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Scientific paper

A Novel Cd(II) Isophthalate Complex with Triethanolamine: Crystal Structure, Fluorescence and Antimicrobial Activity

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Abstract

A mixed ligand Cd(II) complex $[Cd(IsoPht)(TEA)H_2O]\cdot 3H_2O$ was synthesized for the first time by using isophthalic acid ($H_2IsoPht$) and tetradentate triethanolamine (TEA) and characterized by X-ray single-crystal diffraction, FT-IR, and thermogravimetric analysis (TGA). This novel complex crystallizes in the triclinic system with *P-1* space group and distorted monocapped trigonal prismatic geometry. The Cd(II) has seven coordinates with bidentate IsoPht, a TEA in the tetradentate mode, and an aqua ligand. The fluorescence properties of the Cd(II) complex and TEA ligand were investigated at room temperature. The present Cd(II) complex was also tested for its antimicrobial activity by *in vitro* agar diffusion method against some Gram-positive and Gram-negative bacteria and a fungus.

Keywords: Isophthalic acid; triethanolamine; Cd(II) complex; X-ray single crystal; antimicrobial activity

1. Introduction

Triethanolamine (TEA) is a potential ligand that can interact with metal ions to form supramolecular complexes with different structures, and many coordination compounds containing TEA ligands have been reported for the last two decades.[1–6] TEA is also used as a pH regulator in cosmetology, as a corrosion inhibitor in metal-cutting fluids, as a curing agent for epoxy and rubber polymers, in adhesives, antistatic agents, or as a pharmaceutical intermediate.[7–9] TEA generally acts as the tri- or tetradentate ligand, but some metal complexes with mono- or bidentate TEA coordination modes are also known.[10,11] Metal complexes containing TEA ligand can be (neutral or cationic) mono-, bi- and polynuclear structures.[12,13] Some mononuclear mixed ligand complexes were reported for Ni(II) with TEA and orotic acid,[14] Cu(II) with TEA and malonic acid,[15] Zn(II) and Cd(II) with TEA and *p*-nitrobenzoic acid,[16] Zn(II) with TEA and aqua ligand,[17] Cu(II) with TEA, aqua and 1H-imidazole ligands,[18] aqua ligand.[19] Based on the collaborative use of TEA and phthalic acid, mononuclear complexes for Ni(II),[20] Zn(II),[21] Cd(II),[22] and coordination polymer for Cd(II)[23] were also reported. Although TEA has no specific physiological effects except for its low antibacterial activity, as an auxiliary ligand TEA may increase the physiological effect of bioactive substances in mixed ligand metal complexes.[8,9,24] There are preliminary pharmacological studies demonstrating that the transition metal complexes of TEA protect animals from ethanol and carbon monoxide poisoning and have immune-modulating and antiproliferative properties.[25-27] Also, the mixed ligand zinc complex containing TEA has been reported to have anti-angiogenic and anti-atherogenic effects.[28]

Coordination compounds may combine a metal ion, a biocompatible ligand, and some auxiliary ligands in the same molecule to form mixed-ligand coordination types to achieve the desired properties.[29,30] Apart from the TEA ligand, isophthalic acid ($H_2IsoPht$) has been selected as a good candidate for this purpose. Dicarboxylic acids have important advantages in design of coordination compounds compared with other organic ligands. Isophthalic acid has two carboxyl groups that can lose one or two protons to form various coordination modes, act as a hydrogen bond acceptor and donor. So it is a versatile and variable ligand that can bind metal ions in different directions.[31–38] The synthesis of coordination compounds containing O and/or N-donor ligands are very significant

and intriguing in the field of pharmacology due to the discovery of their antimicrobial properties. The biological activity of coordination compounds with O-donor ligand isophthalato (IsoPht) has been studied.[39–42] Antimicrobial activities of Zn-IsoPht complexes were displayed *in vitro* against some Gram-positive, some Gram-negative bacteria and fungus by Radovanović and co-workers, who showed that the most potent inhibitory effect of [Zn(dipya)(IsoPht)]$_n$ (dipya = 2,2'-dipyridylamine) against all the tested microorganisms.[39] Devereux and co-workers demonstrated high antibacterial activity of Mn–phen–pht/IsoPht complexes against *Candida albicans*.[40]

Cadmium coordination compounds containing O and/or N-donor ligands can show promising fluorescence properties.[43–49] In this study, a novel mixed ligand Cd(II) complex with TEA and IsoPht was synthesized and the structure of the complex was identified by using X-ray single-crystal diffraction and FT-IR. Thermal properties of the complex were also examined in detail. The fluorescence and antimicrobial properties of the complex were investigated, too.

