

Computational Analysis of Molecular Surface and Reactivity of a Nickel(II)-EDTA Coordination Polymer

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Abstract

The electronic structure and surface reactivity of poly[ethylenediaminetetraacetato-aqua-disodium-nickel(II)] were investigated using molecular electrostatic potential (MEP) and molecular surface analyses. The calculated MEP surface revealed pronounced charge separation, where the oxygen atoms of the carboxylate groups represent electron-rich regions, while the hydrogen atoms and the coordination environment around the Ni(II) center exhibit positive electrostatic potential. Electron density mapping demonstrated effective charge delocalization between the EDTA ligand and the nickel ion, indicating strong metal–ligand interactions. Surface reactivity analysis further identified the oxygen-containing functional groups as the most favorable sites for electrophilic attack. The balanced distribution of electrostatic potential and electron density suggests high electronic stability and an ordered coordination environment. These findings provide insight into the relationship between the electronic structure and chemical reactivity of the synthesized nickel(II)-EDTA coordination polymer.

Keywords: Nickel(II), EDTA, Molecular Electrostatic Potential, Surface Analysis, Coordination Polymer, DFT, Electronic Structure.

Introduction

The physicochemical behavior of coordination compounds is largely governed by their electronic structure and molecular charge distribution. Understanding electron-density localization and electrostatic potential distributions is essential for predicting chemical reactivity, intermolecular interactions, coordination behavior, and stability. Ethylenediaminetetraacetic acid (EDTA) is a versatile hexadentate ligand capable of coordinating transition metals through four carboxylate oxygen atoms and two nitrogen donor atoms. When coordinated with nickel(II), EDTA forms highly stable complexes characterized by extensive charge delocalization and strong metal-ligand interactions.

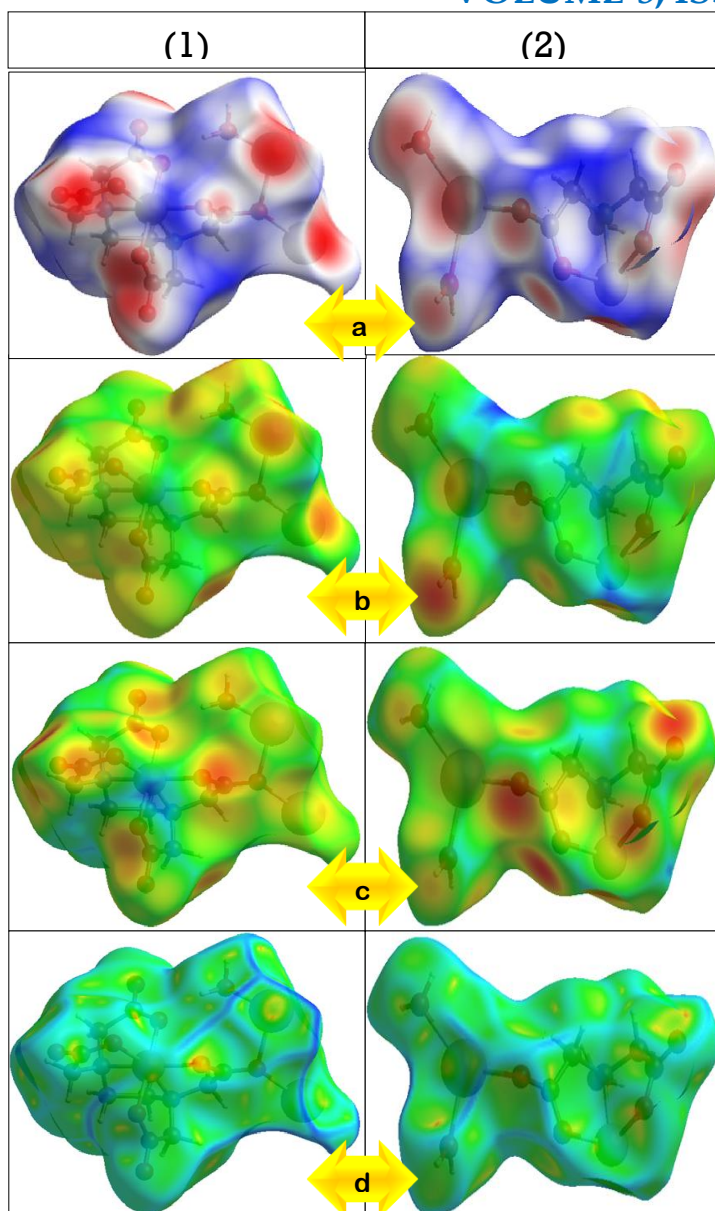


Fig. S1 Hirshfeld surface maps of (1) and (2) (a) d_{norm} (b) d_i (c) d_e and (d) curvedness

(MEP)

(b) Electron Density Surface

(c) Local Charge Distribution Map

(d) Surface Reactivity Descriptor Map

These representations provide complementary information concerning the electronic environment surrounding the nickel center and coordinated EDTA ligand.

Computational surface analysis techniques such as Molecular Electrostatic Potential (MEP), electron density mapping, and molecular surface visualization provide valuable information regarding reactive sites and intermolecular interaction capabilities.

Computational Analysis

The molecular structure of poly[ethylenediaminetetraacetato-aqua-disodium-nickel(II)] was analyzed using molecular surface mapping techniques. The resulting graphical representations illustrate the distribution of electrostatic potential, electron density, local surface polarity, and molecular reactivity descriptors across the coordination framework.

