ISSN: 2582-4686 SJIF 2021-3.261,SJIF 2022-2.889, 2024-6.875 ResearchBib IF: 10.25 / 2025

THE MULTIDISCIPLINARY JOURNAL OF SCIENCE AND TECHNOLOGY

VOLUME-6, ISSUE-6

STRUCTURAL CHARACTERIZATION OF THE COORDINATION POLYMER $[NAFE(EDTA)(H_2O)]_N \cdot H_2O$ ANALYSIS, MOLECULAR ELECTROSTATIC POTENTIAL, AND CRYSTAL PACKING INVESTIGATION

U.U. Ruziev
Department of Chemistry, Termez State University, 43 Barkamol Avlod Street, Termez, 190111, Uzbekistan
Kh.Kh. Turaev
Department of Chemistry, Termez State University, 43 Barkamol Avlod Street, Termez, 190111, Uzbekistan
A.B. Ibragimov
Institute of General and Inorganic Chemistry of Uzbekistan Academy of Sciences, 100170, Mirzo Ulug'bek str., 77a Tashkent, Uzbekistan.
K.B. Kholturaev
Department of Chemistry, Termez State University, 43 Barkamol Avlod Street, Termez, 190111, Uzbekistan

Abstract

The coordination polymer $[NaFe(EDTA)(H_2O)]_n \cdot H_2O$ was comprehensively characterized through elemental and structural analyses, including energy-dispersive X-ray spectroscopy (EDX), molecular electrostatic potential (MEP) surface mapping, and crystal packing investigation. The EDX spectrum revealed prominent Fe Kα and Fe Kβ signals together with the characteristic Na Kα peak, confirming the presence of iron and sodium in the synthesized material and supporting the proposed chemical composition. Molecular electrostatic potential analysis provided valuable information on the charge distribution within the complex, identifying electron-rich regions localized around the carboxylate oxygen atoms of the EDTA ligand and electron-deficient regions associated with coordinated and lattice water molecules. These features indicate favorable sites for intermolecular hydrogen-bonding interactions and contribute to the stabilization of the crystal structure. Crystal packing analysis demonstrated the formation of an extended one-dimensional coordination polymer in which Fe(III) centers are interconnected through EDTA ligands and further stabilized by sodium ions and a network of O-H···O hydrogen bonds involving coordinated and crystallization water molecules. The synergistic combination of coordination bonds, electrostatic interactions, and hydrogen bonding results in a robust supramolecular architecture. The obtained findings provide a deeper understanding of the structural organization, intermolecular interactions, and physicochemical characteristics of this iron-EDTA-based coordination polymer, highlighting the importance of multidentate ligands in the design and construction of extended metal-organic frameworks and related functional materials.

Keywords: Coordination polymer; Fe(III) complex; EDTA ligand; Energy-dispersive X-ray spectroscopy; Molecular electrostatic potential; Crystal packing; Hydrogen bonding; Supramolecular structure.

ISSN: 2582-4686 SJIF 2021-3.261,SJIF 2022-2.889, 2024-6.875 ResearchBib IF: 10.25 / 2025

THE MULTIDISCIPLINARY JOURNAL OF SCIENCE AND TECHNOLOGY

VOLUME-6, ISSUE-6

Introduction

Coordination polymers represent an important class of metal-organic materials that have attracted significant attention due to their fascinating structural diversity and wide range of practical applications in catalysis, ion exchange, gas storage, environmental remediation, magnetism, sensing, and biomedical sciences. The architecture of these materials is largely determined by the coordination behavior of metal ions and the flexibility of the organic ligands employed. Consequently, the rational design of coordination polymers remains an active area of research in modern coordination chemistry and crystal engineering. Among the numerous ligands used for the construction of coordination frameworks, ethylenediaminetetraacetic acid (EDTA) is one of the most versatile multidentate chelating agents. Owing to the presence of four carboxylate oxygen atoms and two nitrogen donor atoms, EDTA can coordinate metal ions in various binding modes, leading to the formation of stable mono-, bi-, and polynuclear complexes as well as extended coordination networks. In addition to strong metal binding, the carboxylate groups of EDTA can participate in hydrogen-bonding interactions, which play a crucial role in the stabilization of supramolecular architectures.