2. Experimental

2. 1. Materials and Instrumentations

Triethanolamine (TEA), Isophthalic acid (H_2IsoPht), and $Cd(NO_3)_2 \cdot 4H_2O$ were purchased from Sigma Aldrich Ltd. IR spectra were obtained with an FT/IR-100 type A Spectrophotometer. Thermal degradation of the complex was performed using a TA Instruments SII-EXTAR-6000 TG/DTA. Experiments were conducted from 30 to 900 °C, with a heating rate of 10 °C min^{-1}, under nitrogen atmosphere using platinum crucibles. Fluorescence spectra of the complex were taken on Agilent Cary Eclipse Fluorescence Spectrophotometer.

2. 2. Synthesis of [Cd(IsoPht)(TEA)H_2O]·3H_2O

5 mmol of $Cd(NO_3)_2 \cdot 4H_2O$ (1540 mg) was dissolved in 30 mL of water. Then, 10 mmol (1.33 mL) TEA was added and reaction solution was stirred for 10 min at 70 °C. After that, 5 mmol (830 mg) of H_2IsoPht was added to the solution and stirred for more 3 hours. 4 weeks later, colorless crystals were obtained by slow evaporation of the clear solution that appeared after filtration at room temperature.

2. 3. X-Ray Crystallography

The reflection intensities of the Cd(II) complex were collected at 296 K using Agilent SuperNova single-crystal diffractometer with Mo-Kα radiation (λ = 0.71073 Å). The structure was solved using the program SHELXT[50] by direct methods, and all non-hydrogen atoms were refined with anisotropic displacement parameters by full-matrix least-squares methods based on F^2 using SHELXL.[51] The molecular graphics were prepared using OLEX^2 program.[52] Detailed information about the crystal data and structure determination are summarized in Table 1. Selected experimental and calculated interatomic distances and bond angles are given in Table 2.

2. 4. Computational Protocol

Quantum chemical calculation of the complex was performed using Gaussian 09 program suits running under Windows.[53] Ground state geometry optimization of the complex was performed by using Minnesota M062X hybrid density functional method with appropriate basis set combinations, 6-31g(d,p) for non-metal atoms and pseudo potential-included SDD for metal atom.

Table 1. Crystallographic data for [Cd(IsoPht)(TEA)H_2O]·3H_2O

Empirical formula	$C_{14}H_{27}CdNO_{11}$
Formula weight	497.76
Temperature/K	293(2)
Crystal system	Triclinic
Space group	$P\bar{1}$
a/Å	9.0749(3)
b/Å	10.7120(3)
c/Å	12.2025(5)
α/°	66.944(3)
β/°	72.272(3)
γ/°	67.510(3)
Volume/Å^3	991.61(7)
Z	1
ρ_{calc}g/cm^3	1.667
μ/mm^1	1.157
F(000)	508.0
Crystal size/mm^3	0.13 × 0.15 × 0.17
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.684 to 52.742
Reflections collected	13143
Independent reflections	4050 [R_{int}= 0.0400, R_{sigma} = 0.0352]
Data/restraints/parameters	4050/3/258
F^2	1.067
Final R indexes [I> = 2σ (I)]	R_1 = 0.0325, wR_2 = 0.0817
Final R indexes [all data]	R_1 = 0.0325, wR_2 = 0.0838
Largest diff. peak/hole / e Å^{-3}	1.44/–0.78

