https://wordlyknowledge.uz/index.php/gpble
Qabul qilingan sana: 07.12.2025
Nashr etilgan sana: 30.01.2026

D.Kh.Saidov, Kh.Kh.Turaev
[1]Termiz State University, Faculty of Chemistry, Termez, Uzbekistan.
Corresponding Author: saidovdilmurod@514gmail.com

SYNTHESIS, CRYSTAL STRUCTURE, THERMAL AND CONDUCTIVE PROPERTIES OF A Cd(II) COORDINATION POLYMER

Abstract: In this paper, a new cadmium-based polymer was synthesized using 1-hydroxy-2-naphthoic acid and cadmium acetate. The structural and physicochemical properties of the obtained polymer were investigated using various analytical techniques. Moreover, electronic transitions. Thermal behavior was examined through differential thermal analysis (DTA) and thermogravimetric analysis (TGA). The crystallinity and phase purity were confirmed by X-ray diffraction (XRD) using a Rigaku MiniFlex 600 diffractometer. In addition, elemental composition was determined via CHNS/O analysis (Thermo Scientific FlashSmart). Additionally, the polymer's electrical properties were evaluated through conductometric measurements.

Keywords - Cadmium-based polymer, 1-hydroxy-2-naphthoic acid, XRD, DTA, TGA.

1.Introduction

Recently, research in the field of coordination polymers (CPs) has expanded significantly, leading to a sharp increase in scientific interest toward this area. CPs are complex chemical systems composed of central metal ions coordinated with organic or inorganic ligands. Through donor atoms, the ligands form coordination bonds with metal ions, resulting in the polymerization process that produces three-dimensional, branched spatial structures possessing diverse structural and functional properties [1, 2]. The structural diversity and high flexibility of these frameworks make CPs highly valuable for both fundamental research and practical applications**.** Their notable features-such as porosity, conductivity, catalytic activity, and environmental safety-open wide opportunities for their utilization in

https://wordlyknowledge.uz/index.php/gpble
Qabul qilingan sana: 07.12.2025
Nashr etilgan sana: 30.01.2026

modern technologies, including energy storage, air pollution reduction, drug delivery, and environmental purification [3, 4]. Consequently, the development of novel synthesis and modification methods of CPs plays a crucial role in materials science. Synthesis based on green chemistry principles guarantees the creation of eco-friendly and sustainable materials [5, 6], promoting their widespread use across diverse industrial sectors [7-9]. Current research efforts are increasingly focused on improving the functional properties and efficiency of CPs through innovative synthetic approaches and advanced design strategies [10].

1-Hydroxy-2-naphthoic acid is used as an intermediate for azo and triphenylmethane dyes and, more recently, for colour film dyes [11]. Complexes of many p-, d-, and 4f-metals with 1-hydroxy-2-naphthoic acid are currently known in the literature [12]. In addition to its use in organic synthesis, [13]. 1-Hydroxy-2-naphthoic acid has found many other applications, such as an intermediate for the production of long-life batteries. The sodium salt of 1-hydroxy-2-naphthoic acid is commonly used to dissolve riboflavin. It can also be used in biochemical studies to determine the content of ammonium, magnesium, and potassium. In this study, the composition and structure of the polymer were studied more deeply than in previous works. According to the results of thermogravimetric analysis (TGA), it was found that ligand L1 retains thermal stability up to 592.85°C, which will allow the synthesis of heat-resistant sorption MOFs (metal-organic frameworks) based on this ligand in the future. The main aim of this work is the study of the new Cd(II) coordination polymer based on 1-hydroxy-2-naphthoic acid and its structure and other properties using modern physicochemical methods.

2. Experimental Part

2.1. Metods

The structural, physicochemical, and functional properties of the synthesized coordination polymer were thoroughly investigated using a comprehensive set of advanced instrumental techniques. The thermal stability and decomposition behavior of the material were systematically evaluated by thermogravimetric and

https://wordlyknowledge.uz/index.php/gpble
Qabul qilingan sana: 07.12.2025
Nashr etilgan sana: 30.01.2026

differential thermal analyses (TGA/DTA). The ionic conductivity and dissociation characteristics of the polymer were examined through conductometric measurements. Moreover, the precise molecular and crystal structure of the coordination polymer was unambiguously determined by single-crystal X-ray diffraction (XRD) analysis, which provided detailed insights into the coordination environments of the metal centers, the ligand coordination modes, and the resulting three-dimensional framework architecture.

