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SYNTHESIS OF A Cd(II)-BASED 2D COORDINATION POLYMER WITH 1-HYDROXY-2-NAPHTHOIC ACID

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Abstract: In this work, a new Cd(II) coordination polymer (HNA-CP) based on 4-hydroxy-1-naphthoic acid (HNA) was synthesized, and its structure was characterized by single-crystal X-ray diffraction. Crystallographic analysis showed that Cd(II) ions have separate coordination media and are combined into an extended two-dimensional polymer frame.

Keywords: X-ray, 2D coordination polymer, 4-hydroxy-1-naphthoic acid (HNA).

Аннотация: В данной работе был синтезирован новый координационный полимер Cd(II) (HNA-CP) на основе 4-гидрокси-1-нафтойной кислоты (HNA), и его структура была охарактеризована методом рентгеновской дифракции на монокристалле. Кристаллографический анализ показал, что ионы Cd(II) имеют отдельные координационные среды и объединены в протяженный двумерный полимерный каркас.

Ключевые слова: Рентген, 2D-координационный полимер, 4-гидрокси-1-нафтоевая кислота (HNA).

Annotatsiya: Ushbu ishda 4-gidroksi-1-naftoik kislotasi (HNA) asosida yangi Cd(II) koordinatsion polimer (HNA-KP) sintez qilindi va uning strukturasini monokristalli rentgen difraksiyasi orqali tavsiflandi. Kristallografik tahlil shuni ko‘rsatdiki, Cd(II) ionlari alohida koordinatsion muhitlarga ega bo‘lib, kengaytirilgan ikki o‘lchovli 2D polimerik ramkaga birlashtiriladi.

Kalit so‘zlar: Rentgen, 2D koordinatsion polimer, 4-gidroksi-1-naftoy kislotasi (HNA).

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 KPs 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. During polymerization, they combine into one-dimensional, two-dimensional, and three-dimensional branched structures, forming multifunctional polymers with unique physicochemical properties [2-4].

In this work, 1-hydroxy-2-naphthoic acid (HNA) was selected as a ligant. HNA has been extensively studied in terms of pharmaceutical, biological, and crystal engineering [23]. 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 [24,25]

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 and potential practical applications of HNA-CP.

Experimental

Synthesis **of Coordination Polymer**

To synthesize the coordination polymer, 0.376 g of 1-hydroxy-2-naphthoate (HNA, 0.1 M) was dissolved in 15 mL of 96% ethanol, followed by the addition of 5 mL of N, N-dimethylformamide (DMF). The solution was stirred magnetically for 30 minutes, resulting in a homogeneous dark brown solution. Separately, 0.266 g of citric acid (CA, 0.1 M) was dissolved in 10 mL of distilled water and gradually added to the ligand solution under continuous stirring. The resulting mixture was filtered through filter paper to obtain a brown filtrate. To promote solvent evaporation, the filtrate was maintained at 50-60°C in a thermostat for 10 days. At the end of this period, dark brown crystals were formed. The final HNA-based coordination polymer was designated as HNA-CP. The schematic representation of the synthesis procedure is shown in Fig. 1.

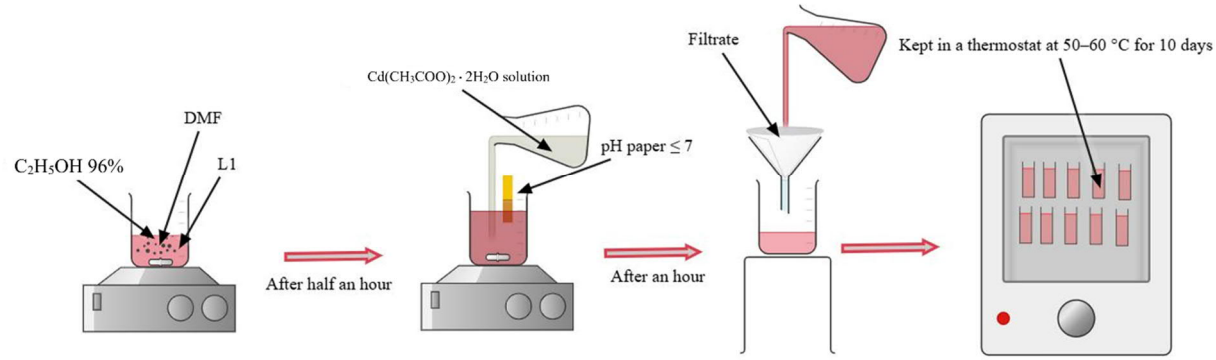

Fig. 1. HNA-CP crystal production scheme.

was performed. Crystallographic data show that the coordination polymer is formed in the presence of Cd (II) ions, HNA, acetic acid (AA), and dimethyl formamide (DMF) solvent molecules. The HNA and AA ligands are fluctuating in the inner coordination region of the Cd (II) centers, while two DMF molecules are located in the outer coordination region. Crystallographic parameters and purification statistics are summarized in Table 1.

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	$-10\leq h\leq 10$, $-22\leq k\leq 23$, $-46\leq l\leq 43$
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

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