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NOVEL Ni(II) COORDINATION COMPOUNDS CONTAINING PHENANTHROLINE DERIVATIVES AND 3-CARBOXY-1-CARBOXYMETHYL-2-OXIDOPYRIDINIUM: SYNTHESIS, STRUCTURE, AND HIRSHFELD ANALYSIS

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ABSTRACT. A novel Ni(II) coordination compound **1**, [Ni(L)(CCP)]·2H_2O, was synthesized under hydrothermal conditions using a combination of ligands with complementary coordination characteristics, where L = 2-(4-fluorophenyl)-1H-imidazo[4,5-f][1,10]phenanthroline and H_2CCP = 3-carboxy-1-carboxymethyl-2-oxidopyridinium. The Ni(II) center adopts a distorted octahedral geometry with six coordination sites, consisting of two nitrogen atoms from the L ligand and four carboxylate oxygen atoms from two deprotonated CCP^{2-} anions. The compounds are connected through π–π stacking interactions, forming a one-dimensional supramolecular chain. Through the C–H···π interactions between the CCP^{2-} anions and L ligands, the one-dimensional chains further assemble into a two-dimensional supramolecular layer. The compound (**1**) was characterized by photoluminescence (PL) spectroscopy and thermogravimetric (TGA) analysis. FT-IR analysis further supports the deprotonation of the carboxylic acid groups and their coordination with the Ni(II) center. Hirshfeld surface analysis quantitatively revealed the contributions of O···H/H···O, F···H/H···F, F···C/C···F, and π···π contacts, indicating their combined contribution to the ordered molecular packing and crystal stability.

KEY WORDS: Coordination compound, Ni(II), Crystal structure, Hirshfeld surface analysis

INTRODUCTION

Coordination compounds are infinite chain or network architectures formed by linking inorganic nodes with organic building units through coordination bonds [1-3]. Compared with conventional inorganic compounds, coordination compounds possess unique structural tunability and property adjustability. By varying the type, valence state, and coordination number of the central metal [4-5], or by modifying the functional groups, framework structure, and coordination modes of the ligands, their optical, electrical, magnetic, catalytic, adsorption–separation, and biological properties can be precisely regulated, enabling the rational design from microscopic molecular structures to macroscopic functional applications [6-7].

At the same time, many coordination compounds lack effective intermolecular interactions, making their frameworks prone to collapse, which limits their practical applications in adsorption, sensing, and catalysis. To address these limitations, the introduction of carboxyl groups into the system is of great significance. As an aromatic polycarboxylate ligand [8-9], 3-carboxy-1-carboxymethyl-2-oxidopyridinium is an excellent candidate for constructing coordination polymers. Aromatic frameworks provide rigid nodes, while O-donor carboxyl groups exhibit strong binding affinity toward metal centers [10-12]. In addition, the presence of multiple coordination sites and diverse coordination modes offers greater structural versatility [13-14].

It is well known that 1,10-phenanthroline (Phen) has been widely used in the construction of supramolecular systems due to its strong coordination ability and its extended conjugated system, which readily facilitates π–π interactions [15-16]. However, comparatively little attention has been paid to its derivative, 2-(4-fluorophenyl)-1H-imidazo[4,5-f][1,10]phenanthroline (L). In