2. 5. Antimicrobial Activity

In vitro antimicrobial screening test of the synthesized compound were carried out for antibacterial and antifungal activity. Antibacterial activity was tested against three bacterial strains; two gram-positive [*Bacillus cereus* (ATCC 10876), *Staphylococcus aureus* (ATCC 29213)] and one gram-negative [*Escherichia coli* (ATCC 25922)] and antifungal activity was tested against one fungal strain [*Candida albicans* (ATCC10231)]. The agar well diffusion method was used in these assays. After nutrient agar was

sterilized in an autoclave at 121 °C for 15 min, it was transferred into sterile Petri plates. Then the agar medium solidified, 8 mm diameter wells were drilled with a sterile metallic applicator. 20 µL of the sample at different concentrations prepared in DMSO was poured into the wells. DMSO served as a negative control, Ampicillin and Fluconazole served as a positive control. The plates were incubated aerobically at 37 °C for 24 h. The diameters of inhibition zones were measured by using a zone reader and were given as millimeters. Evaluation of the inhibition zone was made by averaging the three test results.

3. Results and Discussion

3. 1. The Crystal Structure of [Cd(IsoPht)(TEA)H_2O]·3H_2O

X-ray single-crystal analysis reveals that complex crystallized in the triclinic system with space group *PĪ*. The complex has an interesting monomeric molecular structure which is rarely found for cadmium polycarboxylate complexes. In the complex, H_2IsoPht acts as a bidentate ligand by losing hydrogen atoms while the TEA ligand acts as a tetradentate ligand using all its donor atoms. The Cd1 atom is coordinated by six oxygen atoms and one nitrogen atom, two of which are from IsoPht ligand (O1 and O2), three oxygen atoms, and one nitrogen atom from a TEA ligand (O5, O6, O7, and N1), together with one oxygen atom of aqua ligand, O8W. In crystallization, uncoordinated three water molecules are also part of the molecular structure (Figure 1). Thus, Cd(II) ions are in distorted monocapped trigonal prismatic geometry environments

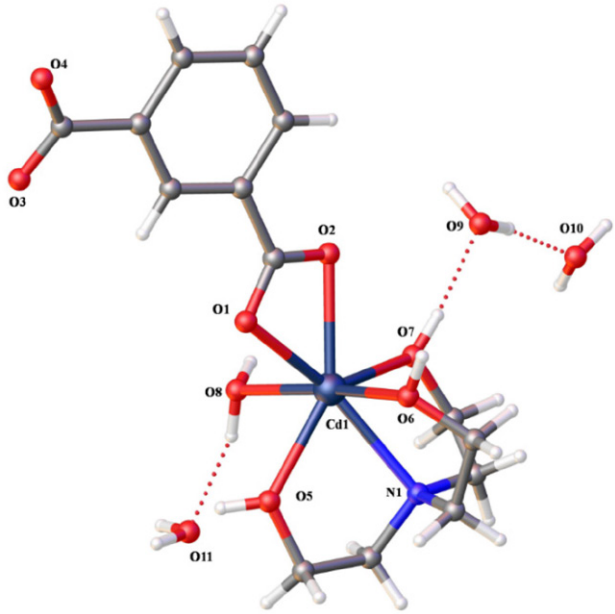

Figure 1. A view of the [Cd(IsoPht)(TEA)H_2O]·3H_2O compound showing the atom-labeling

with CdO_6N chromophores. This seven-coordinate geometry around the Cd(II) ion in the titled complex is similar to the other reported Cd(II) complexes.[1,2]

The Cd1-O bonds are in the range 2.300 (2)–2.399 (2) Å and Cd1-N bond is 2.434 (2) Å (Table 2). The bond lengths between Cd1 and O atoms of IsoPht (O1, O2), 2.329(2) and 2.399(2) Å are comparable to the other Cd(II)-IsoPht complexes.[46,54,55] The bond distances of Cd1-O and Cd1-N between Cd1 and TEA, which are in the range of 2.300(2)–2.353(2) Å (O5, O6, O7) and

Table 2. Selected experimental and calculated coordination bonds and angles of [Cd(IsoPht)(TEA)H_2O]·3H_2O