2.2. Materials and Methods

Cadmium acetate dihydrate, 1-hydroxy-2-naphthoic acid (L1), and acetic acid were used as starting materials. All reagents were purchased from Sigma-Aldrich and used without further purification.

2.3. Synthesis, Element Analysis

A quantity of 0.282 g (0.05 mol) of 1-hydroxy-2-naphthoic acid was dissolved in 30 mL of 96% ethanol, and the resulting solution was magnetically stirred for 30 minutes until a homogeneous dark brown solution was obtained. Subsequently, 0.399 g (0.05 mol) of cadmium acetate dihydrate ($Cd(CH_3COO)_2 \cdot 2H_2O$), previously dissolved in 20 mL of distilled water, was added dropwise to the ligand solution under continuous stirring. The reaction mixture was stirred for an additional 1 hour and then filtered, yielding a brown filtrate. To promote slow solvent evaporation and crystal growth, the filtrate was kept in a thermostat at 50–60 °C for 10 days. At the end of this period, dark brown single crystals suitable for further analysis were obtained with a yield of 73% (see Figure 1).

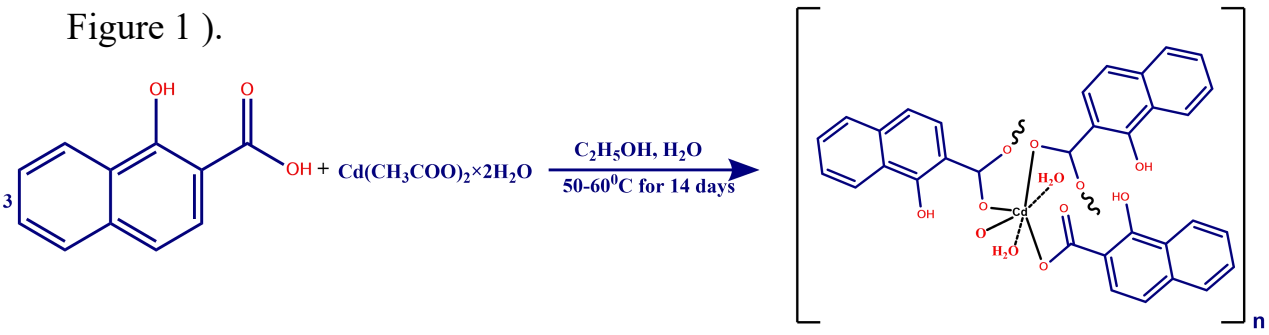


Fig. 2 Polymer synthesis reaction

https://wordlyknowledge.uz/index.php/gpble
Qabul qilingan sana: 07.12.2025
Nashr etilgan sana: 30.01.2026

3.Results and discussion.

3.1.Single-crystal XRD analysis

Crystal Structure Description:

The experimental conditions for single crystal X-ray diffraction and subsequent structure refinement are presented in Table 1, while Table 4 lists the key bond lengths and bond angles. The $[Cd_2(C_{11}H_8O_4)_4(H_2O)_3]_n$ polymer crystallizes in the triclinic crystal system with a noncentrosymmetric space group P-1, reflecting a low-symmetry crystal environment and a slightly distorted molecular geometry within the lattice. The molecular structure of the $[Cd_2(C_{11}H_8O_4)_4(H_2O)_3]_n$ polymer is shown in figure 1(a), with displacement ellipsoids drawn at the 55% probability level, and atoms labelled according to the standard numbering scheme. The overall crystal packing is illustrated in figure 1(b).

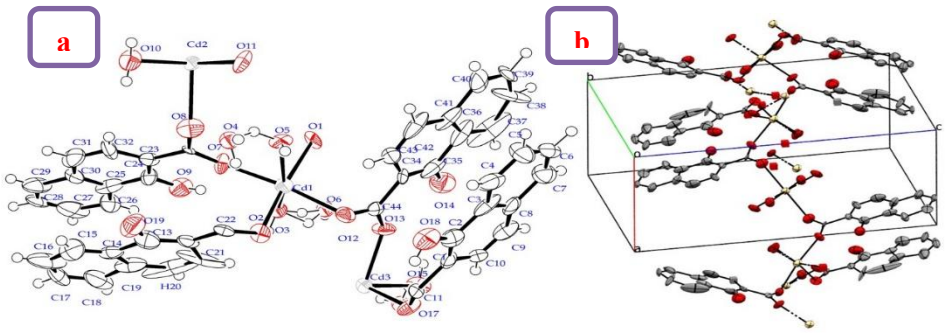


Fig.1 (a) ORTEP of the asymmetric unit of $[Cd_2(C_{11}H_8O_4)_4(H_2O)_3]_n$, showing the atom-numbering scheme with displacement ellipsoids drawn at the 55% probability level. (b) Crystal packing diagram.