Iron-containing EDTA complexes are of particular interest because iron is an environmentally benign and biologically important transition metal. The coordination of Fe(III) ions by EDTA results in highly stable complexes with diverse structural features and physicochemical properties. Furthermore, the incorporation of alkali metal ions such as sodium can significantly influence crystal packing, charge balance, and intermolecular interactions, thereby affecting the overall stability and organization of the resulting coordination polymer. In recent years, the combination of experimental characterization techniques and computational visualization methods has become an effective approach for understanding the structural properties of coordination compounds. Elemental analysis provides information about chemical composition, while molecular electrostatic potential (MEP) mapping reveals the distribution of electron density and identifies potential reactive sites. Crystal packing analysis, on the other hand, offers valuable insight into intermolecular interactions and the supramolecular organization of the crystal lattice. In the present study, the coordination polymer $[NaFe(EDTA)(H_2O)]_n \cdot H_2O$ was investigated using energy-dispersive X-ray spectroscopy (EDX), molecular electrostatic potential (MEP) surface analysis, and crystal structure visualization. The objective of this work was to confirm the elemental composition of the compound, evaluate its electronic surface characteristics, and examine the intermolecular interactions responsible for the formation and stabilization of the polymeric framework. The obtained results contribute to a better understanding of the structural organization and supramolecular behavior of iron-EDTA-based coordination polymers.

Results and Discussion

Energy-dispersive X-ray spectroscopy (EDX) was employed to investigate the elemental composition of the synthesized coordination polymer and to verify the presence of the metal components expected from the proposed chemical formula. The EDX spectrum shown in Figure 1 exhibits distinct characteristic peaks corresponding to sodium and iron, confirming the successful incorporation of these elements into the coordination framework. The most intense signals in the spectrum are observed at approximately 6.40 keV and 7.06 keV, which correspond to the Fe Kα and Fe K emission lines, respectively. The presence of these peaks clearly confirms iron as the central

ISSN: 2582-4686 SJIF 2021-3.261,SJIF 2022-2.889, 2024-6.875 ResearchBib IF: 10.25 / 2025

metal ion in the complex. The high intensity of the Fe Kα peak compared with other detected signals indicates that iron is a major constituent of the coordination polymer and plays a fundamental role in the formation of the polymeric structure. The appearance of both Kα and Kβ transitions also demonstrates the reliability of the elemental identification and excludes the possibility of spectral misassignment.

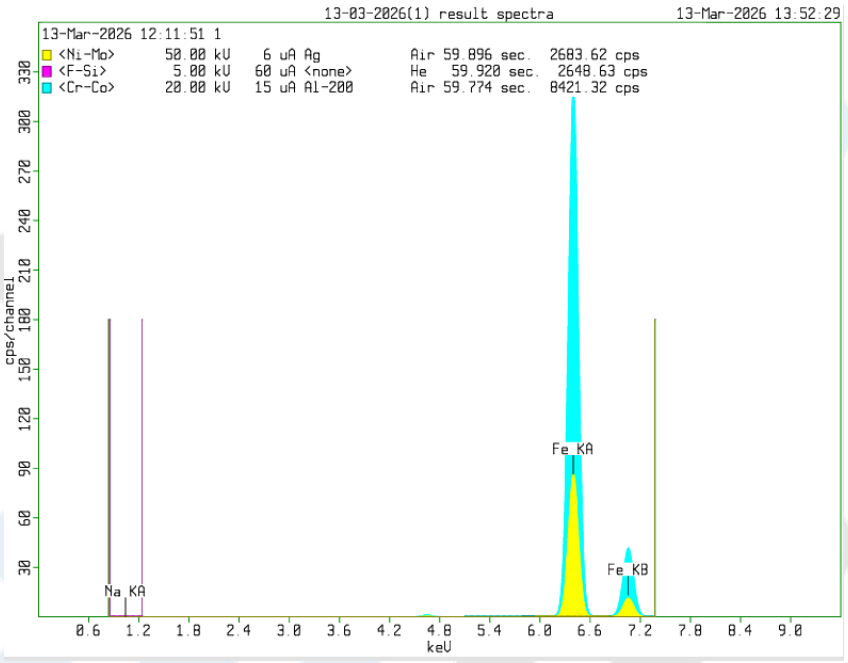

Figure 1. EDX spectrum of the coordination polymer $[NaFe(EDTA)(H_2O)]_n \cdot H_2O$

In addition to the iron peaks, a characteristic signal corresponding to Na Kα is observed near 1.04 keV, providing evidence for the incorporation of sodium ions within the crystal lattice. Sodium ions are expected to contribute to charge compensation and may participate in the stabilization of the extended coordination network through electrostatic interactions. The simultaneous detection of both iron and sodium signals is therefore fully consistent with the proposed composition of $[NaFe(EDTA)(H_2O)]_n \cdot H_2O$.