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addition, in a similar L, the two nitrogen atoms in the imidazole ring exhibit distinct coordination behaviors [17]. The pyrrolic NH can be deprotonated to form a strong coordination site and can also participate in hydrogen-bond interactions, whereas the imine-type nitrogen can directly coordinate to or bridge metal centers [18]. The ligand coordinates with the metal center through two N atoms. Moreover, its relatively large aromatic π surface facilitates π···π stacking interactions [19]. Together with the phenanthroline nitrogen donors, these sites act synergistically to enhance the coordination ability and structural stability of the ligand, while also providing an important structural basis for constructing diverse coordination polymers and tuning the electronic structure and photophysical properties of the complexes [20-21]. Li *et al.* [22] reported [Ni(H_2O)(L)(OBA)](L=2-(4-Fluorophenyl)-1Himidazo[4,5-f][1,10]phenanthroline and OBA= 4,4'-Oxybis(benzoate)), in which OBA^{2-} bridges Ni(II) centers to form two crystallographically distinct one-dimensional chains, which are further extended into a two-dimensional supramolecular structure through π–π interactions. In this work, the [NiL] unit was combined with CCP^{2-}, which differs from OBA^{2-}, resulting in changes in the Ni–O coordination and the subsequent structural construction. The combination of H_2CCP and L shows complementary coordination properties. The former provides multiple O-donor sites and various bridging modes, while the latter is a rigid π-conjugated N-donor ligand with a large aromatic surface [23]. This combination of rigid and flexible coordination features, together with N/O donor sites, may facilitate the formation of extended coordination structures and subsequent supramolecular assembly through π···π stacking and hydrogen-bonding interactions. As the metal center, Ni(II) shows good coordination compatibility with N- and O-donor atoms and can adopt an octahedral coordination environment, supporting the construction of extended coordination structures. The L ligand provides well-defined N, N-donor sites and an extended aromatic surface, while CCP^{2-} offers multiple O-donor sites and various bridging modes. Therefore, the combination of Ni(II) with these ligands results in a stable [NiN_2O_4] coordination environment.

As the metal center, Ni(II) shows good coordination compatibility with N- and O-donor atoms and can adopt an octahedral coordination environment, supporting the construction of extended coordination structures.Based on this, we successfully synthesized a novel Ni(II)-based coordination compound, namely [Ni(L)(CCP)]$_2$·$2H_2O$ (1) (L = 2-(4-fluorophenyl)-1H-imidazo[4,5-f][1,10]phenanthroline, H_2CCP = 3-carboxy-1-carboxymethyl-2-oxidopyridinium). The structure and properties of the compound were characterized by photoluminescence (PL) spectroscopy, infrared (IR) spectroscopy, and thermogravimetric analysis (TGA). Hirshfeld surface analysis was also used to visualize and quantify the intermolecular contacts in the crystal structure. The synergistic effects of hydrogen bonds, weak hydrogen-bond interactions, dispersion forces, and π–π interactions were systematically analyzed and visualized, which may collectively promote ordered molecular packing and contribute to the compactness and thermodynamic stability of the crystal.

EXPERIMENTAL

Materials and measurements

All chemicals used for synthesis and characterization were of reagent grade and obtained from commercial sources without further purification. Thermogravimetric analyses (TGA) was completed on a Perkin-Elmer TG-7 analyzer under N_2 from 25 to 1000 °C. The IR spectrum was acquired on a Perkin-Elmer Spectrum One FTIR spectrometer using the KBr pellet technique over the 4000-400 cm^{-1} region. Fluorescence spectra of solid and liquid samples were measured and analyzed at room temperature with an RF-6000 fluorescence spectrophotometer. Hirshfeld surface analysis and related 2D fingerprints were performed with Crystal Explorer software version 21.5.

X-ray single crystal structure determination

A suitable crystal of compound (**1**) was selected, and diffraction data were collected on a Bruker-AXS Smart CCD diffractometer equipped with graphite monochromated Mo-Kα radiation (λ = 0.71073 Å) at 293(2) K using ω–φ scans. The crystal structure was solved by direct methods using SIR2014 and refined on F^2 by full-matrix least-squares using SHELXL2018/3 [24-25]. All hydrogen atoms were placed geometrically and refined isotropically using a riding model. The results of the single-crystal X-ray diffraction analysis are summarized in Table 1, and selected bond lengths and angles are listed in Table 2.

Table 1. Crystalline data and refinement parameters for **1**.

Formula	$C_{54}H_{36}F_2N_{10}Ni_2O_{12}$
Mr (g.mol^{-1})	1172.35
Crystal system	Triclinic
Space group	$P\bar{1}$
a, b, c [Å]	9.4381(19), 9.6743(19), 14.806(3)
α, β, γ (°)	88.19(3), 77.66(3), 65.60(3)
V (Å^3)	1200.3(5)
Z	1
ρ (g.cm^{-3})	1.622
μ (mm^{-1})	0.872
F(000)	600
Crystal size (mm)	0.203 × 0.185 × 0.171
Temperature (K)	296(2) K
Mo Kα radiation, λ (Å)	0.71073
θ (min-max) (°)	3.067, 27.483
Data set	-12<=h<=12, -12<=k<=11, -19<=l<=19
Tot., Unique data, R_{int}	11907, 5456, 0.0366
Observed [I>2σ(I)] reflections	3531
Nreflections, Nparameters	5456, 361
R[F^2>2σ(F^2)], wR(F^2), S	0.0407, 0.0983, 1.042
$\Delta\rho_{min}$, $\Delta\rho_{max}$ (e.Å^{-3})	-0.298, 0.617

Table 2. Selected bond distances (Å) and bond angles (º) for **1**.