Single-crystal X-ray diffraction analysis reveals that $[Cd_2(C_{11}H_8O_4)_4(H_2O)_3]_n$ forms an extended two-dimensional coordination polymer. In this architecture, each Cd^{2+}centre adopts a distorted seven-coordinate geometry, coordinated by oxygen atoms from carboxylate and hydroxyl groups of four distinct ligands, as well as by water molecules. The carboxylate groups act as μ^3-bridging ligands, connecting three separate Cd^{2+} ions through multiple coordination modes. Specifically, one carboxylate chelates a Cd^{2+} centre via a bidentate κ^2O,O' mode, the hydroxyl group bridges to a second Cd^{2+} ion ($\kappa O'$), and the remaining oxygen coordinates to a third Cd^{2+} ion ($\kappa O''$). This intricate multi-dentate coordination

https://wordlyknowledge.uz/index.php/gpble
Qabul qilingan sana: 07.12.2025
Nashr etilgan sana: 30.01.2026

underpins the formation of the two-dimensional polymeric network. Additionally, the coordinated water molecules enhance structural stability through hydrogen-bonding interactions, further reinforcing the rigidity and extended nature of the polymeric framework. Crystallographic analysis demonstrates that the Cd^{2+} centres exhibit Cd-O bond lengths of 2.245(12)-2.309(12) Å for Cd1, 2.225(13)-2.377(14) Å for Cd2, and 2.215(13)-2.371(12) Å for Cd3, with corresponding average distances of 2.2748, 2.2953 and 2.2777 Å. The Cd-N coordination is characterised by bond lengths of 2.322(4) and 2.328(5) Å, consistent with typical Cd-N interactions in distorted polyhedral environments. Polyhedral analysis of the Cd2 site gives a coordination polyhedron volume of 15.7347 $Å^3$, together with a quadratic elongation of 1.0172 and a bond-angle variance of 53.3614 deg^2, confirming a moderately distorted coordination geometry. The distortion index of 0.02382 indicates a slight deviation from ideal polyhedral geometry, while the effective coordination number of 5.8272 confirms that each Cd^{2+} centre adopts a slightly distorted seven-coordinate environment. Structurally, the compound forms a layered coordination polymer along the a-axis, where individual Cd^{2+} centres are interconnected through bridging carboxylate and hydroxyl groups, giving rise to extended chain-like motifs. These chains further assemble into a columnar supramolecular framework along the b-axis, stabilised by inter-ligand interactions, including hydrogen bonding, which reinforces the rigidity and extended nature of the two-dimensional polymeric network. This description highlights the subtle distortions in the coordination geometry and the overall structural organisation of the polymeric framework.

Table 1. Crystal data and structure refinement details for $[Cd_2(C_{11}H_8O_4)_4(H_2O)_3]_n$

Crystal Data	
Formula	$C_{44}H_{38}Cd_2O_{18}$
Formula Weight	1069.50
Crystal System	triclinic
Spacegroup	P-1(No.2)
a, b, c [Å]	7.3059(5), 14.0348(8), 19.2763(14)

https://wordlyknowledge.uz/index.php/gpble
Qabul qilingan sana: 07.12.2025
Nashr etilgan sana: 30.01.2026

α, β, γ (°)	73.101(6), 84.514(6), 89.955(5)
V [Å^3]	1881.8(2)
Z	2
D (calc) [g/cm^3]	1.905
Mu [mm^{-1}]	9.803
F (000)	1084
Crystal Size [mm]	0.00 x 0.00 x 0.00
Data Collection	
Temperature (K)	102
Radiation [Å]	CuKα 1.54184
Theta Min-Max [°]	2.4, 71.6
Dataset	-8:8; -16: 17; -23: 23
Tot., Uniq. Data, $R_{(int)}$	17737, 7210, 0.159
Observed Data [I>0.0sigma(I)]	4020
Refinement	
Nref, Npar	7210, 598
R, wR2, S	0.1375, 0.3709, 1.06
Max. and Av. Shift/Error	7.53, 0.10
Min. and Max. Resd. Dens. [e/Å^3]	-3.29, 6.41
CCDC	2447454