It should be noted that EDX analysis has inherent limitations in the detection of light elements. Elements such as hydrogen cannot be detected, while carbon, nitrogen, and oxygen generally produce weak signals due to their low atomic numbers and reduced X-ray emission efficiency. Consequently, the organic EDTA ligand and water molecules present in the structure cannot be fully characterized by EDX alone. Nevertheless, the observed elemental profile strongly supports the presence of the inorganic components of the coordination polymer and is in excellent agreement with the expected stoichiometry of the synthesized compound.

The EDX results therefore provide important experimental evidence for the successful synthesis of $[NaFe(EDTA)(H_2O)]_n \cdot H_2O$. Combined with the structural visualization and electrostatic potential analyses discussed in subsequent sections, the elemental analysis confirms the composition and integrity of the coordination framework. These findings demonstrate that the synthesized material contains the essential metal centers required for the formation of the extended polymeric

ISSN: 2582-4686 SJIF 2021-3.261,SJIF 2022-2.889, 2024-6.875 ResearchBib IF: 10.25 / 2025

THE MULTIDISCIPLINARY JOURNAL OF SCIENCE AND TECHNOLOGY

VOLUME-6, ISSUE-6

architecture and establishes a solid basis for further investigation of its structural and physicochemical properties.

Molecular Electrostatic Potential Surface Analysis

The molecular electrostatic potential (MEP) surface analysis was performed to investigate the electronic charge distribution within the $[NaFe(EDTA)(H_2O)]_n \cdot H_2O$ coordination polymer and to identify potential sites involved in intermolecular interactions. MEP mapping is a valuable computational tool for visualizing regions of different electrostatic potential on a molecular surface, thereby providing insight into the reactivity, charge-transfer behavior, and hydrogen-bonding capabilities of a compound.

As illustrated in Figure 2, the electrostatic potential is distributed unevenly over the molecular surface, indicating the presence of both electron-rich and electron-deficient regions. The color gradient ranges from red to blue, where red regions correspond to areas of the most negative electrostatic potential, while blue regions represent areas of positive electrostatic potential. Intermediate colors such as yellow and green indicate regions with moderate charge density.

