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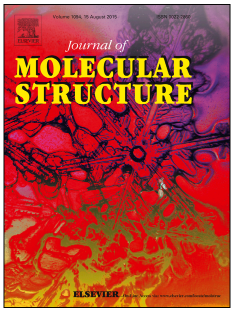

Synthesis, characterization, and crystal structure analysis of Zn(II) and Cd(II) coordination compounds containing 4-((pyridin-4-ylmethylene)amino)phenol Schiff-base ligands

Taraneh Hajiashrafi, Shiva Salehi, Maciej Kubicki, Keith J. Flanagan, Mathias O. Senge

PII: S0022-2860(20)31171-6

DOI: https://doi.org/10.1016/j.molstruc.2020.128846

Reference: MOLSTR 128846

To appear in: *Journal of Molecular Structure*

Received Date: 28 May 2020

Revised Date: 23 June 2020

Accepted Date: 6 July 2020

Please cite this article as: T. Hajiashrafi, S. Salehi, M. Kubicki, K.J. Flanagan, M.O. Senge, Synthesis, characterization, and crystal structure analysis of Zn(II) and Cd(II) coordination compounds containing 4-((pyridin-4-ylmethylene)amino)phenol Schiff-base ligands, *Journal of Molecular Structure* (2020), doi: https://doi.org/10.1016/j.molstruc.2020.128846.

CRediT authorship contribution statement

Taraneh Hajiashrafi: Writing - original draft, review & editing, Software

Shiva Salehi: acquisition of data, analysis and/or interpretation of data

Maciej Kubicki: acquisition of data

Keith J. Flanagan: acquisition of data

Mathias O. Senge: revising the manuscript

Author declaration

1. Conflict of Interest

☒No conflict of interest exists.

We wish to confirm that there are no known conflicts of interest associated with this publication and there has been no significant financial support for this work that could have influenced its outcome.

2. Funding

☒Funding was received for this work.

All of the sources of funding for the work described in this publication are acknowledged below:

We gratefully acknowledge the financial support from the Research Council of Alzahra University- Science Foundation Ireland

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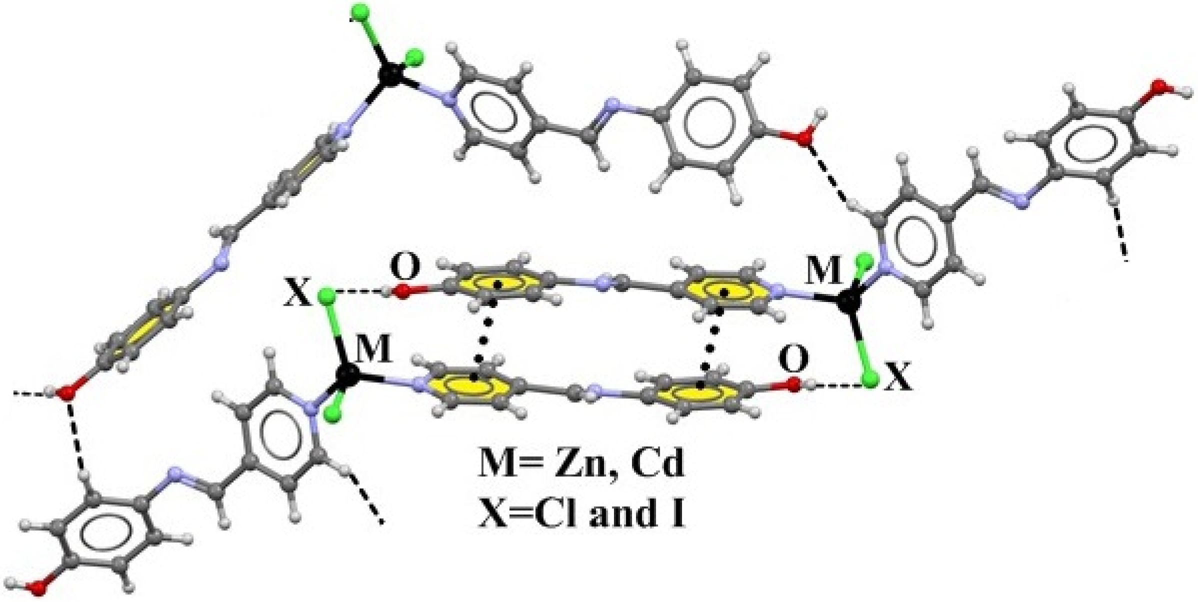
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Synthesis, characterization, and crystal structure analysis of Zn(II) and Cd(II) coordination compounds containing 4-((pyridin-4-ylmethylene)amino)phenol Schiff-base ligands

