

STRUCTURAL ELUCIDATION OF POLY[ETHYLENEDIAMINETETRAACETATO-AQUA-DISODIUM- NICKEL(II)] BY FOURIER TRANSFORM INFRARED SPECTROSCOPY

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Abstract

The coordination behavior of ethylenediaminetetraacetic acid (EDTA) toward transition-metal ions plays a decisive role in determining the structural stability and physicochemical properties of coordination polymers. In the present study, the synthesized poly[ethylenediaminetetraacetato-aqua-disodium-nickel(II)] coordination polymer was investigated by Fourier Transform Infrared (FT-IR) spectroscopy in order to establish the coordination mode of the ligand and verify the metal-ligand bonding environment. The FT-IR spectrum exhibits broad absorption bands at 3461 and 3374 cm^{-1} , which are assigned to the stretching vibrations of coordinated water molecules involved in hydrogen-bonding interactions. Characteristic asymmetric stretching vibrations of coordinated carboxylate groups appear at 1591 and 1475 cm^{-1} , whereas the corresponding symmetric vibrations are observed at 1393 and 1359 cm^{-1} . The frequency separation between these bands confirms that the carboxylate oxygen atoms actively participate in coordination with the Ni(II) center. Additional absorptions at 1316 and 1295 cm^{-1} originate from C–N stretching vibrations, indicating that the nitrogen donor atoms of EDTA are also involved in metal coordination. The appearance of new bands within the 709–444 cm^{-1} region provides direct spectroscopic evidence for the formation of Ni–O and Ni–N coordination bonds.

Keywords: Nickel(II), EDTA, Coordination Polymer, FT-IR Spectroscopy, Metal Complex, Structural Characterization.

Introduction

Coordination polymers based on transition metals and multidentate ligands have attracted considerable attention owing to their structural diversity and potential applications in catalysis, environmental remediation, sensing, and materials science. Ethylenediaminetetraacetic acid (EDTA) is one of the most versatile chelating ligands because it contains two nitrogen donor atoms and four carboxylate oxygen donor

groups, allowing the formation of highly stable metal complexes. Nickel(II) ions readily form coordination compounds with EDTA, producing structures with enhanced thermal stability and unique physicochemical properties. The coordination behavior of EDTA toward Ni(II) has been extensively investigated due to its relevance in environmental chemistry, wastewater treatment, and functional material synthesis. Recent studies have shown that Ni-EDTA complexes exhibit characteristic spectroscopic signatures that provide valuable information regarding metal–ligand interactions and coordination geometry. Among the available characterization techniques, Fourier Transform Infrared (FT-IR) spectroscopy is a powerful method for identifying functional groups involved in coordination and confirming the formation of metal–ligand bonds. Therefore, the present work focuses on the FT-IR characterization of poly[ethylenediaminetetraacetato-aqua-disodium-nickel(II)] and discusses the structural implications of the observed vibrational bands.

Results and Discussion

The FT-IR spectrum of poly[ethylenediaminetetraacetato-aqua-disodium-nickel(II)] exhibits several characteristic absorption bands confirming the successful coordination of EDTA to the nickel(II) ion. A broad absorption region centered at 3461 and 3374 cm^{-1} is assigned to O-H stretching vibrations of coordinated and hydrogen-bonded water molecules. The broad profile of these bands indicates intermolecular hydrogen-bonding interactions commonly observed in hydrated coordination compounds. The absorption band at 3028 cm^{-1} corresponds to C-H stretching vibrations of methylene groups present in the EDTA ligand framework. The presence of this band confirms the structural integrity of the organic ligand after complex formation. A strong absorption band observed at 1673 cm^{-1} is attributed to water bending vibrations coupled with coordinated carboxylate group interactions. The shift of this band compared with free EDTA suggests the participation of carboxylate oxygen atoms in metal coordination.

Prominent peaks at 1591 cm^{-1} and 1475 cm^{-1} are assigned to the asymmetric stretching vibrations, $\nu_{\text{as}}(\text{COO}^-)$, of coordinated carboxylate groups. The corresponding symmetric stretching vibrations appear at 1393 cm^{-1} and 1359 cm^{-1} . The observed separation between asymmetric and symmetric stretching frequencies indicates that the carboxylate groups are directly bonded to the nickel center, consistent with the chelating nature of EDTA. The absorption bands at 1316 cm^{-1} and 1295 cm^{-1} are attributed to C–N stretching vibrations of the coordinated amine groups. These shifts provide evidence that nitrogen donor atoms also participate in coordination with Ni(II), resulting in a hexadentate coordination mode of the EDTA ligand. Several peaks located between 1225 and 1019 cm^{-1} are associated with C–O stretching and skeletal

vibrations of the EDTA backbone. Additional bands at 956, 921, 900, 868, and 816 cm^{-1} correspond to O–C–O deformation modes and chelate ring vibrations. The most convincing evidence of complex formation is provided by the low-

