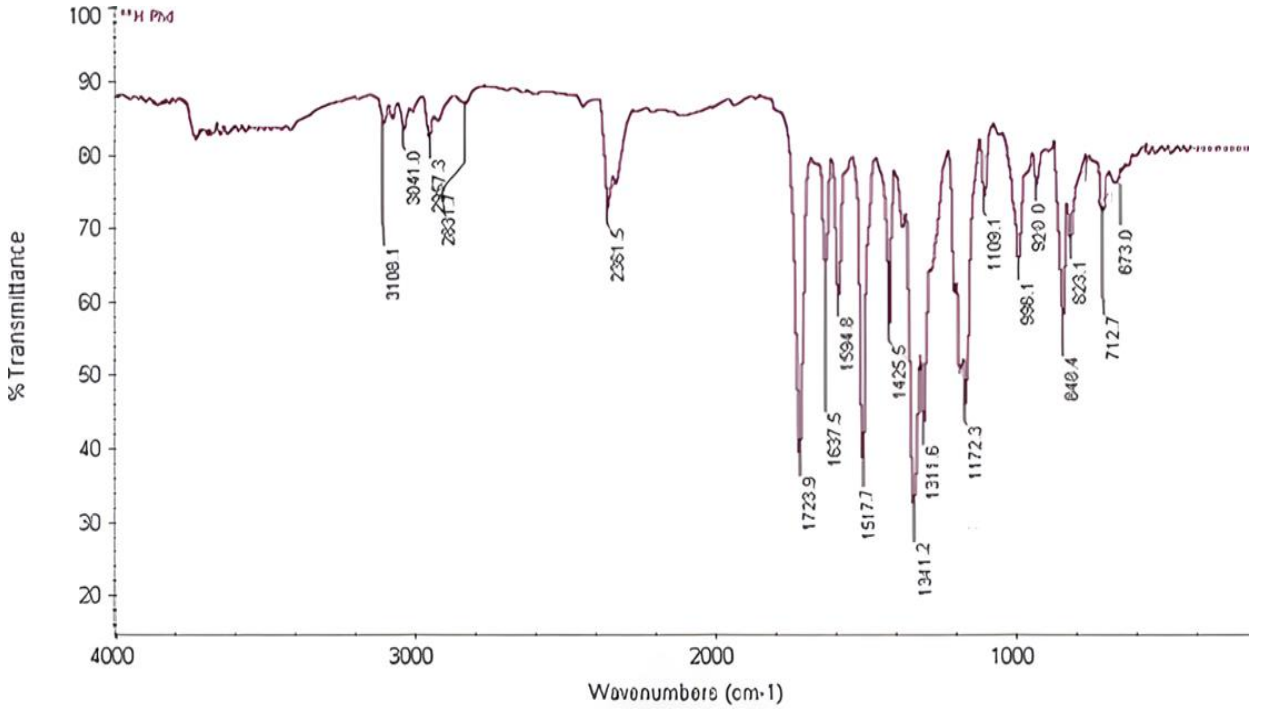

Fig. 3. IR spectrum of Potassium 4-nitrocinnamohydroxamate.

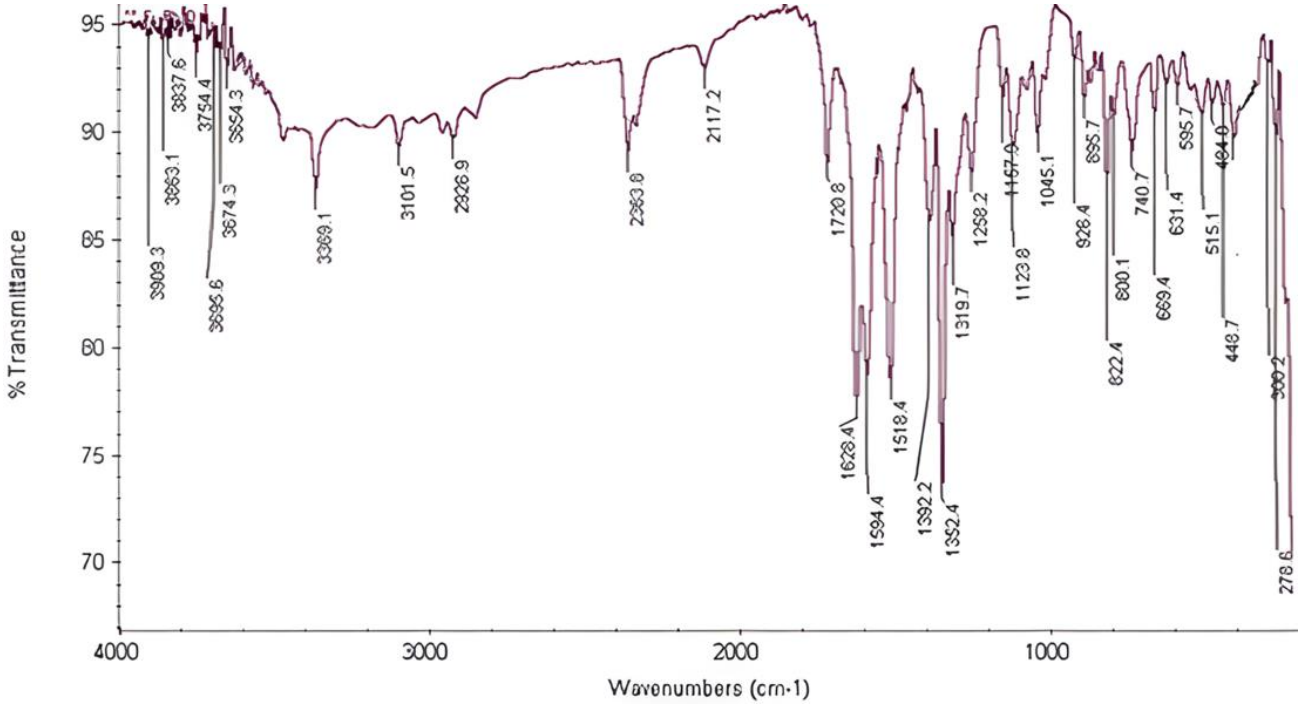

Fig. 4. IR spectrum of tris(4-nitrocinnamohydroxamato)vanadium(III) complex.