Taraneh Hajiashrafi,[a] Shiva Salehi,[a] Maciej Kubicki,[b] Keith J. Flanagan,[c] Mathias O. Senge,[c]*

[a] *Department of Chemistry, Faculty of Physics and Chemistry, Alzahra University, PO Box 1993891176, Tehran, Iran*

[b] *Department of Chemistry, Adam Mickiewicz University, ul. Grunwaldzka 6, 60-780 Poznan, Poland*

[c] *School of Chemistry, Trinity Biomedical Science Institute, Trinity College Dublin, The University of Dublin, 152-160 Pearse Street, Dublin 2, Ireland*

Abstract

Zn(II) and Cd(II) coordination compounds containing 4-((pyridin-4-ylmethylene)amino)phenol ligands were synthesized and then characterized using spectroscopic techniques and single crystal X-ray crystallography. The molecular structure and crystal packing of these complexes, as well as the crystal packing of coordination complexes based on 4-substituted-1-(pyridin-4-yl)methanimine ligand, retrieved from Cambridge Structural Database (CSD), were investigated using structural, Hirshfeld surface analyses, and theoretical calculations. The crystal structure of these coordination complexes is governed by a combination of $\pi\cdots\pi$ stacking, C-H$\cdots\pi$, O-H$\cdots$N, and C-H$\cdots$X hydrogen bonding interactions. This study provides further insight into the understanding of the role of weak non-covalent interactions in the crystal structure of group IIB containing Schiff-base ligand coordination compounds.

Keywords:

Coordination compounds of group IIB; Schiff-base ligand; π-interactions, metallosupramolecular chemistry

1. Introduction

In the last two decades, the supramolecular chemistry of inorganic compounds has attracted increasing interest because of their fascinating structures and their potential applications in various fields such as catalysis[1], gas storage [2], and molecular recognition [3, 4]. It is now well-established that the manner in which molecular building blocks are arranged within supramolecular structures has a tremendous effect on their physical and chemical properties [5, 6]. In this regard, supramolecular chemists have attempted to understand the rules of supramolecular assembly of metal-containing compounds by studying the solid-state structures of these systems using X-ray crystallography data to provide a detailed picture of the supramolecular structure[7, 8]. Crystallographic studies on d-block metal complexes revealed fascinating information about the impact of the ligand structures and denticities [9, 10], nature of the metal center [11, 12], counter-ions [13, 14] and reaction conditions [15, 16] on the crystal structure of metal complexes [17, 18]. Among these, rational selection of the organic ligands plays a decisive role in designing well-defined architectures not only because of their role in directing the dimensionality and topology of the final structure but also due to providing potential interaction sites to generate pre-designed patterns of intermolecular interactions [19-21]. A variety of supramolecular synthons based on highly directional intermolecular interactions such as hydrogen bonding, halogen bonding, and even weak directional π-stacking interactions have been identified and employed as synthetic vectors for the assembly of metal-containing materials [17, 22-25]. It should be noted that although weak interactions such as π-stacking [26] and non-classical hydrogen bonds [26, 27] are usually regarded as weak intermolecular contacts compared to the classical hydrogen bonds [28], there is experimental evidence showing these interactions can even affect the coordination geometry of metal complexes [29-33]. Therefore, supramolecular chemists have a large toolbox of functionalities capable of non-covalent interactions at their disposal, which allow them to design the metal-containing building blocks into well-defined crystal structure according to the chemical information encoded in their molecular structure [34, 35]. In this respect, Hirshfeld surface analysis [36] and the theoretical calculations can be of great help in understanding the role of intermolecular interactions governing the solid-state structure of coordination compounds. Hirshfeld surface analysis is a three-dimensional graphical tool that helps one understands all the intermolecular interactions present in the crystal lattice.

As a continuation of our research interest toward the understanding of the supramolecular organization of group IIB coordination compounds [37-39], three new crystal structures, namely $[Zn(L^{4\text{-}OH})_2Cl_2]$ (**1**), $[Cd(L^{4\text{-}OH})_2I_2]$ (**2**) and $[Cd(L^{4\text{-}OH})_2I_2]\bullet MeOH$ (**3**), containing the 4-((pyridin-4-ylmethylene)amino)phenol ($L^{4\text{-}OH}$) ligand were synthesized and then characterized using spectroscopic techniques and single crystal X-ray crystallography. The crystal structures of these complexes, as well as the crystal packing of coordination complexes based on 4-substituted-1-(pyridin-4-yl)methanimine ligand, retrieved from Cambridge Structural Database (CSD), were investigated using structural, Hirshfeld surface analyses and theoretical calculations. This study reveals the role of π-interactions and hydrogen bonds in the organization and stabilization of these metal-containing crystal structures.