3.2. Thermal Analysis

Thermogravimetric (TGA) and differential thermal analysis (DTA) of the polymer $[Cd_2(C_{11}H_8O_4)_4(H_2O)_3]_n$ were performed (figure 3). The measurement process was continued up to a temperature of 900ºC. For sample analysis, a polymer weighing 3.765 mg was placed in a porcelain dish, and its thermal properties were studied under the influence of temperature.According to the obtained results, the thermogravimetric analysis curve (TG-blue curves) shows changes in three intensive intervals. The sample underwent mass loss in three stages. The first stage mass loss began in the first minutes of thermal exposure, at a temperature of 86.10°C, and ended at 296.71°C at 30.30 min. At this stage, the mass of MOF decreased by 46.454%, which is equal to 1.749 mg. Such mass loss is associated with the evaporation of water and acetic acid contained in the outer layer of the sample. The second stage mass loss began at 296.71°C (at 30.30 min) and continued until 60.49 min. During this stage, which lasted until 592.85°C, the

https://wordlyknowledge.uz/index.php/gpble
Qabul qilingan sana: 07.12.2025
Nashr etilgan sana: 30.01.2026

mass of the sample decreased by 29.668% (1.117 mg). The mass loss at this stage was due to the dissociation of the HNA⁰. In the third stage, at 901.02°C, the sample lost 7.968% (0.3 mg) of mass. At the last stage of the process, the sample was completely decomposed, leaving cadmium oxide and organic residues as the residue.

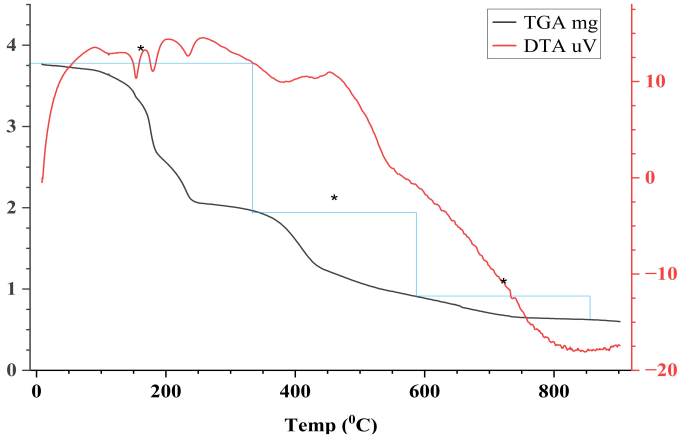


Fig.3 DGA and DTA analysis of the complex

DTA analysis (red curve) showed that the heat absorption, the endothermic process, occurred in four stages. The first stage began at 14.02 min and absorbed a temperature of 135°C. The heat absorption was completed in 17.31 min, when the temperature reached 167.50°C. Energy absorption peaked at 15.98 minutes, occurring at a temperature of 154.05°C.At this stage, -171.38 mJ (-40.94 cal) of heat was absorbed relative to the sample mass, equivalent to 45.52 J/g (10.87 cal/g). Simultaneously, 2.82 mV of energy was released, corresponding to 0.75 mV/mg of the sample mass. Mass loss is primarily associated with the release of adsorbed water and volatile molecules, which determines the initial thermal change of the complex. The second stage endothermic effect began at 17.52 minutes (169.51°C) and ended at 20.64 minutes (200.81°C). The thermal energy change at this stage was 181.28 mJ. At this stage, organic components burn, forming gas, and heat-resistant molecules are released.The third stage endothermic effect began at 21.98 minutes (214.05°C) and ended at 26.05 minutes (254.58°C). The thermal energy change at this stage was -175.97 mJ. In this process, intensive decomposition and carbonation occur, resulting in the combustion of a large amount of organic

https://wordlyknowledge.uz/index.php/gpble
Qabul qilingan sana: 07.12.2025
Nashr etilgan sana: 30.01.2026

matter.The last stage endothermic effect began at 38.82 minutes (380.98°C) and ended at 56.16 minutes (550.71°C). The change in thermal energy at this stage was 2.90 J. This stage is explained by intensive decomposition and the breaking and decomposition of HNA bonds.

Conclusion.

