# Novel Cadmium Dithiocarbamate Complex

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**Abstract:** In this study, a new cadmium(II) complex with ammonium-iminodiacetatedithiocarbamate as ligand, $(NH_4)_3$idadtc, was synthesized. This ligand is interesting because of its polydentate nature and ability to form stable complexes with various transition metals. Through its five donor atoms (two sulfur atoms, two oxygen atoms, and one nitrogen atom), it can behave as a bidentate or tridentate ligand and form four- or five-membered chelate rings with metal ions. The sulfur atoms of the dithiocarbamate group play a particularly important role in its practical application in the chemical industry, agriculture, pharmacy, etc. The coordination behavior of $(NH_4)_3$idadtc, has previously been investigated in reactions with Cu(II), Ni(II), Pd(II), Au(III), Zn(II) and other metal ions, while data on interactions with Cd(II) have not been available in the literature so far. The aim of this work was to investigate the coordination mode of the $(NH_4)_3$idadtc ligand toward the Cd(II) ion. The complex was obtained by reacting cadmium(II) acetate ($Cd(CH_3COO)_2$) with the ligand in a 1:2 molar ratio, in a neutral medium, at room temperature. The obtained product was characterized by IR, UV/VIS, $^1$H and $^{13}$C NMR spectroscopy as well as electrical conductivity measurement. Based on the obtained data, it was concluded that an ionic complex was obtained in which the dithiocarbamato-ligand achieves isobidentate coordination through two sulfur atoms. The assumed composition of the complex is $(NH_4)_4[Cd(idadtc)_2]$.

**Keywords:** Metal complexes, synthesis, spectral characterization

## 1. Introduction

The synthesis of cadmium dithiocarbamate complexes dates back to 1907, when diisobutyldithiocarbamate was first used as a ligand. Since then, numerous cadmium complexes incorporating various aliphatic and aromatic dithiocarbamate ligands have been thoroughly investigated. However, according to existing literature, the well-known dithiocarbamate derivative ammonium-iminodiacetatodithiocarbamate has yet to be explored for the formation of cadmium complexes. This very fact prompted the present study, which aims to investigate the coordination capabilities of ammonium-iminodiacetatodithiocarbamate with cadmium ions.

Obtaining new complexes is an important achievement that advances our understanding of metal–ligand interactions, especially within the coordination chemistry of heavy metals such as cadmium. Cd–DTC complexes have already been utilized as precursors in the synthesis of CdS nanomaterials, in producing semiconductor devices, as photodetectors and sensors, and in biomedical research, where their potential antitumor and antimicrobial activities have been explored [1]. This study creates opportunities to discover additional properties and possible functional applications, thus contributing not only to fundamental chemical knowledge but also to the development of novel materials and pharmacologically active substances.

## 2. Methodlogy

Commercially available reagents were used for the synthesis without further purification.

The ligand $(NH_4)_3$idadtc (0.520 g, 2 mmol), synthesized according to a previously reported procedure [2], was dissolved in 2 mL of distilled water. The resulting aqueous solution was then added to an ethanolic solution of $CdCl_2$ (0.183 g, 1 mmol). Upon mixing, the reaction started immediately, evidenced by the formation of a white precipitate. The reaction mixture was stirred at room temperature using a magnetic stirrer for 20 minutes.

FTIR spectra was recorded in the wavenumber range of 4000 to 400 $cm^{-1}$, at a resolution of 4 $cm^{-1}$, using the ATR technique in reflection mode on a diamond crystal. Measurements were performed on a Spectrum Two FTIR spectrometer (PerkinElmer).

UV/Vis spectra was recorded in the range of 200 to 800 nm using a Cary 50 Scan UV/Visible spectrophotometer (Varian). Aqueous solutions of the complexes at a concentration of 0.05 mmol/L were prepared for the measurements.

NMR spectra were recorded on a Bruker AV1 300 MHz spectrometer using $D_2O$ as the solvent. All measurements were performed at room temperature.