Bond lengths (Å)			
N(1)-Ni(1)	2.0561(18)	N(2)-Ni(1)	2.0465(19)
O(1)-Ni(1)	2.1742(17)	O(2)-Ni(1)	2.133(2)
O(3)-Ni(1)^{i}	2.0204(16)	O(4)-Ni(1)^{i}	1.9686(18)
Bond angles (°)			
O(4)^{i}-Ni(1)-O(3)^{i}	89.38(7)	O(4)^{i}-Ni(1)-N(2)	100.38(8)
O(3)^{i}-Ni(1)-N(2)	96.64(7)	O(4)^{i}-Ni(1)-N(1)	86.25(7)
O(3)^{i}-Ni(1)-N(1)	174.24(7)	N(2)-Ni(1)-N(1)	80.49(7)
O(4)^{i}-Ni(1)-O(2)	160.11(7)	O(3)^{i}-Ni(1)-O(2)	89.48(7)
N(2)-Ni(1)-O(2)	99.48(8)	N(1)-Ni(1)-O(2)	95.90(7)
O(4$^{)i}$-Ni(1)-O(1)	98.69(8)	O(3)^{i}-Ni(1)-O(1)	91.15(7)
N(2)-Ni(1)-O(1)	159.45(7)	N(1)-Ni(1)-O(1)	93.22(7)
O(2)-Ni(1)-O(1)	61.48(7)		

Symmetry code: ^{i} -x+1, -y, -z

Table 3. H-B bonding geometry parameters (Å, °) for **1**.

D-H···A	d(D-H)	d(H···A)	d(D···A)	□DHA
N(3)-H(3A)···O(5)^{iii}	0.86	1.90	2.752(3)	169.0
O(1W)-H(1A)···O(1)	0.85	2.07	2.899(3)	165.9
O(1W)-H(1B)···O(2)^{i}	0.85	2.14	2.990(3)	172.4

Symmetry code: ^{i} -x+1, -y, -z; ^{ii} -x+2, -y, -z+1; ^{iii} x, y, z+1

*Synthesis of **1***

2-(4-Fluorophenyl)-1H-imidazo[4,5-f][1,10]phenanthroline (L) (0.10 mmol, 0.033 g), nickel acetate $Ni(CH_3COO)_2$ (0.15 mmol, 0.038 g), and 3-carboxy-1-carboxymethyl-2-oxopyridinium (H_2CCP) (0.10 mmol, 0.021 g) were accurately weighed and placed in a beaker. An appropriate amount of distilled water was added, and the mixture was magnetically stirred at room temperature for about 5 min until homogeneous. Subsequently, accurately weighed NaOH (0.35 mmol, 0.014 g) and NaCl (0.10 mmol, 0.006 g) were added in sequence. The mixture was further stirred for 20 min until the solids were completely dissolved. The resulting solution was transferred into a 15 mL Teflon-lined stainless steel autoclave, and distilled water was added to reach approximately two-thirds of the reactor volume (about 10 mL). The autoclave was sealed and placed in an oven, where it was maintained at 150 ℃ for 7 days (168 h). After completion of the reaction, the system was cooled to room temperature by programmed cooling. The green block-shaped crystals were collected. Yield: 37% (average) based on Ni.

