CRYSTAL STRUCTURE,

AND BIOLOGICAL ACTIVITY OF A 2D Cd(II) COORDINATION POLYMER BASED ON 1-HYDROXY-2-NAPHTHOIC ACID

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Annotation:

A new two-dimensional (2D) coordination polymer based on Cd (II) was synthesized in the presence of 4-hydroxy-1-naphthoic acid (HNA), acetic acid (AA), N, N-dimethylformamide (DMF), and cadmium acetate. The crystalline structure of the synthesized HNA-CP was determined using single-crystal X-ray diffraction, and it was found that the HNA and AA ligands are fluctually bound with Cd (II) centers in the inner coordination region, while two DMF molecules are located in the outer coordination region. As a result of structural analysis, a classical "oar wheel" type nucleus with a distorted quadratic-pyramidal geometry was identified due to bidentate bridge-forming ligands. Antifungal studies have shown that HNA-CP exhibits significant inhibitory activity against Fusarium oxysporum, F. solani, and F. graminearum. The obtained results confirm that HNA-CP is a promising multifunctional material.

Key words:

4-hydroxy-1-naphthoic acid (HNA), acetic acid (AA), cadmium acetate, 2D, TGA.

Introduction

In recent years, research on coordination polymers (CP) has been rapidly developing, and this area has become a promising direction of great importance in such practical areas as catalysis, sensing, and nanotechnology. The unique structural features of CPs not only arouse fundamental scientific interest but also provide a wide range of practical applications [1]. Coordination compounds are complex systems consisting of central metal ions and organic or inorganic ligands, forming coordination bonds through donor atoms[2]. During polymerization, they combine into one-dimensional, two-dimensional[3], and three-dimensional branched structures, forming multifunctional polymers with unique physicochemical properties[4].

In this work, 1-hydroxy-2-naphthoic acid (HNA) was selected as a ligand. HNA has been extensively studied in terms of pharmaceutical, biological, and crystal engineering[5]. Naphthalene derivatives exhibit a wider range of biological activities, including antimicrobial, antioxidant, anti-inflammatory, cytotoxic, and antiprotozoal effects. It is known that the coordination of such ligands with metal centers significantly enhances or alters their biological profiles, and many studies report an increased antimicrobial effect upon metal complexation[6].

A new two-dimensional Cd (II) coordination polymer (HNA-CP) was synthesized from the 1-hydroxy-2-naphthalene ligand, the structure and properties of which were studied in detail. The structural properties of the polymer were determined by the method of single-crystal X-ray diffraction (SC-XRD), and the coordination medium of Cd (II) ions and the two-dimensional architecture of the polymer frame were confirmed. The results provide important information about the unique structural features[7] and potential practical applications of HNA-CP.

Materials and Methods:

The crystal structure of the synthesized coordination polymer was determined by single-crystal X-ray diffraction using Mo Kα radiation (λ = 0.71073 Å) at room temperature. Data were collected and refined using standard crystallographic methods. Antifungal activity was evaluated in vitro against Fusarium oxysporum, F. solani, and F. graminearum on potato dextrose agar (PDA) by measuring colony growth inhibition compared to control samples.

Results and Discussion:

To understand the structure of the synthesized HNA-CP, single-crystal X-ray diffraction was conducted. Crystallographic data show that the coordination polymer is formed in the presence of Cd (II) ions, HNA, AA, and DMF solvent molecules. The HNA and AA ligands are fluctuating in the inner coordination sphere of the Cd (II) centers, and two DMF molecules are located in the outer coordination sphere. Crystallographic parameters and purification statistics are summarized in Table 1.

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Table 1. Crystal data and structure refinement of the HNA-CP.

CCDC	**2447454**
Empirical formula	$C_{48}H_{42}Cd_3O_{20}$, $2(C_3H_7NO)$
Formula weight	1422.20
Temperature (K)	293(2)
Radiation type	CuKα (1.54184 Å)
Crystal system	Orthorhombic
Space group	*Pbca(No. 61)*
a, b, c (Å)	8.2917(3), 18.5711(6), 36.8982(12)
α, β, γ (°)	90, 90, 90
Volume ($Å^3$)	5681.8(3)
Z	4
Density (calculated) (g/cm^3)	1.663
Absorption coefficient (mm^{-1})	9.604
F(000)	2856
Crystal size (mm^3)	0.11 x 0.12 x 0.14
Theta range for data collection	4.8, 79.0°
Index ranges	-10≤h≤10, -22≤k≤23, -46≤l≤43
Reflections collected	37207
Independent reflections	5925 [R(int) = 0.101]
Data/parameters	4456/375
Goodness-of-fit on F^2	1.11
Absorption correction	multi-scan
Max. and min. transmission	-1.23 and 1.43
Refinement method	Full-matrix least-squares on F^2
Final R indices [I>2sigma(I)]	R1 = 0.0490, wR2 = 0.1279