Bond lengths (Å)					
Bond	Exp.	Calc.	Bond	Exp.	Calc.
Cd1-O1	2.329(2)	2.2216	Cd1-O6	2.353(2)	2.5327
Cd1-O2	2.399(2)	2.2723	Cd1-O7	2.325(3)	2.3801
Cd1-O5	2.300(2)	2.4193	Cd1-O8	2.324(2)	2.4119
Cd1-N1	2.434(2)	2.4485			
Bond angles (°)					
Angle	Exp.	Calc.	Angle	Exp.	Calc.
O1-Cd1-O2	55.12(7)	58.86	O5-Cd1-O7	131.11(10)	126.59
O1-Cd1-O6	86.17(9)	92.92	O7-Cd1-O2	80.08(8)	103.19
O8-Cd1-O2	94.06(8)	131.99	O7- Cd1-O1	134.14(8)	132.58
O8-Cd1-O1	88.16(9)	87.74	O7-Cd1-O6	103.78(11)	123.19
O8- Cd1-O6	170.64(9)	152.86	O1-Cd1-N1	150.55 (8)	152.40
O8-Cd1-O7	85.50(11)	73.38	O2-Cd1-N1	140.73 (7)	127.47
O6-Cd1-O2	88.80(8)	69.16	O5-Cd1-N1	70.83 (8)	74.03
O5-Cd1-O2	146.41(8)	130.20	O6-Cd1-N1	72,15 (8)	69.51
O5-Cd1-O1	91.61(8)	83.14	O7-Cd1-N1	72.00 (8)	74.64
O5-Cd1-O8	78.85(9)	69.84	O8-Cd1-N1	110.61(8)	98.47
O5- Cd1-O6	93.86(10)	83.29			

2.434(2) Å (N1), are similar within the reported seven-coordinated mixed ligand complexes.[16,23] However, these bond lengths are shorter than those of the reported eight-coordinated complexes.[3,22] In addition, the bond angles between the Cd1 and O atoms vary between 55.12° (7) and 170.64° (9) in Table 2. The bond angles of the complex are normal compared with those of the related complexes.[1,2,16] The crystal structure is further stabilized by multiply intermolecular hydrogen bonds. The uncoordinated water molecules play an important role in the supramolecular architecture. The hydrogen-bonding interactions, which are assembled into 2D layers parallel to by O-H···O weak hydrogen bonds (Table 3), formed where the TEA donate hydrogen atoms to the neighboring carboxylate and water oxygens (Figure 2). It can be seen from Figure 2 that the hydrogen bonds between the TEA ligands and the carboxylate groups of IsoPht, giving rise to R_3^2 (8) and R_4^4 (20) ring motives. The molecules located along the [010] direction (Figure 3(a)), are linked by π···π stacking [π···π d = 3.556 Å] (Figure 3(b)). The π···π stacking interaction between the benzene ring of the IsoPht ligand is stronger than in the related {[Cd(HFlu)(IsoPht)(H_2O)] · H_2O}n (HFlu = fluconazole) complex [π···π d = 3.705 Å] in literature.[46]

An extensive network of hydrogen bonds, π···π stacking, and van der Walls interactions embed the complex in a three-dimensional lattice. Figure 4 shows the packing diagram of the complex along the [100] direction.

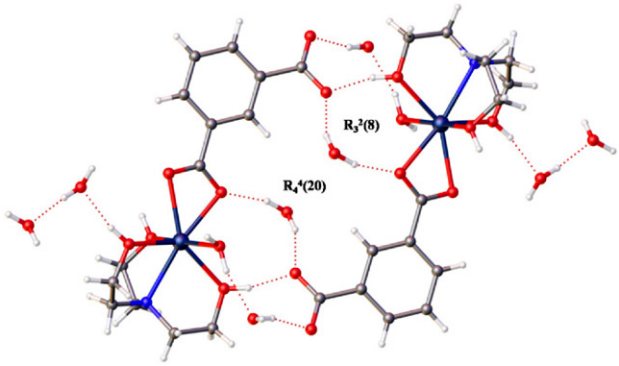

Figure 2. Part of the crystal structure of [Cd(IsoPht)(TEA)H_2O]·3H_2O, showing the formation of R_3^2(8), and R_4^4(20) rings by the O-H···O hydrogen bonds