The absorption band due to υ(C-N) mode occurring at 1341 cm^{-1} in free ligand has appeared band at 1352 cm^{-1} in complex. The absorption band due to υ(N-O) mode occurring at 920 cm^{-1} in free ligands have been observed to shift to higher wave number at 926 cm^{-1} in complex. A shift in υ(C=O) mode to lower wave numbers and that of υ(N–O) mode to higher region is suggestive of bonding through carbonyl and hydroxylamine oxygen atoms (O,O coordination), establishing thereby bidentate nature of ligands. The absence of bands in 400-300 cm^{-1} region, due to υ(V-Cl) mode further substantiated that all chlorines have been replaced by hydroxamate ions [37]. The occurrence of bands in 596 cm^{-}

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[1]and 515 cm^{-1} region have been assigned to υ(V-O) mode [38].

3.2. Electronic Spectra

Electronic spectra of VCl_3 display absorption bands at 697, 284, 230 cm^{-1} in agreement with literature [39]. Electronic spectra of complex was recorded in 200-900 nm range exhibited two bands at 700 and 545 nm has been assigned to MLCT and LMCT transition respectively in consonance with previous reports on nonoxovanadium complexes [40, 41]. In addition intense high energy bands at 419 nm and 385 nm is ascribed to intraligand charge transfer transition. The two low energy intense bands may be ascribed to spin allowed d-d transitions $^3T_{1g}$ (F) → $^3T_{2g}$ (F) and $^3T_{1g}$ (F) → $^3T_{1g}$ (P) [26]. The higher energy transitions may be ascribed to charge transfer bands and hydroxamate intra-ligand π→π* transitions.

3.3. Mass Spectra

The complex of composition [V(4-NO_2-C_6H_4CH=$CHCONHO)_3$] exhibited base peak at m/z 208 has been assigned to formation of ligand (Figure 5). The peak at m/z 717 (16.43) and 675 (53.33) has been ascribed to $[M+3CH_3]^+$ and $[M+3H]^+$ respectively. The other most abundant fragment ions occurring are at m/z 579 (32.39), 466 (33.65) have been ascribed to $[M-2NO_2-H]^+$, $[M-HL+H]^+$ respectively (Table 1).

Fragmentation pattern of complex is given in scheme 2.

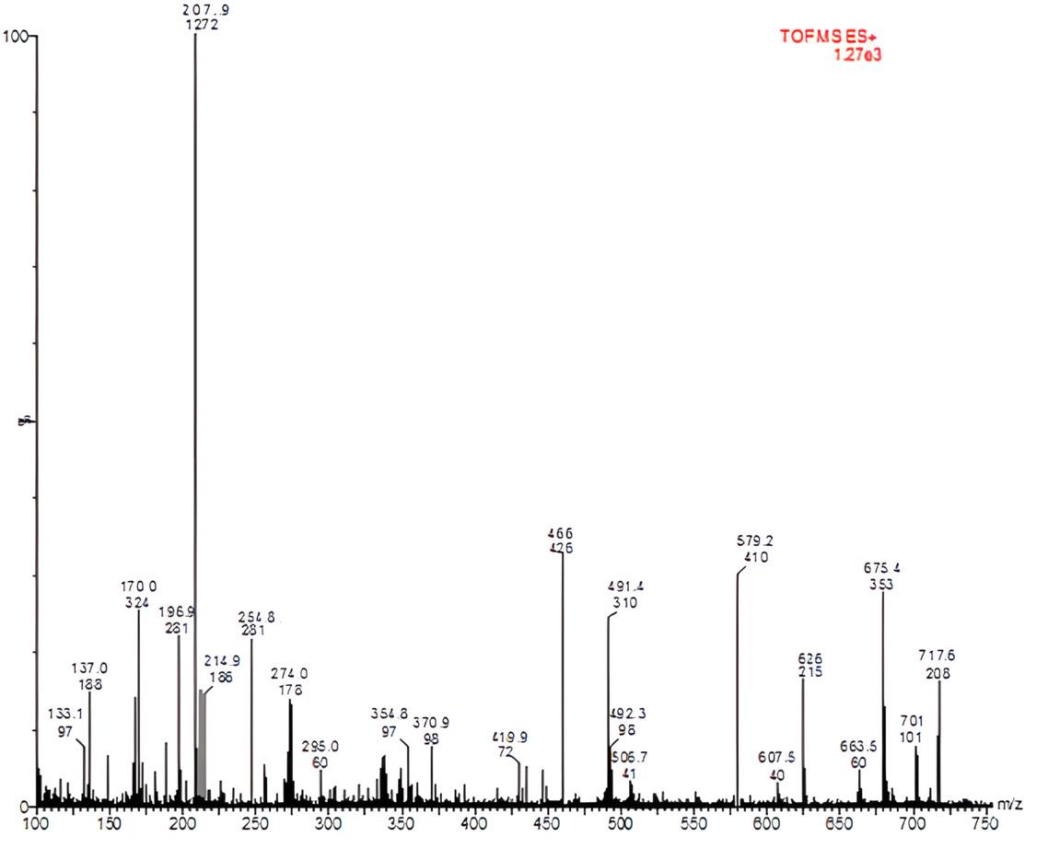

Fig. 5. Mass spectrum of tris(4-nitrocinnamohydroxamato)vanadium(III) complex.

Table 1. Mass spectral data of tris(4-nitrocinnamohydroxamato)vanadium(III) complex.