RESULTS AND DISCUSSION

TG analysis

Compound 1 was placed under a nitrogen atmosphere and heated to 1000 ℃ at a rate of 10 ℃·min^{-1} to evaluate its thermal stability. As shown in Figure 1, the first weight loss of 3.0% between 28-122 ℃ corresponds to the removal of free water molecules (calculated value: 3.1%). The second weight loss occurs in the range of 398-782 ℃. It is mainly attributed to the decomposition of the $C_8H_5O_4N$ group in the organic acid anion and L ligands. The observed weight loss is 84.5%, which is in good agreement with the calculated value of 84.6%. Due to the overlapping decomposition processes of the organic components at this stage, the individual weight-loss steps cannot be clearly distinguished. The weight of the resulting residue corresponds to NiO, with an observed residue of 12.3%, close to the calculated value of 12.5%. A slight increase in mass was observed in the temperature ranges of 150-370 ℃ and 800-950 ℃. This phenomenon may be mainly attributed to buoyancy and baseline effects associated with changes in the density of the surrounding N_2. In the low-temperature region (150-370 ℃), the adsorption of N_2 within nearby intermolecular voids or porous regions may also contribute to the apparent increase in mass [26]. At higher temperatures (800-950 ℃), after the organic framework has largely decomposed, the residual inorganic species may undergo slight reactions with trace oxygen impurities in the nitrogen atmosphere, potentially contributing to the observed increase in mass [27]. Overall, the thermogravimetric analysis results are in good agreement with the crystal structure analysis.

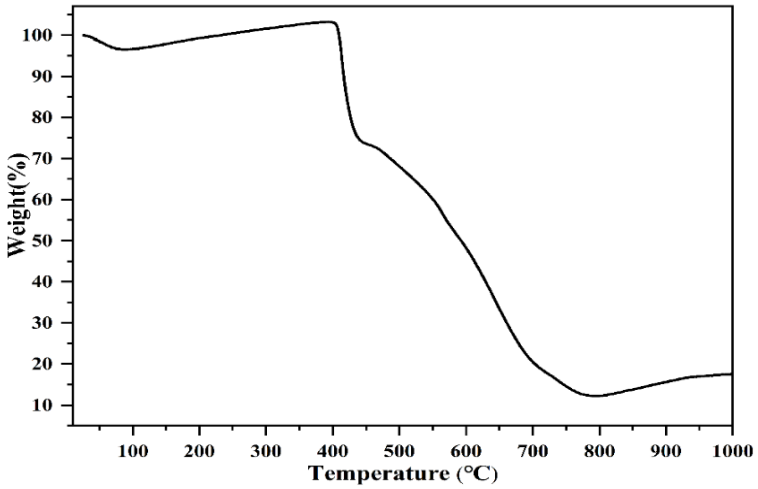


Figure 1. The TGA of compound **1**.

IR analysis

The FT-IR spectrum of compound (**1**), L, and H_2CCP were depicted in Figure 2. The broad absorption peak at 3448 cm^{-1} is assigned to the O–H stretching vibration of hydroxyl groups, which may originate from residual water molecules in the system or hydrogen-bond interactions involving the carboxyl groups of the ligands. H_2CCP exhibits a broad absorption band in the range of 3000–2500 cm^{-1}, which can be attributed to the O–H stretching vibration of the carboxylic acid (-COOH) group. The band nearly disappears in the spectrum of the compound, suggesting that the carboxylic acid group is deprotonated and that H_2CCP participates in coordination. H_2CCP shows a relatively broad absorption band in the range of 1800–1700 cm^{-1}, which is characteristic of the C=O stretching vibration of the free carboxylic acid (-COOH) group [28]. The band nearly disappears in the spectra of L and the compound, while new bands appear at 1478 and 1314 cm^{-1}, which can be assigned to the asymmetric (ν_{as}) and symmetric (ν_s) stretching vibrations of the carboxylate($-COO^-$) group, respectively. The frequency difference between these two bands ($\Delta\nu = \nu_{as} - \nu_s$) is 134 cm^{-1}. This value ($\Delta\nu < 200$ cm^{-1}) suggests that CCP^{2-} coordinates with the metal center as a carboxylate ligand in a bidentate chelating mode. The peak at 1111 cm^{-1} may correspond to the C–O stretching vibration of the pyridine ring or the carboxyl group. The weak band near 3069 cm^{-1} corresponds to the stretching vibration of aromatic C–H bonds. The multiple peaks in the range of 724–839 cm^{-1} are attributed to out-of-plane bending vibrations of aromatic C–H bonds, reflecting the substitution pattern of the aromatic ring.