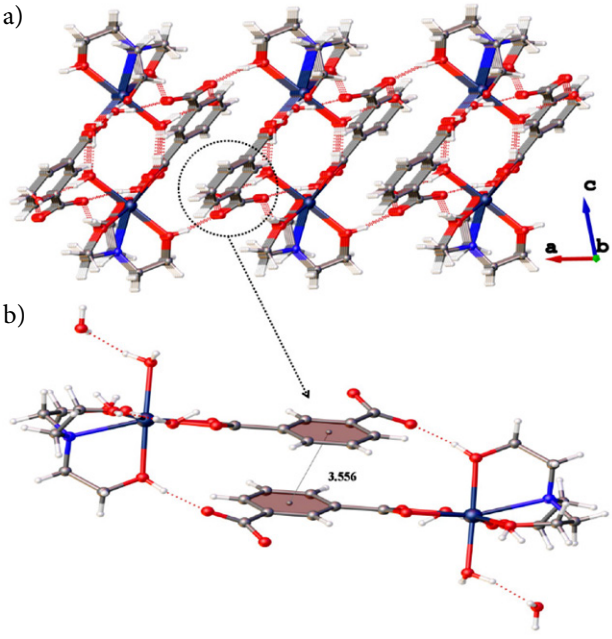

Figure 3. ((a) 2-D supramolecular network along the [010] direction in [Cd(IsoPht)(TEA)H_2O]·3H_2O complex. (b) π···π interaction

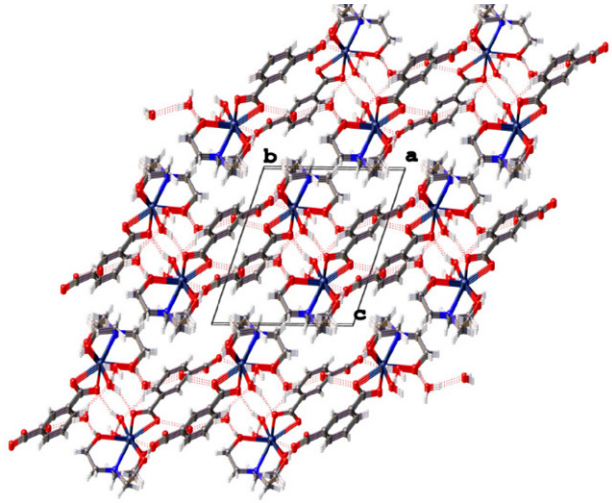

Figure 4. Packing diagram of [Cd(IsoPht)(TEA)H_2O]·3H_2O complex along the [100] direction

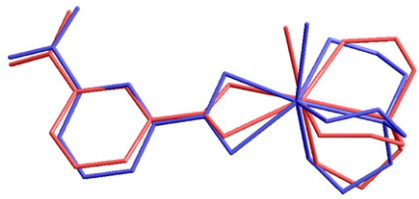

Figure 5. Superimposition of X-ray(red) and optimized(blue) geometries of [Cd(IsoPht)(TEA)H_2O]·3H_2O

Table 3. Hydrogen bond interactions for [Cd(IsoPht)(TEA)H_2O]·3H_2O

Hydrogen-bonds				
D-H· · ·A	D-H	H···A	D···A	D-H···A
O8-H8-O9^{i}	0.85	2.08(4)	2.895(4)	161.9
O8-H8-O11	0.85	1.98	2.818(4)	167.2
O6-H6-O4^{ii}	0.89(5)	1.71(5)	2.598(3)	176(5)
O5-H5-O3^{iii}	0.73(5)	1.81(5)	2.536(4)	169(6)
O9-H9-O10	0.85	1.84	2.693(4)	176.2
O9-H9-O8^{i}	0.85	2.26	2.895(4)	132.0
O10-H10-O1^{iv}	0.85	2.01	2.808(3)	156.1
O10-H10-O3^{i}	0.85	1.91	2.743(4)	165.0
O11-H11-O4^{iii}	0.85	2.11	2.928(4)	162.5

Symmetry transformations used to generate equivalent atoms: (i) x, 1-y, 1-z; (ii) x, 2-y, 1-z; (iii) 1-x, 2-y, 1-z; (iv) +z, -1 +y, +z

Quantum chemical optimized geometry of the complex exhibited reasonable accordance with experimental X-ray geometry with a RMSE deviation of 0.622 Å. Superimpositions of the X-ray and calculated geometries of the complex are given in Figure 5. In general, there is a pleasant consistence between optimized and X-ray geometries according to the results and as expected, the general tendency of gas-phase optimizations in favour of somewhat extending the bond distances was introduced.