2. Experimental Section

2.1 Apparatus and reagents

Starting materials for the synthesis of compounds **1** and **2** were purchased from Aldrich Chemical Company and used without further purification. The Fourier transform infrared spectra were recorded at room temperature on a Nicolet Fourier Transform IR (Nicolet 100 spectrometer) in the range 500-4000 cm^{-1} using KBr pellets. Elemental analyses (carbon, hydrogen, and nitrogen) were determined using an ECS 4010 CHN-O made in Costech, Italy. Melting points were measured by an Electrothermal 9100 melting point apparatus and were corrected.

2.2 Synthesis of [Zn(L^{4-OH})$_2$Cl$_2$] (1), [Cd(L^{4-OH})$_2$I$_2$] (2) and [Cd(L^{4-OH})$_2$I$_2$].MeOH (3)

The synthesis of L^{4-OH} ligand was reported previously by some of us [38]. [Zn(L^{4-OH})$_2$Cl$_2$] (**1**), [Cd(L^{4-OH})$_2$I$_2$] (**2**), and [Cd(L^{4-OH})$_2$I$_2$]•MeOH (**3**) were synthesized according to the reported procedure by some of us [38]. Scheme 1 shows the L^{4-OH} ligand and **1-3** complexes syntheses.

To a solution of 0.1 mmol MX_2 (M=Zn or Cd; X=Cl or I) in 5 mL methanol, a solution of L^{4-OH} (0.1 mmol) in 5 mL of methanol was added with stirring. The mixture was heated at 50 ˚C for about 15 minutes, followed by a reduction of the solvent volume, resulting in the immediate formation of bright yellow solid. Stirring was continued for 10 min and then the mixture was filtered with a filter paper. The solid residue was washed with a little cold methanol, dried in *vacuo* and then dissolved in 20 mL of hot methanol. Upon slow evaporation of the filtrate at room temperature, colorless crystals of **1** and **2** suitable for X-ray diffraction were collected within a week. Notably, two different crystals were obtained for compound **2** including the yellow prism crystals (**2**) and colorless block crystals (**3**). The crystal structure analysis revealed that compound **3** was the methanol solvate of compound **2**. Also, it should be noted that other zinc and cadmium halide complexes with L^{4-OH} ligand that would have been of interest here could not be studied because no suitable crystals were obtained.

L^{4-OH} FT-IR (KBr pellet, cm^{-1}): 3272(w), 3065(w), 2998(w), 2947(w), 2880(w),2804(w), 2737(w), 2677(w), 2603(w), 1603(vs), 1575(vs), 1506(m), 1463(s), 1414(m), 1251(vs), 1155(vs), 1002(m), 840(s). Melting Point: 201-203°C [38].

*Compound **1** (yield 75%).* Anal. calcd for $C_{24}H_{20}Cl_2N_4O_2Zn$: C, 54.11; H, 3.78; N, 10.52. Found: C, 54.18 H, 3.86; N, 10.46. IR (KBr pellet, cm^{-1}): 3759(w), 3351(vs), 1619 (vs), 1585(vs), 1503(s), 1429(s), 1373(w), 1334(s), 1267(s), 1206(vs), 1156(w), 1027(m), 837(vs), Figure S2a. Melting Point: 172-173 °C. Photoluminescence properties, $\lambda_{excitation}$(nm): 400 and $\lambda_{emission}$(nm):580

Compounds ***2*** *(yield 60% (2+3)*).* Anal. calcd for $C_{24}H_{20}Cd\ I_2N_4O_2$ (**2**): C, 37.80; H, 2.64; N, 7.35. Found: C, 37.78 H, 2.61; N, 7.35. FT-IR (KBr pellet, cm^{-1}): 3444(w), 3423(br), 3139(br), 1614 (s), 1574(vs), 1540(s), 1509(w), 1458(m), 1423(m), 1376(w), 1284(s), 1238(s), 1160(s), 1010(s), 835(s), 544(w), Figure S2(b) and (c). Melting Point: 177–179 °C. Photoluminescence properties, $\lambda_{excitation}$(nm): 400 and $\lambda_{emission}$(nm):530