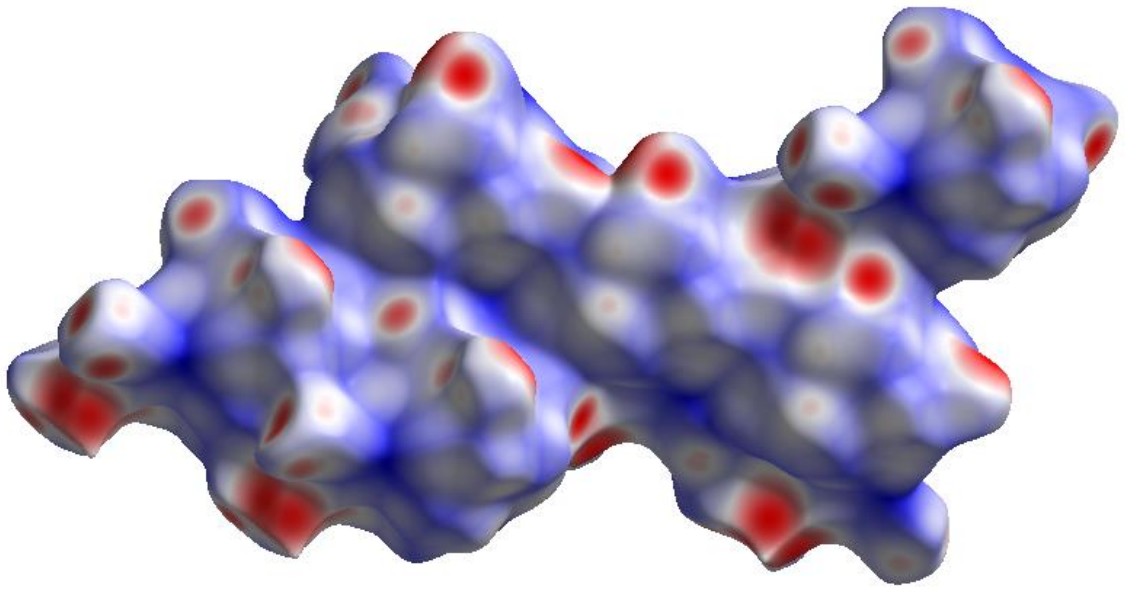

Figure 2. Molecular electrostatic potential (MEP) surface of $[NaFe(EDTA)(H_2O)]_n \cdot H_2O$**.**

The most negative electrostatic potential values are concentrated around the oxygen atoms of the carboxylate groups belonging to the EDTA ligand. These oxygen atoms possess a high electron density due to the presence of lone electron pairs and the partial negative charge associated with the carboxylate functionality. As a result, these sites are expected to serve as strong hydrogen-bond acceptors and play a significant role in intermolecular recognition processes. Furthermore, the localization of negative potential around the oxygen donor atoms is consistent with their involvement in coordination to the Fe(III) center, highlighting the important contribution of the EDTA ligand to the stabilization of the coordination environment.

In contrast, regions of positive electrostatic potential are primarily observed around the hydrogen atoms of coordinated and lattice water molecules. These hydrogen atoms exhibit electron-deficient character and therefore act as potential hydrogen-bond donors. The presence of such positively

ISSN: 2582-4686 SJIF 2021-3.261,SJIF 2022-2.889, 2024-6.875 ResearchBib IF: 10.25 / 2025

charged regions suggests that water molecules actively participate in the formation of intermolecular O-H···O hydrogen bonds with neighboring carboxylate oxygen atoms. These interactions contribute significantly to the cohesion and stability of the crystal structure.

The MEP surface also provides valuable information regarding the influence of the metal center on the electronic structure of the complex. Coordination of the EDTA ligand to the Fe(III) ion results in a redistribution of electron density throughout the molecule, generating distinct regions of charge accumulation and depletion. This redistribution enhances the polarity of the coordination framework and promotes electrostatic interactions between adjacent molecular units. Such interactions are particularly important in coordination polymers, where the overall stability of the structure depends not only on metal-ligand bonds but also on secondary supramolecular forces.

Crystal Packing and Intermolecular Interactions

The crystal packing structure of $[NaFe(EDTA)(H_2O)]_n \cdot H_2O$, illustrated in Figure 3, provides valuable insight into the three-dimensional organization of the coordination polymer and the intermolecular forces responsible for its structural stability. The packing diagram reveals that the compound forms an extended coordination network in which the metal centers, ligand molecules, sodium ions, and water molecules are arranged in a highly ordered manner throughout the crystal lattice. The regular arrangement of these structural components contributes to the formation of a robust supramolecular architecture that extends in multiple crystallographic directions.

At the molecular level, the Fe(III) center is coordinated by the multidentate EDTA ligand through its nitrogen and oxygen donor atoms, producing a stable chelated environment around the metal ion. The strong metal-ligand coordination bonds serve as the primary structural framework of the polymer. The EDTA ligand acts as an efficient bridging unit, allowing the formation of repeating coordination motifs that propagate throughout the crystal. Such coordination behavior is characteristic of EDTA-based complexes and demonstrates the ability of this ligand to generate extended architectures through multiple donor sites.