The conductivity measurements were carried out on aqueous solutions of the complex at a concentration of $10^{-3}$ mol/$dm^3$, using a Mettler Toledo SevenDirect SD23 pH/conductometer.

## 3. Results and Discussion

The complex was isolated in excellent yield: 97.58% (0.5826 g), as a white powder, which is highly soluble in water but poorly soluble in organic solvents. Its molar conductivity in water (427,5 S·$cm^2$/mol) corresponds to a 1:4 electrolyte type.

### *3.1. FTIR spectra studies*

The FTIR spectrum (Fig. 1) shows a band at 3161 $cm^{-1}$, which can be attributed to N–H stretching vibrations, indicating the presence of ammonium ions. The region between 950 and 1050 $cm^{-1}$, typical for C–S vibrations, features a sharp singlet at 992 $cm^{-1}$ in the complex.

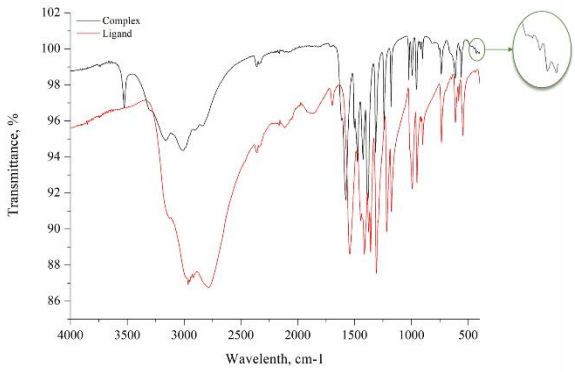


**Figure 1.** Side-by-side comparison of the ligand and complex IR spectra.

This band is assigned to asymmetric C–S stretching and supports the conclusion that the ligand coordinates isobidentately [3]. A slight shift of the band related to symmetric C–S stretching, observed at 614 $cm^{-1}$, further confirms coordination through sulfur atoms. A sharp band at 1238 $cm^{-1}$ corresponds to C–N stretching within the $–NC(H_2)COO^-$ group, while the band at 1577 $cm^{-1}$ is linked to C–N vibrations in the $–NCS_2$ group. Bands that do not appear in the free ligand's spectrum but become evident in the complex are attributed to newly formed metal–ligand bonds. A weak band at 404 $cm^{-1}$ is associated with delocalized electrons involved in δ(SCdS) vibrations, part of a broader conjugated system that also includes δ(SCS) and δ(CNC) contributions. Finally, the band at 427 $cm^{-1}$, characteristic of Cd–S stretching vibrations, confirms the coordination of sulfur atoms from the ligand to the cadmium ion in the complex [4].

*3.2. $^1H$ NMR and $^{13}C$ NMR spectra studies*

In the $^1H$ NMR spectrum of the ligand, recorded in $D_2O$, a signal at 4.90 ppm corresponds to the residual solvent proton and serves as a reference. A signal at 4.66 ppm is assigned to $CH_2$ protons within the ligand structure. In the complex spectrum (Fig. 2a), this signal shifts downfield to 4.49 ppm, indicating interaction with the metal centre.

The $^{13}C$ NMR spectrum of the complex (Fig. 2b) shows chemical shifts compared to the free ligand, reflecting changes due to metal coordination. The CSS carbon shifts from 211 ppm (ligand) to 206.89 ppm (complex), and the carboxylate carbon ($COO^-$) shifts from 176.36 ppm to 174.89 ppm—both indicating increased electron density [2]. In contrast, $CH_2$ carbons shift from 59.00 ppm to 60.90 ppm, suggesting reduced electron density.