Phytopathogenic Fungal Strains Studies: In this study, the antifungal activity of the synthesized coordination polymer Cd (II) (HNA-CP) was assessed against three phytopathogenic species: *Fusarium oxysporum*, *Fusarium solani, and Fusarium graminearum.* For antifungal testing, four preparations were prepared: (1) HNA-CP, (2) $Cd(CH_3COO)_2 \cdot 2H_2O$, (3) DMSO, and (4) 1-hydroxy-2-naphthoic acid, each at a concentration of 2.5% (Table 2) using DMSO as a solvent[8].

8 Saidov, D. X., & Turayev, X. X. AB Ibragimov coordination polymer based on 1-hydroxy 2-naphthoic acid and Cd ($CH_3COO)_2 \cdot 2H_2O$// republican scientific an
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Table 2. Elemental Composition.

Sl. No.	Composition	Concertation
1	HNA-CP	2.5%
2	$Cd(CH_3COO)_2 \cdot 2H_2O$	2.5%
3	DMSO	2.5%
4	1-Hydroxy-2-naphthoic acid	2.5%

The experiments were conducted according to the method of N. S. Yegorov. 1 ml of the fungal mycelium suspension was evenly distributed on the PDA plates, after which four pits were created in each Petri dish. 0.5 ml of the test solution was administered into each well.