Complex [V(4-NO_2-C_6H_4CH=$CHCONHO)_3$] [M]	m/z	Int.(%)
$[M+3CH_3]^+$	717	16.43
$[M+3H]^+$	675	53.33
$[M-NO_2]^+$	626	16.99
$[M-2NO_2-H]^+$	579	32.39
$[M-HL^3+H]^+$	466	33.65
$[M-HL^3-NO_2+H]^+$	420	1.58

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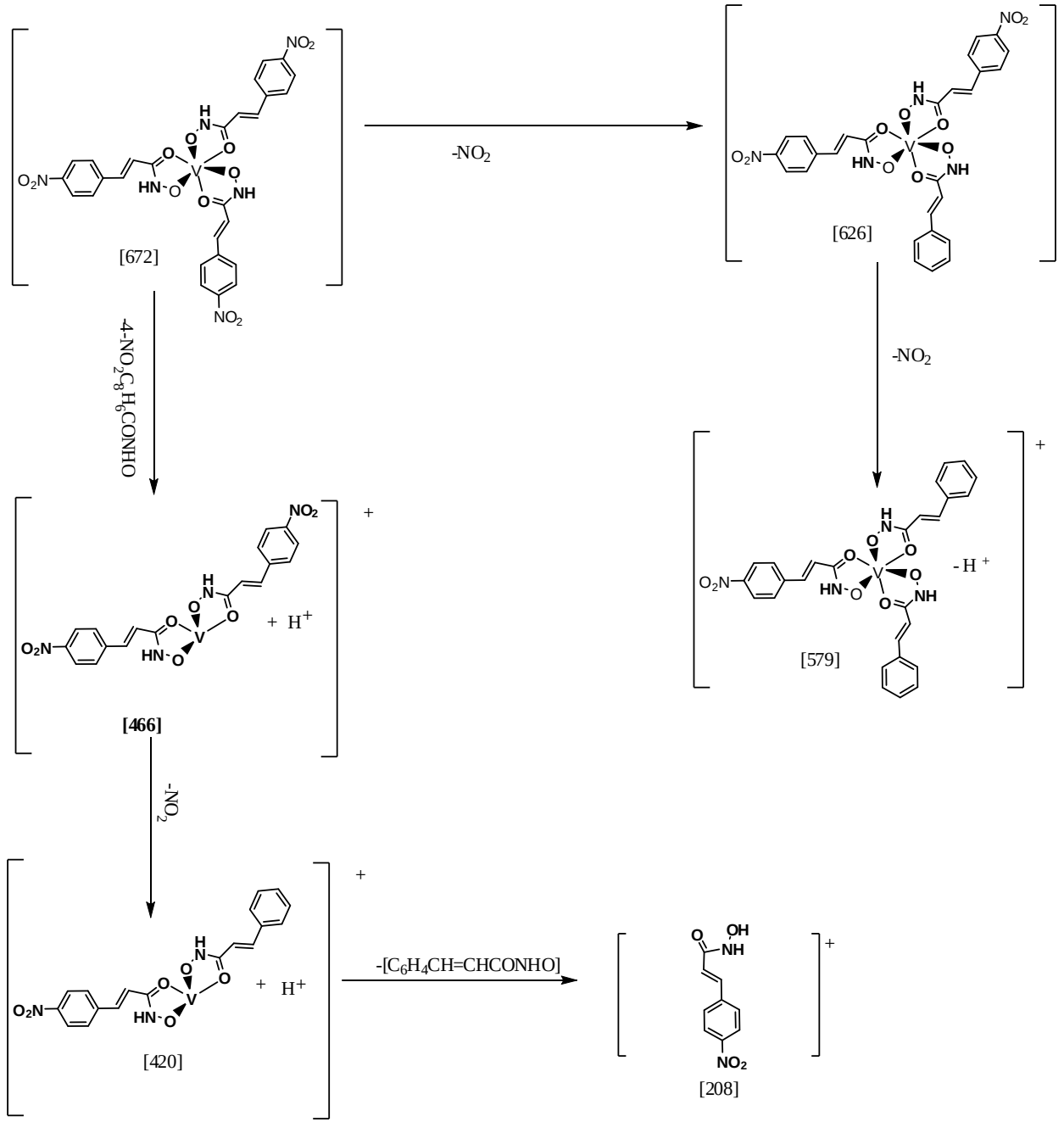
$[HL+H]^+$	208	100



Scheme 2. Fragmentation pathways of $[V(4\text{-}NO_2\text{-}C_6H_4CH{=}CHCONHO)_3]$.

3.4. DFT Calculations

The energy-minimized structures of the ligand and its complex have been displayed in Figure 6 (a and b). The final single point energy for the ligand and the complex has been calculated to be -2.06×10^4 and -8.74×10^4eV respectively. Electronic properties information has been obtained through the frontier molecular orbital (FMO) analysis of the ligand and its complex. For the ligand, the highest occupied molecular orbital (HOMO) is mainly localized on the alkene double bond and the hydroxamate group, while the lowest unoccupied molecular orbital (LUMO) is placed on the whole molecular system, with a band gap of 1.4193 eV. In the case of the complex, HOMO is concentrated on the central part of the molecule, i.e., the donor site of the ligand and the metal ion surrounding it, while the LUMO orbitals are delocalized

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over the entire molecular system, having a band gap of 1.3267 eV. The negative values of the energies of E_{HOMO} and E_{LUMO} for the V(III) complex confirm its stability.