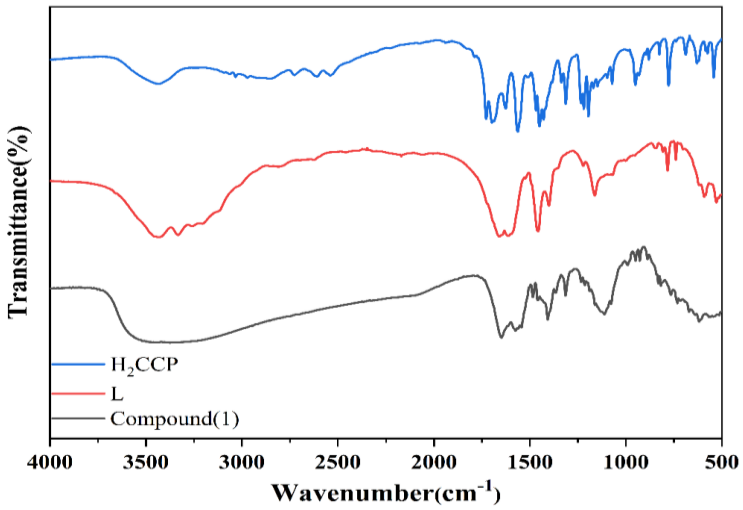


Figure 2. The FT-IR spectrum of compound **1**.

PL analysis

The photoluminescence spectra of 1, H_2CCP, and L were measured at room temperature. As shown in Figure 3, H_2CCP exhibits the strongest emission peak at 383 nm, which can be attributed to π→π* or n→π* electronic transitions of its aromatic ligand [29]. The ligand L exhibits a broad emission band centered at 555 nm, which is mainly associated with the π→π transitions within the ligand and its extended π-conjugated system. Compound 1 exhibits a strong emission at 509 nm, showing a blue shift relative to the free ligand L (555 nm). As a coordination compound, 1 exhibits an emission peak similar in profile to that of the L ligand, suggesting that its emission properties may arise from interactions between the ligand and the metal center (such as ligand-to-metal charge transfer or intraligand electronic transitions) [30-31]. The emission of L originates from its intrinsic electronic transition processes. The differences in emission peak positions and intensities among these species reflect the influence of molecular structure and coordination environment on their fluorescence properties.

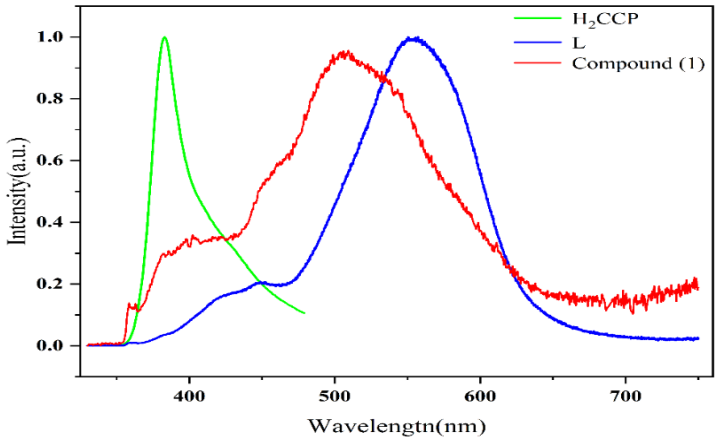


Figure 3. The PL of compound **1**.