3. 2. FT-IR Study

In the FT-IR spectrum of the Cd(II) complex, the broad absorption band between 3500 and 3100 cm^{-1} with maxima at 3427, 3385 and 3146 cm^{-1}, which are assigned to stretching vibrations υ(O–H) of uncoordinated water molecules, aqua and TEA ligand (Figure S1). The FT-IR stretching band at 3373 cm^{-1} belongs to the hydroxyl group (O–H) of the TEA ligand and has been observed to shift to lower wavelength (3146 cm^{-1}) during complexation. The FT-IR bands identified at 3079, 2975, 2898 and 2844 cm^{-1} are associated with aromatic and aliphatic υ(C–H) stretching vibrations. The bands in the spectral region 1700–1300 cm^{-1} of complex shows five peaks with frequencies 1601, 1538, 1479, 1442 and 1390 cm^{-1}. These bands can be attributed to stretching vibrations of aromatic ring $\nu(C_{Ar})$ and carboxylate groups υ(C=O). The peaks corresponding to a strong asymmetric stretching υ_{asym}(C=O) as 1689 cm^{-1} and a weak symmetric stretching υ_{sym}(C=O) as 1417 cm^{-1} of the H_2IsoPht were observed at lower frequencies (1538 cm^{-1} and 1390 cm^{-1}, respectively). This situation demonstrates that the Isopht ligand coordinated to the Cd(II) via the oxygen atoms of the carboxylate group. The difference between the υ_{asym}(C=O) and υ_{sym}(C=O) stretching vibrations observed in the IR spectra of the complexes (Δυ), [$\Delta\upsilon = \upsilon_{asym}(C=O) - \upsilon_{sym}(C=O)$] is used to determine the coordination type of the carboxylate group. The frequency difference, $\Delta\upsilon > 200$ cm^{-1} generally associated with unidentate coordination, a possible exception involving highly unsymmetrical bridging, i.e. "pseudo-unidentate" coordination. $\Delta\upsilon > 105$ cm^{-1} and < 200 cm^{-1} indicates chelating and/or bridging carboxylate groups. Accordingly, the value of Δυ 148 cm^{-1} for the complex indicated that the chelate coordination mode of the carboxyl group of the IsoPht.[56,57] The coordination mode of IsoPht ligand is also approved by the single-crystal X-ray structure examined. The band observed at 434 cm^{-1} is due to the metal-oxygen (M–O) bond.[58]

3. 3. Thermal Analysis

Thermal stability and behavior of the Cd(II) complex were examined by simultaneous TG/DTG/DTA in nitrogen atmosphere. The TG-DTG and DTA curves of the complex are shown in Figure 6. The complex underwent complete degradation in two main stages. The first stage (44–118 °C), is related to the removal of both crystal water and aqua ligand at DTG_{max} 88 °C with a 13.98% mass loss. This exhibits an endothermic peak at 89 °C in the DTA curve. The anhydrous complex stays stable up to 179 °C. Over this temperature, it can be suggested that the TEA and IsoPht ligands removed successively from the structure in the temperature range of 179–657 °C (DTG_{max}: 378 °C). The final solid product of thermal decomposition is associated with CdO formation (found 27.7, calcd. 25.8%).