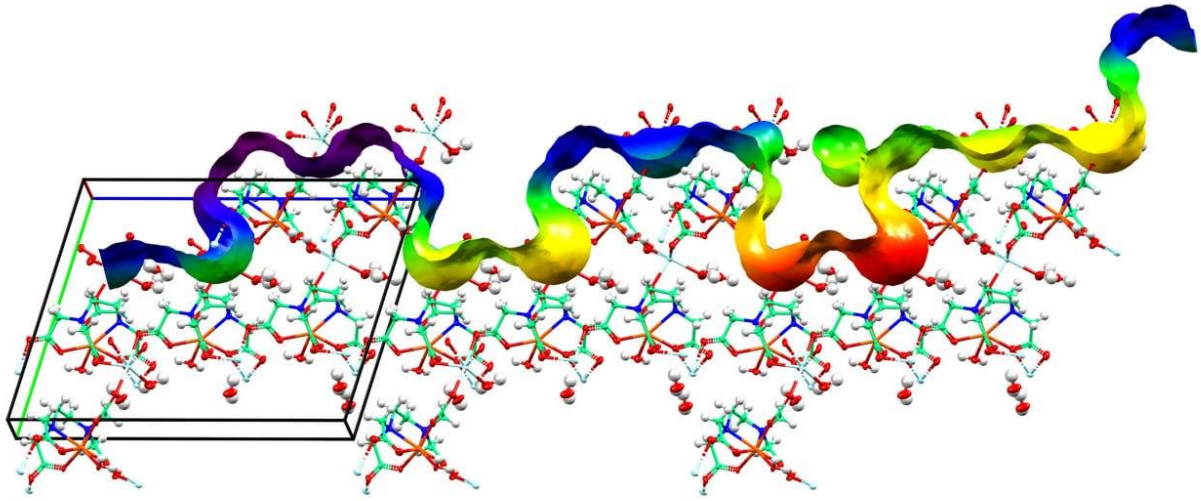

Figure 3. Crystal packing arrangement of $[NaFe(EDTA)(H_2O)]_n \cdot H_2O$**.**

The crystal packing arrangement further indicates that sodium ions play an important role in the overall organization of the structure. Besides maintaining charge neutrality, the sodium ions

ISSN: 2582-4686 SJIF 2021-3.261,SJIF 2022-2.889, 2024-6.875 ResearchBib IF: 10.25 / 2025

contribute to the stabilization of the polymeric framework through electrostatic interactions with neighboring oxygen-containing groups. These interactions help connect adjacent coordination units and reinforce the integrity of the crystal lattice. The participation of sodium ions in the packing arrangement highlights their significance in controlling the geometry and organization of the coordination polymer.

An important feature of the crystal structure is the presence of both coordinated and lattice water molecules. Coordinated water molecules occupy positions within the coordination sphere of the iron center, while lattice water molecules are located between neighboring polymeric chains. These water molecules act as key participants in the supramolecular assembly by forming an extensive network of hydrogen bonds. The hydrogen atoms of water molecules interact with the oxygen atoms of carboxylate groups, generating numerous O-H···O hydrogen-bonding contacts throughout the structure. These interactions effectively link adjacent polymeric units and contribute significantly to crystal stabilization.

The packing diagram suggests the existence of continuous intermolecular contact pathways extending along the polymeric direction. Such pathways create a three-dimensional network of non-covalent interactions that complement the coordination bonds present within the framework. The combination of strong metal-ligand interactions and weaker hydrogen-bonding contacts produces a highly interconnected structure capable of resisting lattice distortion. Consequently, the crystal exhibits enhanced rigidity and structural coherence.

Furthermore, the arrangement of neighboring chains indicates that electrostatic attractions between positively charged and negatively charged regions of the structure contribute to the overall packing efficiency. The negatively polarized carboxylate oxygen atoms of the EDTA ligand interact favorably with positively polarized hydrogen atoms of water molecules and sodium-containing regions, resulting in additional stabilization of the crystal lattice. These electrostatic interactions operate synergistically with hydrogen bonding to strengthen the supramolecular framework.

The observed crystal packing pattern demonstrates that the stability of $[NaFe(EDTA)(H_2O)]_n \cdot H_2O$ is not solely dependent on coordination bonds but also on a complex network of secondary interactions. Hydrogen bonding, electrostatic attractions, and van der Waals contacts collectively contribute to the formation of a densely packed and energetically favorable crystal structure. Such cooperative interactions are commonly encountered in coordination polymers and play a decisive role in determining their physical and chemical properties.