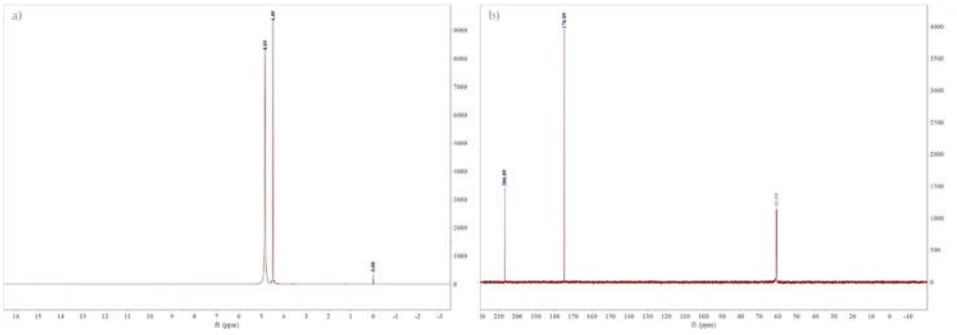

**Figure 2. a)** $^{1}H$ NMR spectra of complex; **b)** $^{13}C$ NMR spectra of complex

*3.3. UV visible spectra studies*

The UV/Vis spectrum of the ligand (Fig. 3) shows two absorption bands in the ultraviolet region. The band at 259 nm is attributed to intraligand π→π* transitions, associated with electron transitions within the $NCS_2$ group. This indicates the presence of conjugated π-electrons capable of absorbing UV radiation. The second band, observed at 287 nm, is assigned to n→π* transitions from the lone electron pair on the sulfur atom.

Upon coordination with $Cd^{2+}$ ions, shifts in these absorption bands are observed in the complex. The bands appear at 258 nm and 282 nm, reflecting changes in the ligand's electronic structure due to cadmium coordination. A new band at 223 nm is attributed to intraligand charge transfer (ILCT) induced by cadmium binding. Additionally, a weak band at 336 nm is observed and assigned to ligand-metal "charge transfer" (LMCT).

Based on obtained data, the proposed formula of the complex is $(NH_4)_4[Cd(idadtc)_2]$, shown in Fig. 4.

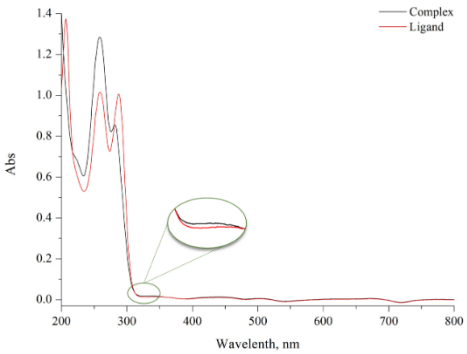


**Figure 3.** Side-by-side comparison of the ligand and complex UV/Vis spectra

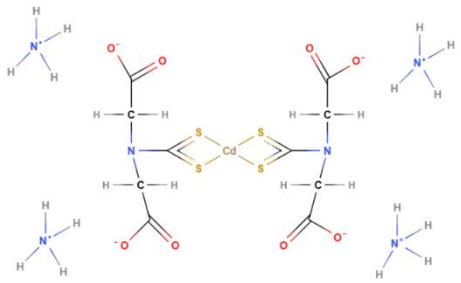

**Figure 4.** The proposed structure of complex $(NH_4)_4[Cd(idadtc)_2]$

## 4. Conclusions

In this study, a new cadmium(II) complex with ammonium-iminodiacetatedithiocarbamate ($(NH_4)_3$idadtc) ligand was successfully synthesized. Spectroscopic characterization by IR, UV/VIS, and $^{1}H$ and $^{13}C$ NMR spectroscopy, together with electrical conductivity measurements, confirmed the formation of an ionic complex with the proposed composition

$(NH_4)_4[Cd(idadtc)_2]$. The IR spectral shifts of characteristic C–S and Cd–S vibrations indicated that the ligand coordinates to the cadmium ion through sulfur atoms in an isobidentate mode. Changes observed in the NMR chemical shifts further supported the interaction between the ligand and the metal center, while UV/VIS spectroscopy revealed modifications in the ligand's electronic structure upon coordination, including the appearance of metal-to-ligand charge transfer (MLCT) bands.

**References**


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