The calculated HOMO-LUMO energy gap for the complex is lower than that of the ligand, strongly supporting complexation. The bond parameters, such as bond lengths and bond angles, for the ligand and the respective complex, have been combined and represented in Table 2. The chemical reactivity parameters were also determined to define the chemical reactivity of a system like Ionization Potential, electron affinity, chemical potential, electronegativity, electrophilicity index, chemical hardness, softness, etc. These are calculated by the energies of HOMO-LUMO orbitals using the expressions:

Electronegativity (χ) = $-(E_{LUMO}+E_{HOMO})/2$

Electrophilicity Index (ω) = $\mu^2/2\eta$

Chemical Potential (μ) = $-\chi = (E_{LUMO}+E_{HOMO})/2$

Hardness (η) = $(E_{LUMO}-E_{HOMO})/2$

The Koopmans' theorem states that ionization potential (I) and electron affinity (A) are the negative energy eigenvalues of the HOMO and LUMO, respectively. It is determined by the energy gap between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) in the frontier molecular orbitals. A complex with a shorter gap between HOMO and LUMO is considered less stable or more reactive compared to the ligand (Figure 7a and b). The higher the electronic chemical potential, the less stable or more reactive the system is. The electrophilicity index (ω) measures the ease with which a species can accept electrons. A high value of ω indicates a good electrophile, while a low value of ω indicates a good and more reactive nucleophile. For V(III), the value of ω is 9.84 eV, which is much greater than for KHL (0.019). This suggests that the complex is a stronger electrophile and electron acceptor than the KHL ligand, which can easily act as a good electron donor and more reactive nucleophile with a lower ω value.

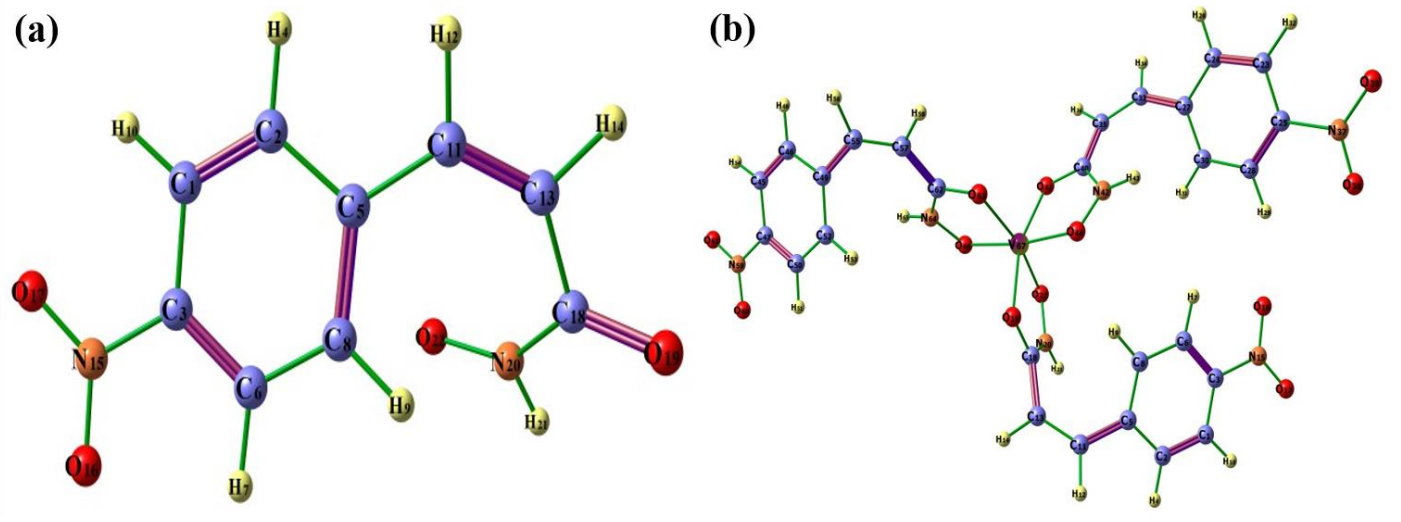

Fig. 6. Energy-optimized geometry for (a) the ligand, and (b) the complex.

Table 2. Chemical reactivity parameters calculated from HOMO-LUMO energies.

Chemical reactivity parameters	KHL	Complex
Final Single Point Energy (eV)	-2.06×10^4	-8.74×10^4
I.E.(eV)	0.5451	4.2778
E.A.(eV)	-0.8742	2.9511
Dipole Moment (D)	3.6122	3.2216
χ	-0.1645	3.6145
η(eV)	0.7101	0.6633
S	0.7041	0.7538
μ(eV)	0.1645	-3.6145
ω (eV)	0.01905	9.848