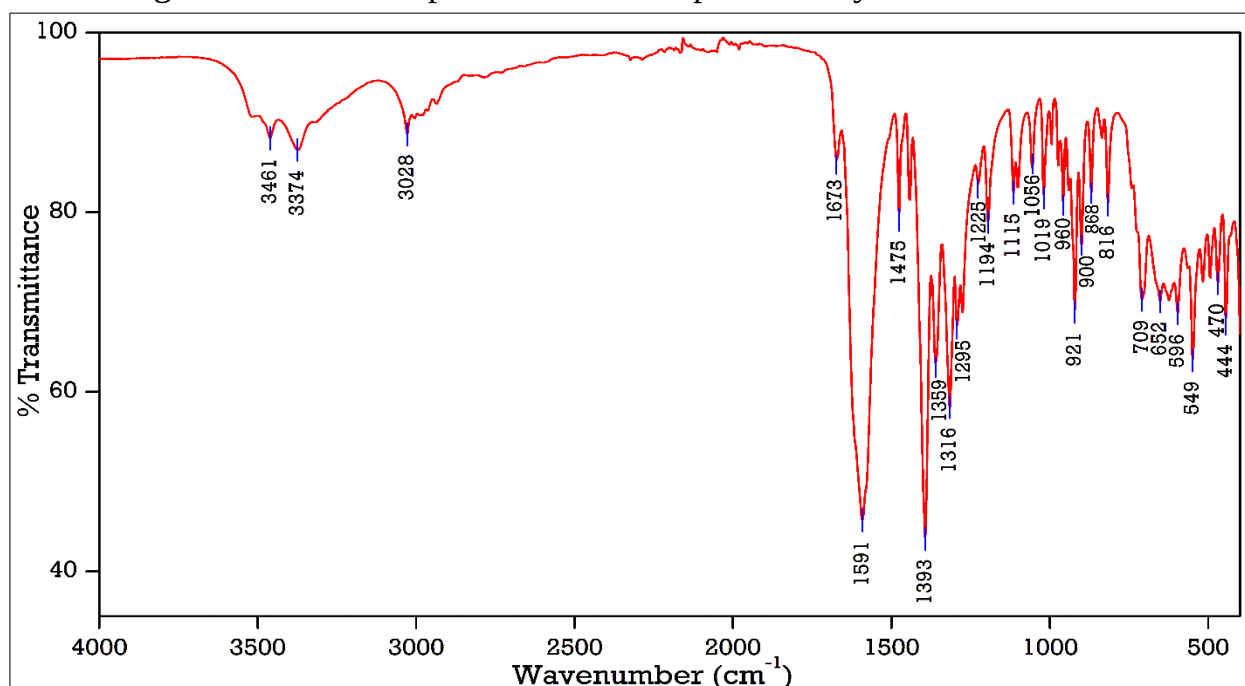


Figure 1. FT-IR spectrum of poly[ethylenediaminetetraacetato-aqua-disodium-nickel(II)].

Frequency bands observed at 709, 682, 596, 549, 470, and 444 cm^{-1} . These absorptions are characteristic of Ni–O and Ni–N stretching vibrations and confirm the direct interaction of nickel(II) with both oxygen and nitrogen donor atoms of EDTA. Based on these spectral features, the nickel ion is proposed to adopt a distorted octahedral geometry in which EDTA acts as a hexadentate ligand while water molecules complete the coordination sphere. Similar vibrational characteristics have been reported in recent studies on transition-metal EDTA complexes.

Table 1. FT-IR Assignments of Poly[ethylenediaminetetraacetato-aqua-disodium-nickel(II)]

Wavenumber (cm^{-1})	Assignment
3461, 3374	O-H stretching of coordinated water
3028	C-H stretching (CH_2)
1673	H-O-H bending / coordinated carboxylate vibration
1591, 1475	vas(COO^-)
1393, 1359	vs(COO^-)
1316, 1295	C-N stretching
1225-1019	C-O and skeletal vibrations
956-816	O-C-O deformation

709-549	Ni-O stretching
470, 444	Ni-N stretching

Conclusion

The FT-IR analysis of poly[ethylenediaminetetraacetato-aqua-disodium-nickel(II)] confirmed the successful coordination of EDTA to the nickel(II) center through both carboxylate oxygen and amine nitrogen donor atoms. The presence of characteristic $\nu_{as}(\text{COO}^-)$ and $\nu_s(\text{COO}^-)$ bands, together with metal-ligand vibrations observed below 700 cm^{-1} , provides strong evidence for the formation of Ni-O and Ni-N bonds. Broad O-H stretching bands indicate the presence of coordinated water molecules involved in hydrogen bonding. Overall, the spectral data support the formation of a hydrated nickel(II)-EDTA coordination polymer possessing an octahedral coordination environment around the metal center.

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