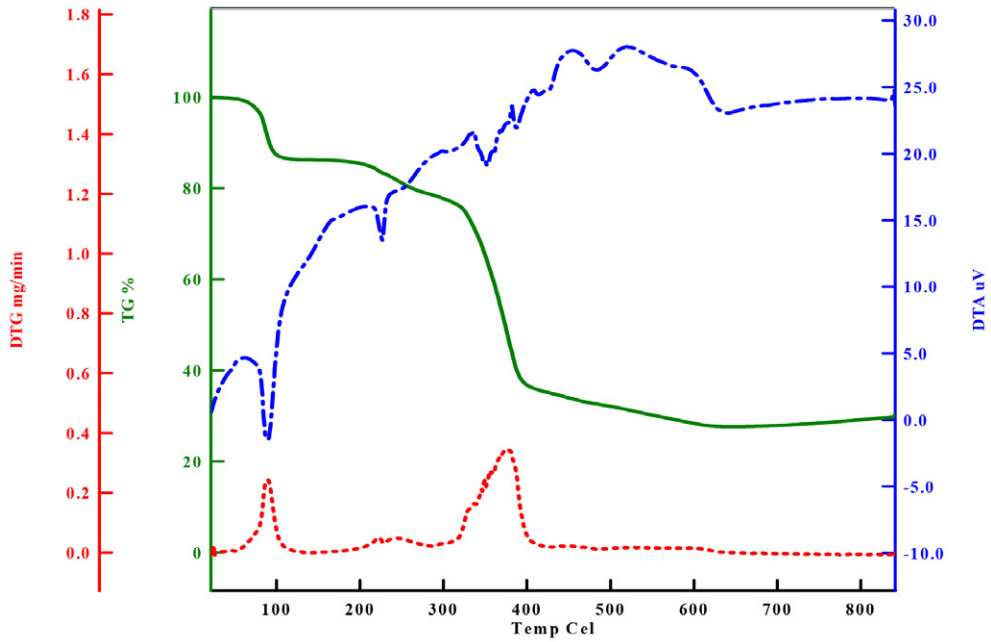

Figure 6. TGA curves of [Cd(IsoPht)(TEA)H_2O]·3H_2O complex

3. 4. Fluorescence Properties

The fluorescent properties of the TEA ligand and Cd(II) complex have been examined at room temperature. The resulting emission spectrum is given in Figure 7. Due to the fluorescence quenching of carboxyl groups of IsoPht (which are strong electron-attracting groups), this ligand shows very low fluorescence emission at room temperature.[48,59] While the TEA ligand shows the emission peaks at 312 and 346 nm with the excitation at 270 nm, the complex exhibits emission bands at 357 and 423 nm with the excitation at 270 nm. Compared with the emission of the TEA ligand, the emission peaks of the complex were observed to redshift (ca.45 nm and 77 nm). The solid-state fluorescence of the complex may be assigned to MLCT or LMCT transitions.[60]

3. 5. Antimicrobial Activity

The antimicrobial activity of the prepared $[Cd(IsoPht)(TEA)H_2O]\cdot 3H_2O$ complex against three bacteria and one fungus was studied. Saturated solution and inhibition zones (mm) of the Cd(II) complex are given in Table 4. In the different concentrations of the complex, various inhibition values were observed for *B. cereus, S. aureus, E. coli,* and *C. albicans* between 10–25 mm, 7–20 mm, 16–18 mm, and 8–15 mm respectively. It was shown more efficacy than positive control against all three bacterial zones, especially at concentrations of 40000 and 20000 ppm.

Recently, it has been reported that Cu(II) complexes of TEA with salts of salicylic, cinnamic, and succinic acids,[6] Zn(II) and Cu(II) cinnamate with TEA complexes[61] showed antimicrobial activity against bacteria *E. coli, S. aureus, M. smegmatis,* fungi *C. albicans* and *A. niger*. In addition, it has been shown that TEA with Cu(II) picrate and Ag(I) complexes appeared to exhibit mild to moderate activity towards *S. marcescens, S. japonicum, S. maltophilia* and *S. aureus*.[62,10] Compared to these previous studies, it can be said that the Cd(II) complex synthesized in this study has a moderate inhibitory activity against similar strains.