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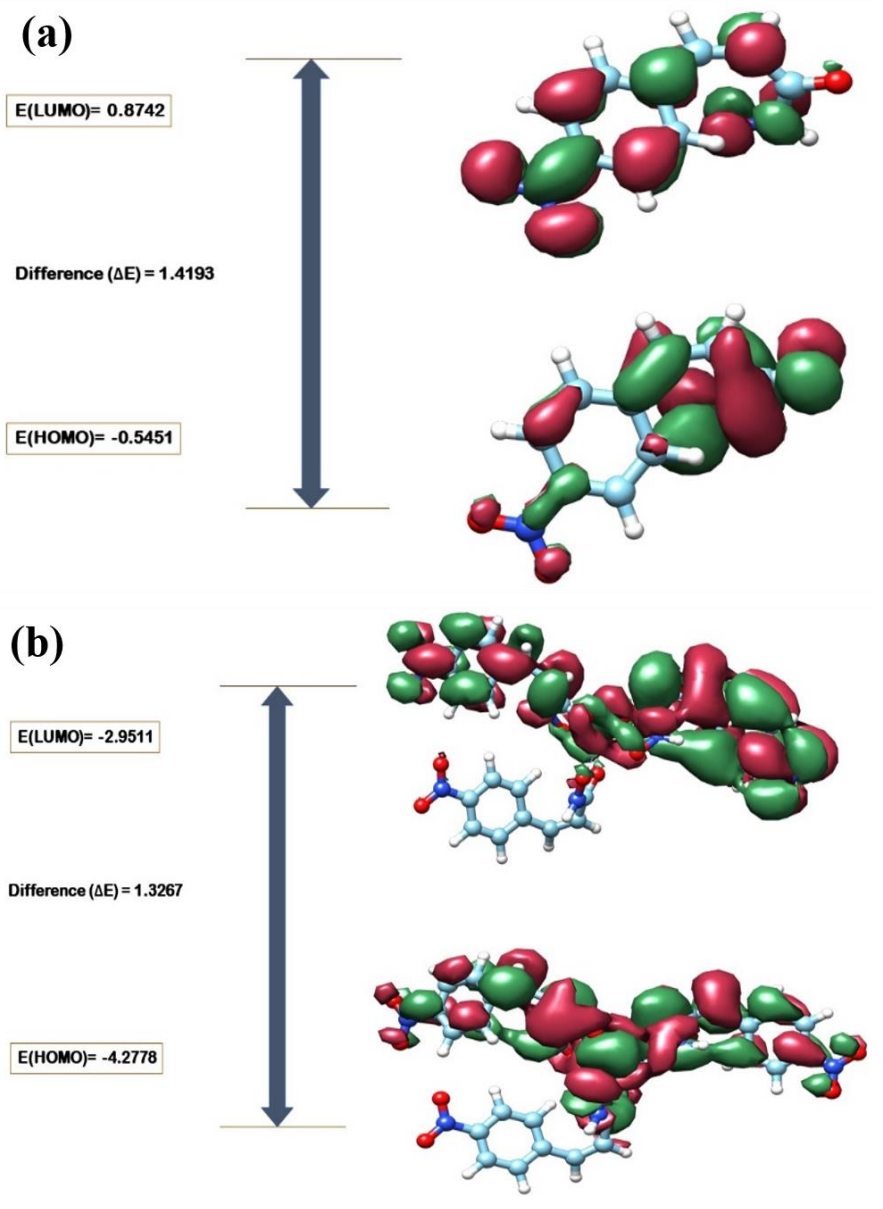
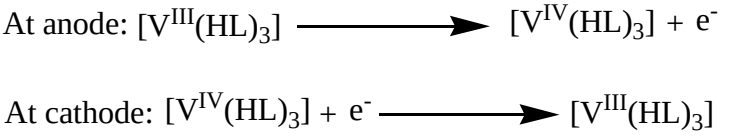


Fig. 7. (a and b) Representation of HOMO-LUMO band gap for ligand and the complex

On the basis of computational, physicochemical and spectrophotometric studies; FTIR, electronic and mass spectral studies, a distorted octahedral geometry has been proposed around vanadium for the complex.

3.5. Electrochemical studies

The potential of the electrode was scanned from a value where no redox reaction occurs to one where reduction or oxidation of the analyte takes place. The voltammogram is then displayed as peaks in current-potential plot on both forward and reverse scans (Figure 8). Chemical reversibility is robust requirement for catalytic activity. In order to prove electrochemical properties of newly synthesized vanadium(III) complex, the cyclic voltammetric measurements in MeOH/H_2O (5:95) was studied. Complex have displayed single anodic and cathodic peak corresponding to the electrode process as (Scheme 3):



Scheme 3. Electrochemical reactions of tris(4-nitrocinnamo-hydroxamato)vanadium(III) complex.

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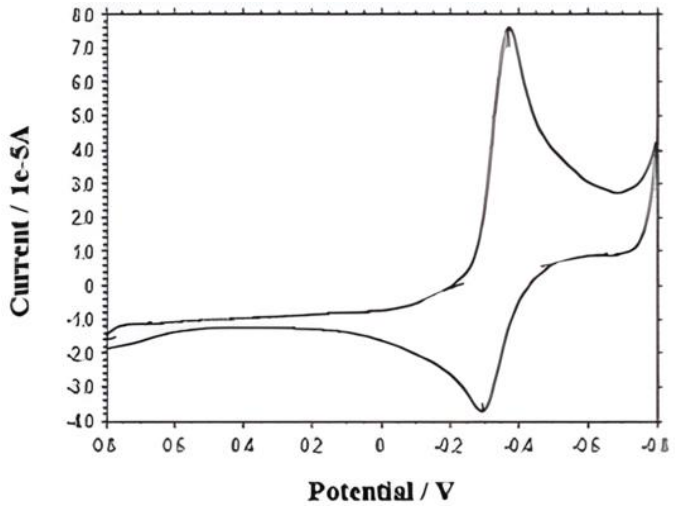

Fig. 8. Cyclic voltammogram of tris(4-nitrocinnamo-hydroxamato)vanadium(III) complex.

3.6. Thermal Studies

Of various physical and chemical methods of investigation, thermal analytical techniques have undergone remarkable advancements [42] and have developed systematically over the years to such an extent that thermal analysis in recent years has acquired considerable prominence in virtually all branches of science and technology. Thermal stability of complex has been studied by TG/DTA technique under N_2 atmosphere. The TG curve of complex has shown it to be thermally stable up to 200ºC after which temperature complex decompose in single step (Figure 9). The total mass loss of 87.82% corresponds to formation of VO_2 as the ultimate decomposition product with some organic matter. The formation of VO_2 is quite noteworthy as most of vanadium complexes decompose to V_2O_5. The formation of VO_2 was confirmed by recording IR and XRD of residue [43].

3.7. Biological Activities

3.7.1. Antibacterial activity

The precursor, ligand and newly synthesized complex were tested *in vitro* for antibacterial activity against *Gram +ve* bacteria viz *Staphylococcus aureus, Staphylococcus epidermidis and Gram –ve bacteria Escherichia coli, Salmonella typhi, Salmonella paratyphi and Klebsiella pneumoniae* employing MIC method (Table 3). A comparative study of results of treated control, commercial antibiotic tetracycline hydrochloride (THC) was done. Standard drug (THC) inhibited bacteria under study in 7.81-15.62 µg/mL range and VCl_3 inhibits *E. coli* at 500 µg/mL and is not effective against other bacterial strains.