Conclusion

In this study, the coordination polymer $[NaFe(EDTA)(H_2O)]_n \cdot H_2O$ was successfully investigated through a combination of elemental and structural characterization techniques, including energy-dispersive X-ray spectroscopy (EDX)**,** molecular electrostatic potential (MEP) surface analysis**,** and crystal packing visualization**.** The integrated application of these methods provided valuable information regarding the composition, electronic properties, and supramolecular organization of the compound.

The EDX analysis confirmed the presence of the principal metallic components, namely iron and sodium, thereby supporting the proposed chemical formula and demonstrating the successful synthesis of the coordination polymer. The observed characteristic Fe Kα, Fe Kβ, and Na Kα signals were consistent with the expected elemental composition and indicated the high purity of the obtained material.

The molecular electrostatic potential analysis revealed a distinct distribution of charge density throughout the coordination framework. Electron-rich regions were predominantly localized around the carboxylate oxygen atoms of the EDTA ligand, whereas electron-deficient regions were associated mainly with the hydrogen atoms of coordinated and lattice water molecules. This charge distribution indicates a strong tendency toward intermolecular hydrogen-bond formation and highlights the important role of electrostatic interactions in stabilizing the crystal structure.

References

1. Suyunov J. R. et al. Synthesis, crystal structure and Hirshfeld surface analysis of diaquabis (o-phenylenediamine-κ2N, N′) nickel (II) naphthalene-1, 5 disulfonate //Structure Reports. – 2023. – Т. 79. – №. 11. – С. 1083-1087. Martell, A. E., & Smith, R. M. (1974). *Critical Stability Constants, Volume 1: Amino Acids*. Plenum Press, New York. *Acta Cryst.* (2023). https://doi.org/10.1107/S2056989023009350

2. Juraev Azamat Shoymurot ugli, et al. "Synthesis, crystal structure, supramolecular architecture and electronic structure analysis of a new iron (III)-EDTA complex salt." *Journal of Molecular Structure* (2026): 146273. https://doi.org/10.1016/j.molstruc.2026.146273

3. Ruziev, U., Djumayeva, Z., Toirova, G., Kholturaev, K., Ibragimov, A., & Balakrishnan, C. (2026). Crystal Structure, Vibrational Spectroscopic Characterization, and Bond Valence Sum (BVS) Analysis of a Copper (II)-H_2EDTA-Based Coordination Polymer $[Cu(H_2EDTA)]_n$ H_2O. *TerDU xabarlari*, *1*(1). https://journals.tersu.uz/index.php/1/article/view/83

4. Yuldasheva, N. N., Abdullaev, I. I., Takhirov, Y. R., Khudaynazarovich, T. K., Ruziev, U. U. U., Tashpulatov, J. J., ... & Ibragimov, A. B. (2026). Synthesis, structure and effect on cotton seed germination and seedling vigor of bis (2-hydroxybenzoate) bis (pyridine-3-carboxamide) copper (II). *Zeitschrift für Kristallographie-Crystalline Materials*, *241*(1-2), 9-23. https://doi.org/10.1515/zkri-2025-0044

5. Khabibjonovich, A.A., Yusupboyevich, Y.Y., Zamirovich, A.B., Khamidjanovich, R.A., Sadullayevich, N.A., Bakhtiyarovich, I.A., Akhtar, M.N., AlDamen, M.A. and Gao, J., 2024. A coordination polymer of Na-Fe (III) with EDTA: synthesis, characterization, electrical conductivity, adsorption properties and Hirshfeld surface analysis. *Adsorption*, *30*(6), pp.1407-1418. https://doi.org/10.1007/s10450-024-00504-4

6. Sanchiz, J., Domínguez, S., Mederos, A., Brito, F. and Arrieta, J.M., 1997. Tetramethyl Carboxylic Acids Derived from o-Phenylenediamines as Sequestering Agents for Iron (III): Thermodynamic Studies. X-ray Crystal Structure of Sodium Aqua (4-chloro-1, 2-phenylenediamine-N, N, N ‘, N ‘-tetraacetato) ferrate (III)− Water (1/1.5). *Inorganic Chemistry*, *36*(18), pp.4108-4114. https://doi.org/10.1021/ic9700617

7. Braga, D., Grepioni, F., & Tedesco, E. (1998). Crystal engineering and hydrogen-bonded networks. *Chemical Reviews*, 98(4), 1375-1406. https://doi.org/10.1021/cr960011m