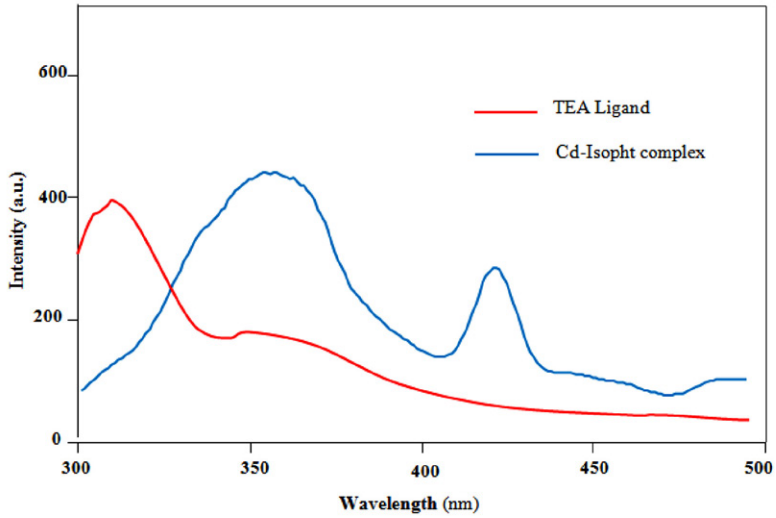

Figure 7. Fluorescence spectrum of $[Cd(IsoPht)(TEA)H_2O]\cdot 3H_2O$ complex and TEA ligand in the solid-state (λ_{ex} = 270 nm)

Table 4. Diameter of zones of inhibition (mm) of $[Cd(IsoPht)(TEA)H_2O]\cdot 3H_2O$ complex

ppm	*S.aureus*	*B.cereus*	*E.coli*	*C.albicans*
40000	20	25	18	15
20000	20	25	16	15
10000	15	20	0	12
5000	13	16	0	8
2500	9	15	0	0
1250	7	15	0	0
625	0	14	0	0
312.5	0	10	0	0
[a]DMSO	–	–	–	–
[b]Ampicilin (10μg/mL)	18	20	15	–
[b]Flukonozol (25μg/mL)	–	–	–	20

a: negative control; b: positive control

The antimicrobial activity of mixed ligand metal complex was determined by various factors such as the chelate effect, i.e. bidentate, tridentate or tetradentate ligands, the nature of ligand, the total charge of the complex, and metal ion located in the center.[63] In light of this information, it can be said that despite the weak antimicrobial activity of TEA alone,[8,9] the complex formed by combining with Cd(II) ion shows moderate antimicrobial activity against all tested strains.

4. Conclusions

A novel mixed ligand $[Cd(IsoPht)(TEA)H_2O]\cdot 3H_2O$ complex was synthesized and structurally characterized. The revealed X-ray structure clearly showed that the complex has a distorted monocapped trigonal prismatic geometry by binding to Cd(II) ion as TEA tetradentate and IsoPht bidentate. Thermal stability and behavior of the complex in the nitrogen atmosphere were investigated. The complex was completely degraded in two main stages. Fluorescence properties of cadmium complex having d^{10} electron configuration at room temperature were also measured. In the fluorescence spectrum, the red-shift of the peaks of the complex may be attributed to the LMCT or MLCT transitions. In addition, the antimicrobial properties of the complex were investigated against three bacteria and one fungus. Data on the antimicrobial activity of the Cd(II) chelate complex formed by the tetradentate TEA and bidentate IsoPht ligands shows supported that it demonstrated moderate activity to inhibit the growth of all tested strains.

Supplementary Data

Crystallographic data have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication No. CCDC 1977619. Copies of the data can be obtained, free of charge, on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (fax: +44-1223-336033 or e-mail: deposit@ccdc.cam.ac.uk).

Acknowledgments

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Povzetek

Z uporabo izoftalne kisline (H_2IsoPht) in tetradentatnega trietanolamina (TEA) smo sintetizirali nov kadmijev(II) kompleks s formulo [Cd(IsoPht)(TEA)H_2O]·3H_2O in dobljeno spojino karakterizirali z monokristalno rentgensko difrakcijo, FT-IR in termogravimetrično analizo (TGA). Spojina kristalizira triklinsko v prostorski skupini *P-1* s popačeno trikotno prizmo z dodatnim ligandom nad stransko ploskvijo. Cd(II) je sedemštevno koordiniran z bidentatnim IsoPht, tetradentatnim TEA in akva ligandom. Preučevali smo fluorescenčne lastnosti kadmijevega kompleksa in liganda TEA. Raziskovali smo tudi antimikrobno aktivnost sintetiziranega Cd(II) kompleksa z *in vitro* metodo difuzije v agarju proti gram pozitivnim in gram negativnim bakterijam ter glivam.