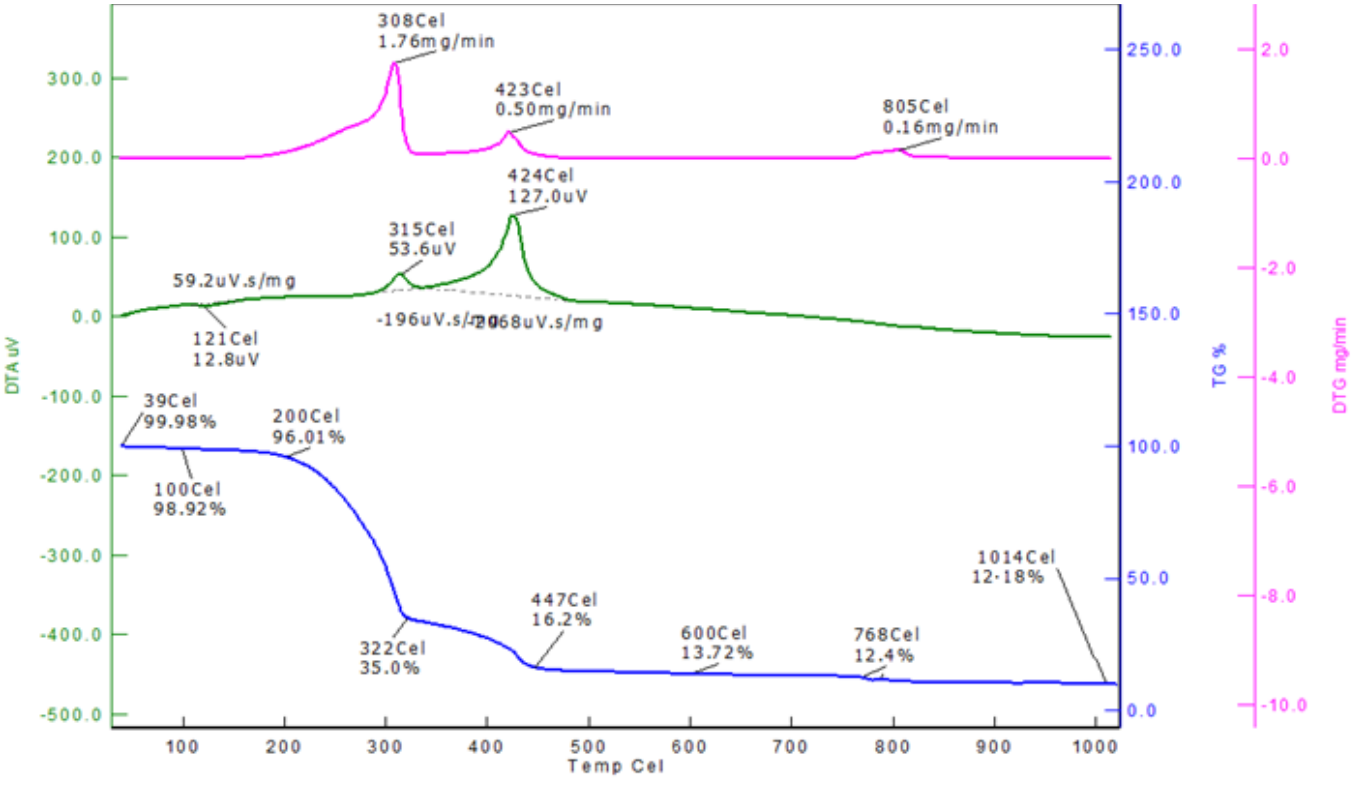

Fig. 9. TG/DTA curve of tris(4-nitrocinnamohydroxamato)vanadium(III) complex.

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Table 3. Antibacterial activity of potassium hydroxamate, precursor and tris(4-nitrocinnamohydroxamato)vanadium(III) complex by MIC method in µg / ml.

Compound	*E. coli*	*S. aureus*	*S. epidermidis*	*S. typhi*	*S. paratyphi*	*K. pneumoniae*
$[VCl_3]$	500	-	-	-	-	-
$[4\text{-}NO_2\text{-}C_6H_4CH{=}CHCONHOK](KHL)$	125	250	250	125	125	250
$[V(4\text{-}NO_2\text{-}C_6H_4CH{=}CHCONHO)_3]$	62.5	62.5	62.5	3.9	15.63	31.25
Standard Drug/Tetracyclinhydrochloride	15.63	15.63	7.81	15.63	15.63	15.63

Table 4. Antifungal activity of potassium hydroxamate, precursor and tris(4-nitrocinnamohydroxamato)vanadium(III) complex by MIC method in µg/ml.

Compound	*A.niger*	*B.fulva*	*M.circinelloids*
VCl_3	500	500	250
$[4\text{-}NO_2\text{-}C_6H_4CH{=}CHCONHOK]$	250	250	62.5
$[V(4\text{-}NO_2\text{-}C_6H_4CH{=}CHCONHO)_3]$	31.25	31.25	15.63
Standard Drug/Fluconazole	3.9	3.9	3.9

Free 4-nitrocinnamohydroxamate ligand inhibits *S. aureus*, *S. epidermidis* and *K. pneumoniae* at 250 µg/mL and at 125 µg/mL for *S. typhi, S. paratyphi, E. coli* as shown in Figure 10**.** The activity of complex has been reported to enhanced considerably (3.9-62.5 µg/mL) and it is even more effective than standard drug for *S. typhi* having MIC of 3.9 µg/mL and almost similar activity to standard drug i.e. 15.63 µg/mL for *S. paratyphi.*

3.7.2. Antifungal activity

The antifungal activity of complex, potassium 4-nitrocinnamohydroxamate and vanadium precursor was tested in vitro on selected fungi viz. *A. niger, B. fulva, M. circenelloids* using MIC method**.** The results were compared with standard antifungal drug fluconazole (treated control) which inhibits the fungi under study at 3.9 µg/mL (Table 4).