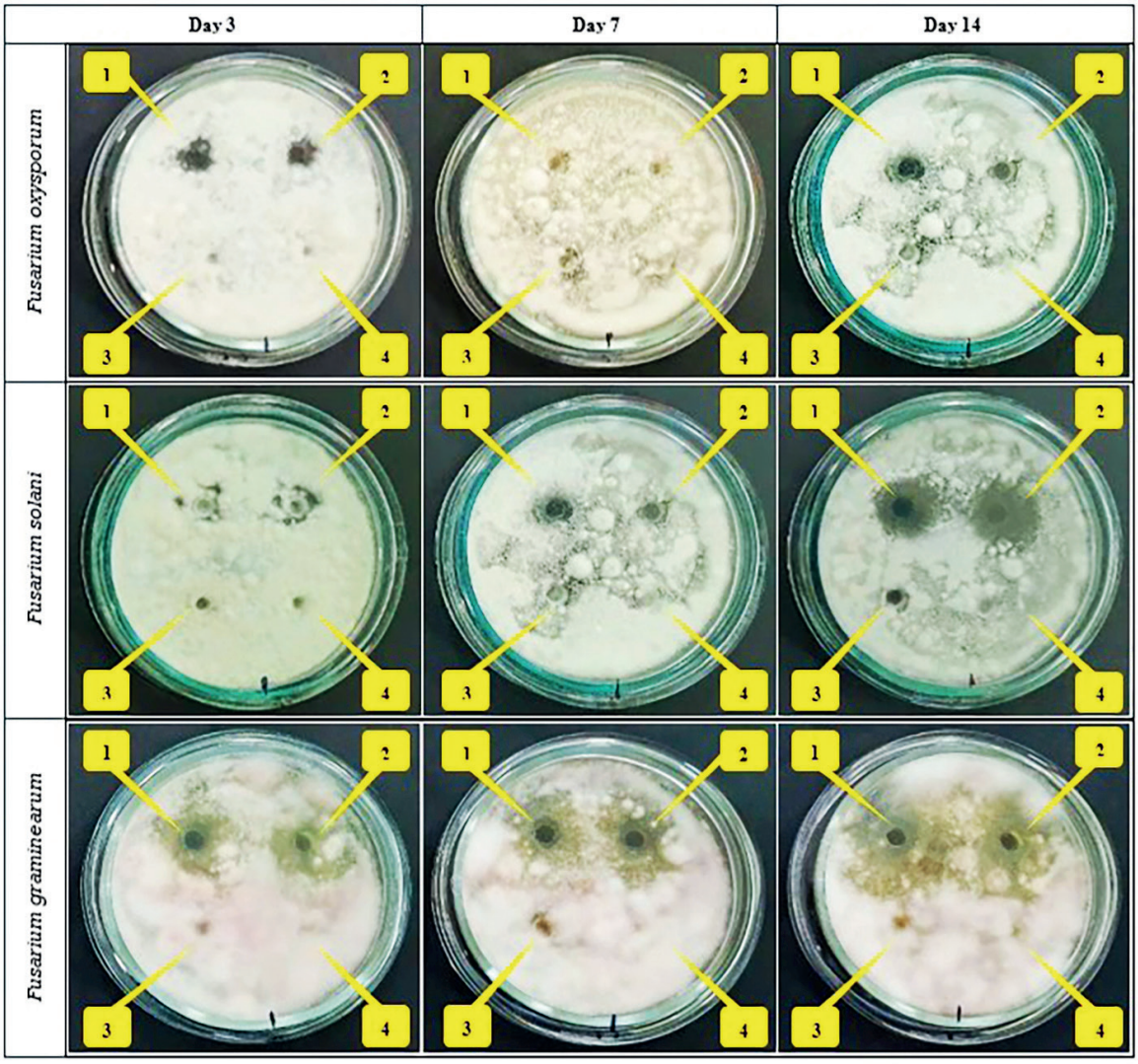

Fig. 1 Antifungal activity of the tested compounds against Fusarium oxysporum, Fusarium solani, and Fusarium graminearum. Numbers 1-4 correspond to: (1) HNA-CP, (2) Cd(CH3COO)2·2H2O, (3) DMSO, and (4) 1-hydroxy-2-naphthoic acid.

The plates were incubated for 14 days in an artificial climate chamber, stored at a temperature of 25-26°C during the day and 20-21°C at night. Antifungal effect was assessed by measuring the diameter of the inhibition zone (d, mm) on days 3, 7, and 14. Control of DMSO and 1-hydroxy-2-naphthoic acid showed insignificant inhibition zones during the experimental period, which confirmed their low antifungal activity. Cd $(CH_3COO)_2 \cdot 2H_2O$ caused only moderate[9] inhibition, which indicates limited effectiveness. On the contrary, HNA-CP showed consistently high inhibitory activity against three types of fungi. The overall inhibitory effects are illustrated in Fig. 1.

TGA/DTA Studies:

The thermal stability of the synthesized HNA-CP was analyzed using differential thermal and thermogravimetric studies. 18.339 mg of polymer crystals were used for the analysis, and the process was carried out at temperatures up to 800 °C (Fig. 2). The thermogravimetric analysis (TG) curve of HNA-CP showed two important stages of mass loss. The mass loss in the temperature range of 57.62-215.95 °C was caused by the decomposition of the complex and the complete removal of acetic acid and DMF, which led to a decrease in the total mass by 54.77%. This value indicates a significant mass loss from the compound. At this stage, mass loss was observed in the range from 219.96 to 638.04 °C, resulting in a 36.03% decrease in the total mass due to the decomposition of HNA acid. At the end of this process, cadmium (II) oxide remained[10]. Differential thermal analysis (DTA) of the complex revealed the following: This stage is an endothermic process, occurring in the temperature range from 69.75 °C to 83.41 °C, the change in thermal energy is -17.45 J. Mass loss occurs mainly due to the separation of water and other small molecules stuck to the surface, which indicates the first change in the complex due to heat. The reactions are also endothermic, occurring in the temperature range from 116.59 °C to 146.92 °C, with a change in thermal energy of -1.4 J. At this stage, organic components burn to form gas and release heat-resistant molecules.

Table 3 Analysis of the results of the TGA and DTA curves of the obtained HNA-CP.

Sl. No	Temp. (°C)	Mass lost [mg (18.339)]	Mass loss (%)	Amount of energy consumed (μV*s/mg)	Time spent (min)	dw (mg)	dw/dt (mg/min)
1	50	0.0159	0.0867	2.997	3.05	18.323	0.00521
2	100	0.227	1.23	2.674	68.43	18.112	0.00331
3	200	8.447	46.06	-9.152	78.46	9.892	0.10765
4	300	11.485	62.62	0.080	88.36	6.854	0.12997
5	400	13.849	75.51	-13.641	98.575	4.49	0.14049
6	500	15.146	82.58	-25.573	108.775	3.193	0.13924
7	600	16.352	89.1	-31.385	118.875	1.987	0.13755
8	700	17.163	93.28	-47.937	129.21	1.176	0.13283
9	800	17.282	94.23	-59.488	139.66	1.057	0.12374