Crystal structure

Based on single-crystal X-ray diffraction analysis, the Ni(II) compound crystallizes in the triclinic crystal system with the $P\bar{1}$ space group. The asymmetric unit consists of a Ni(II) ion, one bidentate chelating neutral L ligand, one deprotonated CCP^{2-} anion, and two free water molecules. As shown in Figure 4(a), the central Ni(II) ion adopts a six-coordinate distorted [NiN_2O_4] octahedral geometry. The equatorial plane is formed by two nitrogen atoms, N(1) and N(2), from the L ligand (N(1)–Ni(1) = 2.0561(18), N(2)–Ni(1) = 2.0465(19) Å), and two carboxylate oxygen atoms, O(1) and O(2), from the CCP^{2-} anion (O(1)–Ni(1) = 2.1742(17), O(2)–Ni(1) = 2.133(2) Å). The axial positions are occupied by two bridging oxygen atoms, $O(3)^i$ and $O(4)^i$ ($O(3)–Ni(1)^i$ = 2.0204(16), $O(4)–Ni(1)^i$ = 1.9686(18) Å), which originate from the CCP^{2-} anion of adjacent units. The Ni–O and Ni–N distances in 1 are consistent with those observed in other analogous compounds $\{[Ni(1,4\text{-NDC})(L)(H_2O)_2]\cdot 2H_2O\}_n$ (1,4-H_2NDC = 1,4-naphthalenedicarboxylic acid, L = 1-(1H-imidazo[4,5-f][1,10]phenanthrolin-2-yl)naphthalen-2-ol) [32]. The two carboxylates and the phenolic hydroxyl of the CCP^{2-} anion bridge two Ni(II) atoms in a μ_2-η^1:η^1:η^1:η^1:η^0 mode (Figure 4(b)). In such a manner, two Ni(II) atoms are connected by two CCP^{2-} anions to give a dimeric $[Ni(CCP)]_2$ discrete dinuclear coordination unit with the Ni···Ni distance of 6.343 Å (Figure 5). The two L ligands are situated at two sides of the dimer by chelating the Ni(II) atom, providing π-π stacking interactions, thereby forming a $[Ni(L)(CCP)]_2$ discrete dinuclear coordination unit [N(1)/C(1)–C(5), N(1)/C(1)–C(5) at (1–x, –y, 1–z), centroid-to-centroid distance 3.6808(15) Å and dihedral angle of 0.00(12)°, and slippage of 1.309 Å]. As shown in Figure 5, adjacent dimers are generated into a one-dimensional supramolecular chain by these π-π stacking interactions. Additionally, there exist the N–H···O hydrogen bond (N(3)–H(3A) = 0.86 Å, $H(3A)\cdots O(5)^{iii}$ = 1.90 Å, $N(3)\cdots O(5)^{iii}$ = 2.752(3) Å, ∠$N(3)–H(3A)\cdots O(5)^{iii}$ = 169.0°, symmetric codes: ^{iii} x, y, z+1) in 1, which further make the supramolecular layer structure of 1 stable (Table 3). Noticeably, there exist C–H···π interactions between the C(25) atom of CCP^{2-} anion and the phenanthroline ring [N(1)/C(1)–C(4)/C(7)–C(12)/N(2)/C(6)/C(5) at (2–x, –y, –z)] of the L ligand (2.80 Å, and an angle of 2.75°). When these C–H···π interactions are accounted for, the one-dimensional chains are extended into a two-dimensional supramolecular layer (Figure 6).

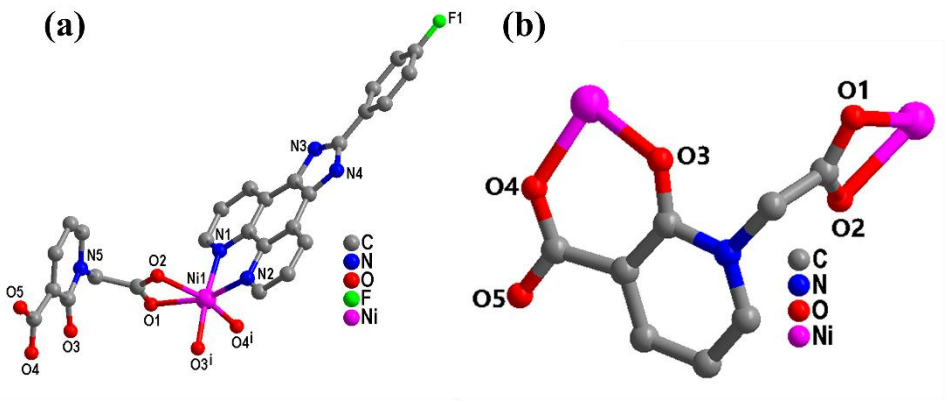


Figure 4. (a) The coordination environment of Ni(II) atoms (symmetric code: ^{i} -x+1,-y,-z), (b) The coordination mode of the CCP2- anion.