In this study, the structure and properties of the new cadmium (II) polymer $[Cd_2(C_{11}H_8O_4)_4(H_2O)_3]_n$, synthesised on the basis of the HNA ligand, were comprehensively studied. Monocrystalline X-ray diffraction analysis confirmed the formation of an extended two-dimensional coordination architecture of the polymer and the stable coordination of Cd^{2+} centers through carboxylate, hydroxyl groups, and water molecules. Thermogravimetric analysis (TGA/DTA) showed that the material has a gradual decomposition and sufficient thermal stability. The obtained data indicate that this coordination polymer has potential practical applications due to such properties as stable structure, flexible functional groups, and conductivity.

References

1. Dzhardimalieva G. I., Uflyand I. E. Design and synthesis of coordination polymers with chelated units and their application in nanomaterials science //RSC advances. - 2017. - T. 7. - №. 67. - C. 42242-42288. https://doi.org/10.1039/C7RA05302A
2. Heine T., Dinca M., Zhu G. Physical Phenomena in Porous Frameworks //Accounts of chemical research. - 2025. - T. 58. - №. 3. - C. 327-329. https://doi.org/10.1021/acs.accounts.4c00835
3. Engel E. R., Scott J. L. Advances in the green chemistry of coordination polymer materials //Green Chemistry. - 2020. - T. 22. - №. 12. - C. 3693-3715. https://doi.org/10.1039/D0GC01074J
4. Masoomi M. Y., Morsali A. Applications of metal–organic coordination polymers as precursors for preparation of nano-materials //Coordination Chemistry Reviews. - 2012. - T. 256. - №. 23-24. - C. 2921-2943. https://doi.org/10.1016/j.ccr.2012.05.032
5. Engel E. R., Scott J. L. Advances in the green chemistry of coordination polymer materials //Green Chemistry. - 2020. - T. 22. - №. 12. - C. 3693-3715. https://doi.org/10.1039/D0GC01074J

https://wordlyknowledge.uz/index.php/gpble
Qabul qilingan sana: 07.12.2025
Nashr etilgan sana: 30.01.2026

6. Un H. I. et al. Defect-tolerant electron and defect-sensitive phonon transport in quasi-2D conjugated coordination polymers //Nature communications. - 2025. - T. 16. - №. 1. - C. 6628. https://doi.org/10.1038/s41467-025-61920-w
7. D.X.Saidov, X.X.To‘rayev, A.B.Ibragimov, B.Z.Adizov, A.Sh.Jo‘rayev, Z.V.Nurullayeva. Study of the structure and properties of a mixed-ligand polymer synthesized using 1.10-phenanthroline, tartaric acid, and copper nitrate // uzbek chemical journal Toshkent- 2025, №2 S 42-50
8. Kh.T.K., Ibragimov A.B., Kh.S.D. Synthesis and structural analysis of a mixed-ligand coordination polymer with Cd(II) based on 1-hydroxy-2-naphthoic and acetic acids // Journal of Universal Science Research. - 2025. - T. 3. - № 5. - C. 120-122.
9. Turaev Kh.Kh., Ibragimov A.B., Saidov D.Kh., B.CH.Tursunov, R.U.Ruziyev, Nurullaeva Z.V. Structure and properties of a mixed-ligand coordination polymer synthesized from 3,5 dimethylpyrazole, fumaric acid, and cobalt(ii) chloride hexahydrate //uzbek chemical journal Toshkent- 2025, №3 S
10. Turaev Kh.Kh., Ibragimov A.B., Saidov D.Kh., Xolto‘rayev Q.B., Nurullaeva Z.V. Obtaining crystalline structure and thermal properties of a new mixed-ligand coordination polymer of magnesium //uzbek chemical journal Toshkent- 2025, №3 S 66-74
11. J. Bailey, L. A. Williams in K. Venkataraman (ed.): Chemistry of Synthetic Dyes, vol. IV, Academic Press, New York, 1971 Hardback ISBN: 9780127170046
12. Elsayed S. A. et al. New complexes of 2-hydroxy-1-naphthoic acid and X-ray crystal structure of [Pt (hna)(PPh3) 2] //Journal of Molecular Structure. - 2013. - T. 1036. - C. 196-202. https://doi.org/10.1016/j.molstruc.2012.09.018
13. Ahatov A.A, Turaev Kh.Kh., Toshkulov A.Kh. Synthesis, crystal structure and properties of tris(benzene-1.2-diamine-N,N′)-cadmium naphthalene-1,5-disulfonate trihydrate complex compound. Indian Journal of Chemistry. Vol. 63, October 2024, pp. 1036-1043. https://doi.org/10.56042/ijc.v63i10.12760.