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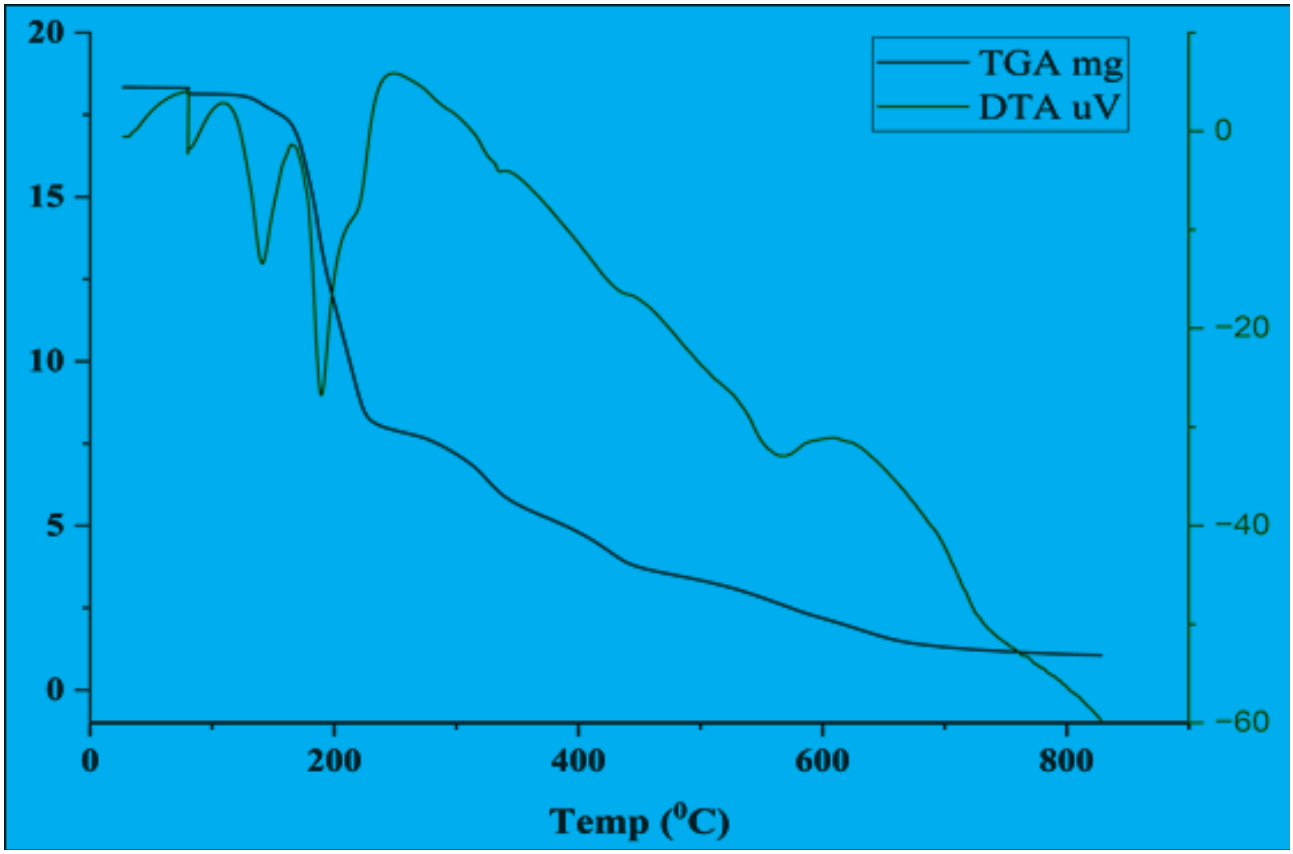

This stage is characterized by endothermic reactions in the temperature range from 165.94 °C to 178.06 °C; the change in thermal energy is -3.46 J. At this stage, a large amount of decomposition and carbonation occurs, which leads to the complete combustion of a significant amount of organic material, leaving only a small amount of mineral oxides. Table 3 shows the data of THA and DTA for the prepared HNA-CP[11].

Conclusion: In this work, a new Cd(II) coordination polymer (HNA-CP) based on 1-hydroxy-2-naphthoic acid (HNA) was successfully synthesized. Its two-dimensional structure was determined by single-crystal X-ray diffraction, revealing a distorted quadratic-pyramidal coordination geometry around the Cd(II) centers caused by bidentate ligands. Thermogravimetric analysis (TGA) demonstrated that HNA-CP exhibits good thermal stability, with initial weight loss attributed to the removal of coordinated and/or lattice solvent molecules, followed by a major decomposition step corresponding to the collapse of the polymeric framework[12]. Antifungal studies showed that HNA-CP possesses significant inhibitory activity against *Fusarium oxysporum*, *F. solani*, and *F. graminearum*. These results confirm the potential of HNA-CP as a promising multifunctional material with combined structural, thermal, and biological properties.

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