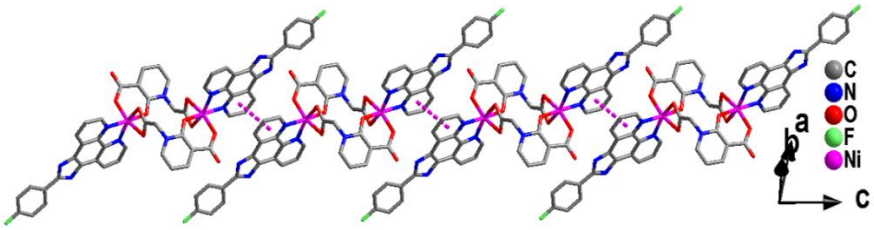


Figure 5. The 1D chain structure of compound 1 by π-π interactions.

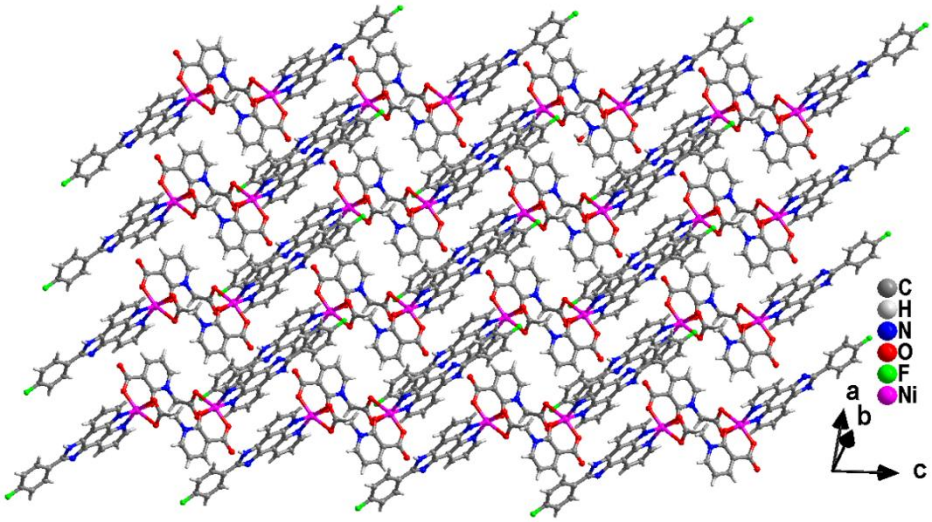


Figure 6. View of the 2D supramolecular architecture of **1** by C–H···π interactions.

Hirshfeld surface analysis

To further investigate the intermolecular interactions in the crystal structure of compound 1, Hirshfeld surface analysis was performed using CrystalExplorer 21.5 software [33-34].

In Figure 7, the bright red spots on the dnorm map clearly indicate N–H···O hydrogen-bonding interactions between the N(3)–H(3A) group of the imidazole ring in the L ligand and the carboxyl oxygen atom O(5) of the (H_2CCP) anion (N(3)–H(3A)···O(5)^{iii}). In addition, the O–H···O hydrogen bonds formed by the hydrogen atoms of the lattice water molecule O(1W) with the coordinated oxygen atom O(1) and the carboxyl oxygen atom O(2) (O(1W)–H(1A)···O(1), O(1W)–H(1B)···O(2)^{i}) appear as pale red regions on the surface map. The red and blue triangular patterns observed in the shape index map indicate π–π stacking interactions between the imidazo-phenanthroline ring of the L ligand and the fluorophenyl group of adjacent molecules [35]. The curvedness map shows extensive green flat regions, corresponding to the planar nature of the large conjugated imidazo-phenanthroline system in the L ligand, while the blue boundaries outline the contour of the pyridine ring in the CCP^{2-} anion.

The 2D fingerprint plots (Figure 8) quantitatively reveal the relative contributions of different types of intermolecular interactions. H···H contacts account for the highest proportion, reaching 30.0%, mainly arising from hydrophobic interactions between the fluorophenyl group of the L ligand and aliphatic chains, which effectively fill the lattice voids and enhance packing