The surface maps displayed in Figure 1 (a-d) represent different electronic descriptors commonly used in computational coordination chemistry:

(a) Molecular Electrostatic Potential

Results and Discussion

Molecular Electrostatic Potential (MEP) Analysis

The molecular electrostatic potential (MEP) surface of poly[ethylenediaminetetraacetato-aqua-disodium-nickel(II)] is presented in Figure 4a. The MEP map provides valuable information regarding the charge distribution and possible reactive sites within the coordination framework. The red-colored regions correspond to areas of negative electrostatic potential, indicating zones of high electron density. These regions are predominantly localized around the oxygen atoms of the carboxylate groups and coordinated water molecules.

The accumulation of negative charge on these oxygen centers demonstrates their strong electron-donating character and confirms their important role in coordination to the nickel(II) ion. In contrast, the blue-colored regions represent areas of positive electrostatic potential and are mainly distributed around hydrogen atoms and portions of the coordination environment surrounding the metal center. These regions are electron deficient and therefore more susceptible to nucleophilic interactions.

The pronounced separation between positive and negative electrostatic potential regions suggests effective ligand-to-metal charge transfer and strong coordination interactions between EDTA donor atoms and the Ni(II) center. The MEP analysis further indicates that oxygen atoms constitute the most favorable sites for electrophilic attack, whereas positively polarized regions may participate in hydrogen-bonding interactions and intermolecular recognition processes.

The observed electrostatic potential distribution confirms the highly polarized nature of the coordination polymer and contributes to its remarkable thermodynamic stability.

Electron Density Surface Analysis

The electron density surface represented in Figure 4b illustrates the spatial distribution of electron clouds throughout the molecular framework. The surface demonstrates that electron density is concentrated primarily around the donor atoms involved in metal coordination. Oxygen atoms exhibit the highest electron density because of their electronegativity and participation in carboxylate coordination. Significant electron density is also observed around nitrogen donor atoms of the EDTA ligand. The electron density around the nickel center is relatively uniform due to extensive orbital overlap between the metal ion and coordinating atoms. Such distribution suggests efficient electron delocalization throughout the coordination sphere. The absence of highly localized electron accumulation indicates strong electronic communication between the ligand and metal center. This behavior is

characteristic of stable coordination compounds in which charge is distributed over the entire molecular framework rather than concentrated at isolated atomic centers.

The observed electron density pattern therefore supports the formation of a robust coordination network stabilized through extensive metal–ligand interactions.

Local Ionization Potential Analysis

The local ionization potential surface shown in Figure 4c provides insight into the regions of the molecule most susceptible to electron removal and oxidative processes. The surface reveals significant variations in local ionization energy across the molecular framework. Regions exhibiting lower ionization potential are mainly associated with oxygen-rich domains and donor atom environments. These sites can more readily participate in electron-transfer processes because electrons are less tightly bound. The areas surrounding the coordinated oxygen atoms display enhanced reactivity, suggesting that these sites are the most likely locations for interaction with external electrophilic species. Conversely, regions exhibiting higher ionization potential indicate greater electronic stability and lower susceptibility to oxidation. The distribution of local ionization potential confirms that the electronic properties of the complex are strongly governed by the coordinated EDTA ligand and its donor atoms. The relatively uniform transition between high- and low-energy regions further demonstrates efficient charge redistribution within the molecular structure.

Local Electron Affinity Analysis

Figure 4d presents the local electron affinity surface of poly[ethylenediaminetetraacetato-aqua-disodium-nickel(II)]. Electron affinity mapping provides information regarding the ability of different molecular regions to accept additional electron density. The surface shows moderate electron-accepting capability distributed throughout the coordination framework, with localized enhancement near certain oxygen-containing functional groups. The relatively homogeneous surface distribution indicates that the molecule possesses balanced electronic characteristics and does not contain highly unstable electron-deficient regions. Such behavior is consistent with the strong chelating ability of EDTA and the stabilizing influence of nickel coordination. The electron affinity analysis suggests that the complex can effectively participate in intermolecular interactions involving charge transfer while maintaining overall electronic stability. These characteristics contribute to the chemical robustness and coordination stability of the nickel(II)-EDTA framework.

Reactivity and Stability Assessment

The combined surface analyses provide a comprehensive understanding of the electronic structure and reactivity of the synthesized coordination polymer. The MEP map demonstrates the existence of distinct electron-rich and electron-poor regions, indicating favorable conditions for intermolecular interactions. Electron density analysis confirms efficient charge delocalization throughout the molecular framework, while ionization potential and electron affinity surfaces reveal balanced electronic behavior and moderate chemical reactivity. The most reactive regions of the complex are associated with:

Conclusion

Computational molecular surface analysis revealed significant information regarding the electronic structure and reactivity of poly[ethylenediaminetetraacetato-aqua-disodium-nickel(II)]. The molecular electrostatic potential map demonstrated pronounced charge separation, with oxygen donor atoms representing the most electron-rich regions of the complex. Electron density and charge distribution analyses confirmed strong ligand-to-metal electronic interactions and extensive charge delocalization throughout the coordination framework. Surface reactivity mapping indicated that oxygen-containing functional groups and coordinated water molecules constitute the primary reactive sites within the structure. The balanced electrostatic environment and efficient charge delocalization contribute significantly to the stability of the nickel(II)-EDTA coordination polymer. These findings provide valuable insight into the electronic behavior, intermolecular interaction potential, and chemical stability of the synthesized complex.

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