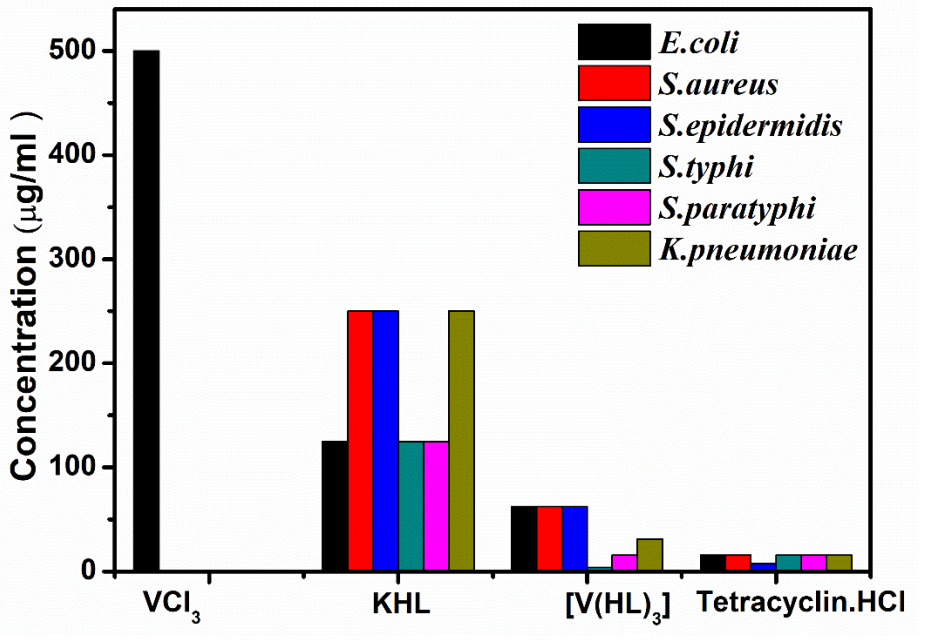

Fig. 10. Graph for the antibacterial activity of precursor, ligand, complex and standard drug.

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The VCl_3 inhibits the growth of selected fungi *A. niger, B. fulva* at 500 µg/mL and *M. circenelloids* at 250 µg/mL. Analysis of data has shown that potassium 4-nitrocinnamohydroxamate inhibit fungi at 250 µg /mL for *A. niger*, *F. fulva* and at lower concentration 62.5 µg/mL for *M. circenelloides.* Newly synthesized vanadium (III) complex shows inhibition at 15.63-31.25 µg/mL. Antifungal activity of complexes increased considerably on complexation although it is less effective than reference drug **(**Figure 11**)**. A significant increase in biological activity on complexation is due to biological significance of hydroxamate and efficient diffusion through cell membrane. The partial sharing of positive charge of metal center with the ligand on coordination reduces its polarity. This is responsible for increasing the hydrophobic character and liposolubility of the molecule in crossing cell membrane of the microorganism [44-47].

3.7.3. Cytotoxicity

Cytotoxic assays of VCl_3, potassium 4-nitrocinnamohydroxamate and newly synthesized complex was performed at several concentrations by means of colorimetric microculture MTT assay. The results were compared with standard drug simvastatin. Complex exhibits appreciable viability of 33.0 % at 2mM concentration (Table 5, Figure 12). Newly synthesized complex was found to be very less toxic than standard drug, but, it has been observed that with increase in concentration of test complex cytotoxicity gets enhanced.

Table 5. Cytotoxic assay of hydroxamate ligands, precursor and tris(4-nitrocinnamohydroxamato)vanadium(III) complex against Hep2C cell line

Compound	Cell inhibition (%) at the selected test compound concentration								
	Control	0.25 mM	0.50 mM	1 mM	2 mM	4 mM	8 mM	20 mM	28mM
VCl_3	100	14.3	18.7	18.7	30.8	30.8	28.6	27.0	28.8
4-NO_2-C_6H_4CH=CHCONHOK (KHL)	100	20	27.6	22.6	69.2	71.4	74.2	75.1	78.9
[V(4-NO_2-C_6H_4CH=CHCONHO)$_3$]	100	16.7	17.8	27.4	33.0	31.9	31.9	28.6	28.6
Simvastatin	100	86	88.3	90.1	92	94.3	95.7	97.9	98.3