compactness, thereby forming the basis of the dense crystal packing. C···H/H···C interactions contribute 21.9%, including multiple weak C–H···O hydrogen bonds involving C–H groups on the imidazo-phenanthroline ring and neighboring molecules, which regulate molecular orientations and the stacking arrangement of aromatic rings, thereby optimizing the crystal packing configuration. O···H/H···O contacts account for 19.3%, encompassing the aforementioned N–H···O and O–H···O hydrogen bonds as well as C–H···O interactions. These hydrogen-bond interactions show clear directionality and may contribute to the formation of a stable intermolecular hydrogen-bond network, which helps stabilize the crystal structure and promotes its ordered assembly. Notably, C···C interactions contribute 8.3%, which can be attributed to π–π stacking between the imidazo-phenanthroline ring and the fluorophenyl group in the L ligand. F···H/H···F contacts account for 6.1%, reflecting weak interactions between fluorine atoms and neighboring C–H groups. N···H/H···N interactions account for 5.8%, mainly arising from interactions between nitrogen-containing heterocycles. F···C/C···F contacts account for only 2.8%, indicating that the interaction between fluorine atoms and aromatic carbon atoms is relatively weak. For the fluorine-containing structure, the weak F···H/H···F hydrogen-bond interactions and F···C/C···F dipole–dispersion interactions may further influence the molecular arrangement and interlayer packing, thereby contributing to the stability of the crystal structure. The synergistic effect of these weak interactions collectively stabilizes the ordered packing of the molecular structure, contributing to the compactness and thermal stability of the crystal.

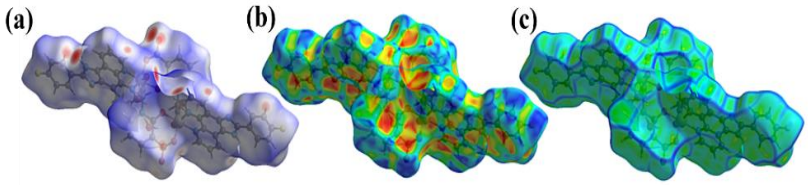


Figure 7. Hirshfeld surfaces of 1 mapped over (a) d_{norm}, (b) shape index, (c) curvedness.

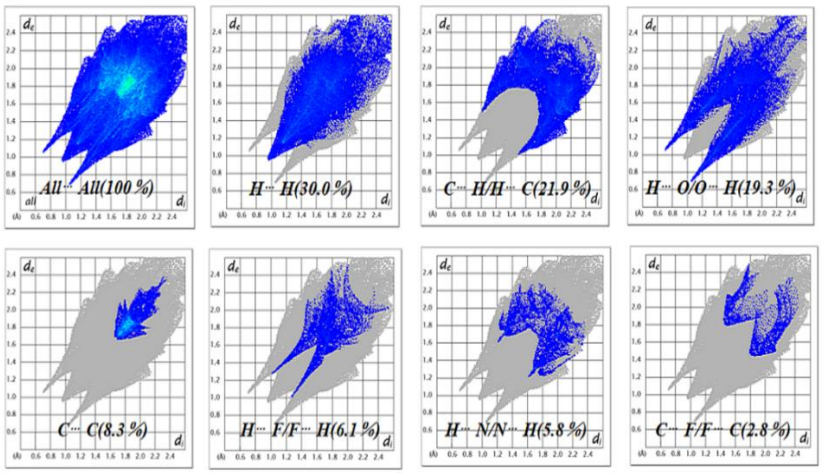


Figure 8. 2D fingerprint plots for 1.

CONCLUSION

A new Ni(II) coordination compound, [Ni (L)(CCP)]·$2H_2O$ (**1**), has been hydrothermally synthesized and fully characterized. The CCP^{2-} anion bridges two Ni(II) atoms in a μ_2-η^1:η^1:η^1:η^1:η^0 mode, forming a dinuclear $[Ni(L)(CCP)]_2$ unit. The L ligands on both sides of the dimer coordinate with Ni(II) ions, and the resulting π–π stacking extends to link adjacent dimers into a one-dimensional supramolecular chain, further stabilized by hydrogen bonds. C–H···π interactions between CCP^{2-} and L ligands assemble these chains into a two-dimensional supramolecular layer. The structure of compound (1) in the solid state was characterized by IR, PL, TGA, and Hirshfeld surface analysis.

ACKNOWLEDGEMENTS

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Supplementary data

Crystallographic data have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication number CCDC 2542499. Copies of this information may be obtained free of charge from The Director, CCDC, 12 Union Road, Cambridge, CB2 1EZ, UK (fax: +44-1223-336033; email: deposit@ccdc.cam.ac.uk or www: http://www.ccdc.cam.ac.uk).

Ethical standard

All ethical guidelines have been followed.

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