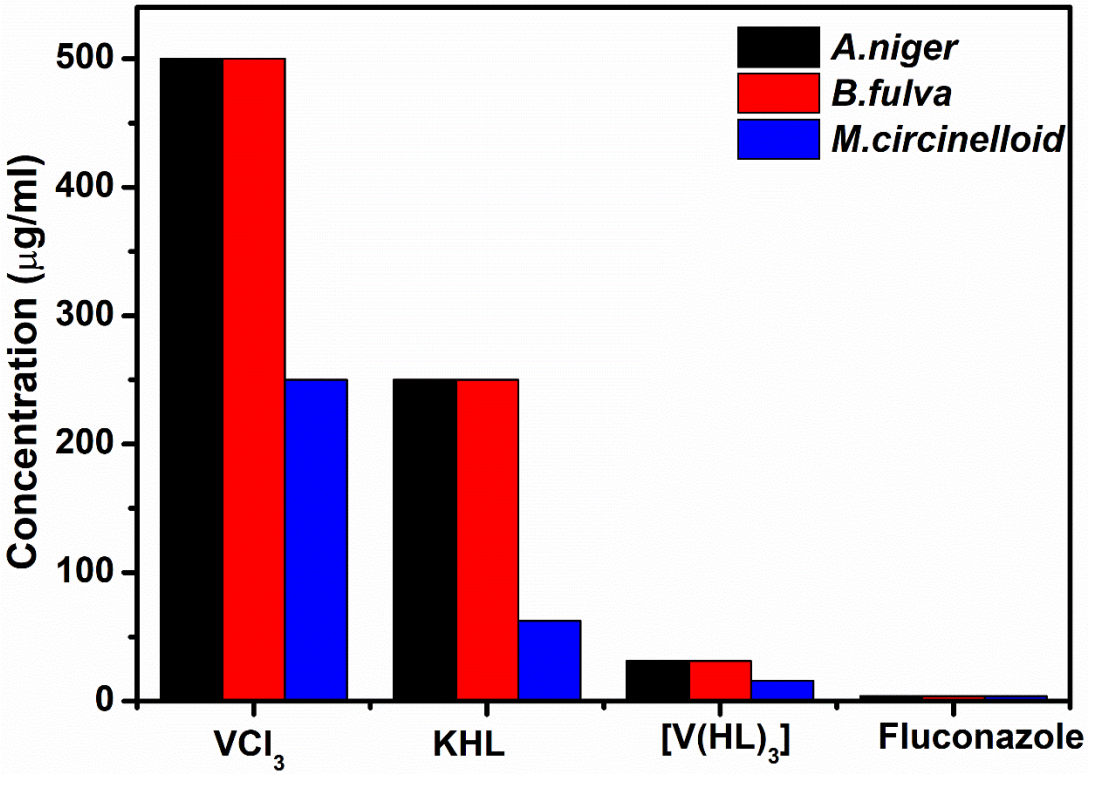

Fig. 11. Graph for the antifungal activity of precursor, ligand, complex and standard drug.

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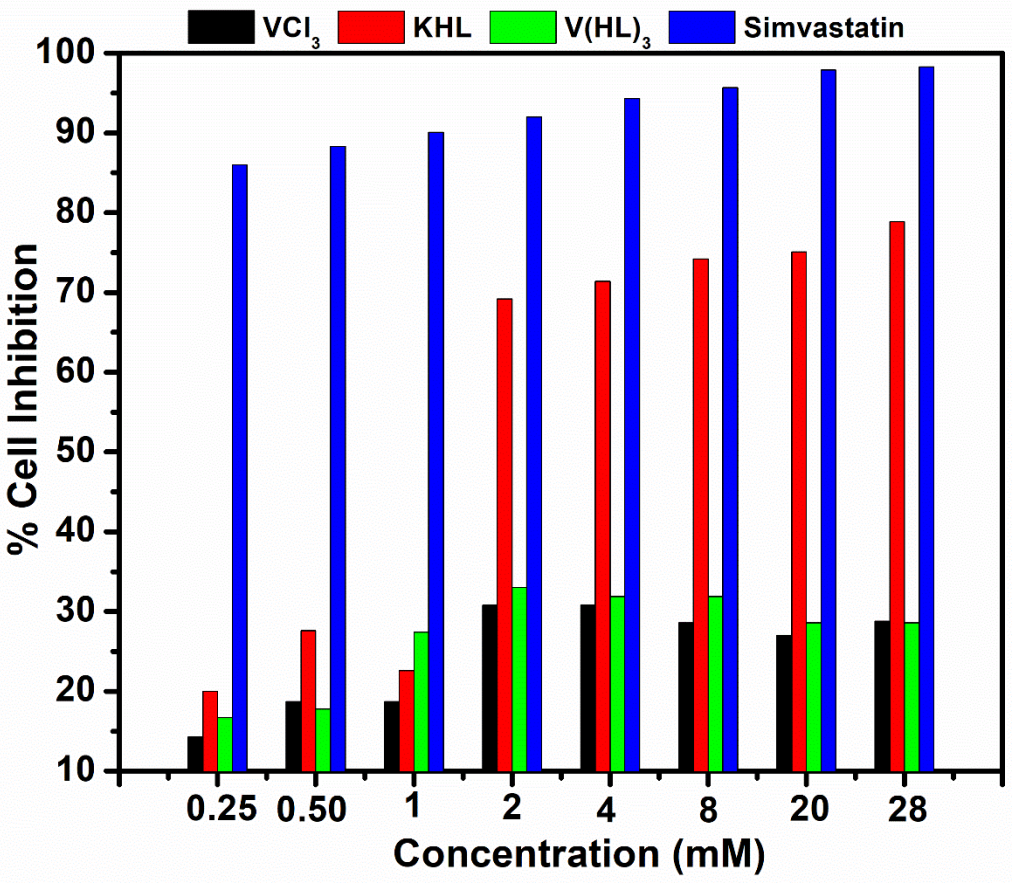

Fig. 12. Graph for the cytotoxicity of precursor, ligand, complex and standard drug.

4. CONCLUSIONS

A facile and convenient method has been devised for the synthesis of vanadium (III) 4-nitrocinnamohydroxamate complex and a remarkable chelating property of ligand has been demonstrated. The synthesized complex is mononuclear and exhibit (O, O) coordination mode through carbonyl and hydroxylamine oxygen. Mononuclear nature of complex has further been supported by mol. wt. determination by cryoscopic measurements and mass spectral data. The complex formation and its stability are strongly confirmed from the negative value of energies for HOMO and LUMO of the complex as compare to ligand in DFT calculations. The complex undergoes single step decomposition and is stable upto 200°C. Vanadium (III) hydroxamate complex exhibit remarkable biological activity against pathogenic bacteria and fungi. Cytotoxicity assay of complex exhibits appreciable viability of 33.0 % at 2mM concentration and cytotoxicity gets significantly enhanced with increase in concentration.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interests.

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