Compounds ***3****.* Anal. calcd for $C_{26}H_{28}Cd\ I_2N_4O_4$ (**3**): C, 37.77; H, 3.41; N, 6.78. Found: C, 37.75 H, 3.45; N, 6.75. FT-IR (KBr pellet, cm^{-1}): 3423(br), 3127(br), 1613 (s), 1573 (vs), 1541(s), 1509(w), 1457(m), 1418(m), 1374(w), 1284(s), 1237(s), 1158(s), 1008(s), 834(s), 541(w). Melting Point: 175–177 °C. Photoluminescence properties, $\lambda_{excitation}$(nm): 405 and $\lambda_{emission}$(nm):542

[*] We were more interested in the crystal than the synthesis so they weren't completely separated and that further studies will be conducted to investigate and control this formation as it would be interesting for other complexes too. The lower yields are due to removing the mother liquor which would contain some of the compounds but in a mixture of impurities and solvents that can't crash out due to the concentration of the liquid. "(yield 60% (2+3) Compounds 2 and 3 were formed in 60:40 ratio)"

2.3 Single-Crystal Diffraction Studies

X-ray diffraction data were collected for **1** at 130(1) K on a Rigaku four-circle SuperNova diffractometer with Atlas CCD detector and mirror-monochromated CuK_α radiation (λ = 1.54178 Å); for **2** at 100(1) K on a Rigaku four-circle Xcalibur diffractometer, with Eos CCD detector and graphite-monochromated MoK_α radiation (λ = 0.71069 Å), and for **3** at 100(1) K on a Bruker APEX-II four-circle diffractometer, with graphite-monochromated MoK_α radiation (λ = 0.71069 Å). The data were corrected for Lorentz-polarization as well as for absorption effects [40]. Precise unit-cell parameters were determined by a least-squares fit of 3293 (**1**), 11830 (**2**), and 9793 (**3**) reflections of the highest intensity, chosen from the whole experiment. The structures were solved with SHELXT-2013 and refined with the full-matrix least-squares procedure on $|F^2|$ by SHELXL-2013 [41]. All non-hydrogen atoms were refined with anisotropic thermal parameters, hydrogen atoms were placed in idealized positions and refined as 'riding model' with isotropic displacement parameters set at 1.2 (1.5 for methyl groups) times U_{eq} of appropriate carrier atoms. In **1** the central C-CH=N-C group was found disordered over two alternative positions, site occupation factors of 0.5 were ascribed for both sites, Figure S1. The crystallographic information is listed in Table 1 and further experimental and refinement detail can be found in the SI. CCDC-1993550 (for **1**), 1993551 (for **2**), and 1993553 (for **3**) contains the supplementary crystallographic data for this paper.

Hirshfeld surface analysis and two-dimensional fingerprint plots were generated by using Crystal Explorer 3.1 software [36]. These surfaces visually summarize the spatial arrangement and relevance of intermolecular interactions by their color code.

2.4 Theoretical methods

DFT calculations of the non-covalent interactions were carried out using the ORCA quantum chemistry suite [42]. The BLYP exchange-correlation functional [43] with the recent D3 empirical dispersion correction (BLYP-D3) was used to evaluate the binding energies[44]. The basis set superposition error (BSSE) is not taken into consideration because small BSSE effects are assumed to be absorbed by the D3 empirical potential [45]. The decomposition of the interaction binding energy was also computed at BLYP-D3/TZ2P. To evaluate the interactions in the solid-state, we have used the crystallographic coordinates. This procedure and level of the theory have been successfully used to evaluate similar interactions [46-48]. An all-electron triple-zeta basis-set with two polarization functions, TZ2P, has been used to describe all the atoms. The core electrons were treated by using frozen core approximation. The zeroth-order regular approximation (ZORA) was applied for treating the relativistic effect.

3. Results and Discussion

3.1 Synthesis and crystal structure analysis

Schiff-base ligands are easily prepared ligands that can form stable complexes with metal ions [49, 50]. The substituted-1-(pyridin-4-yl)methanimine ligands are suitable building blocks for crystal engineering studies of coordination compounds, since they are capable of coordinating to the metal ion in a predictable manner while providing potential interaction sites to generate self-assembled structures.

Compounds (**1**) and (**2**) were synthesized by reacting 4-((pyridin-4-ylmethylene)amino)phenol ligand with the corresponding metal halide salts. Two different crystals were obtained for compound **2** from the same growth solution, the **3** entity is referred as **2** solvate, which is further supported by single crystal X-ray diffraction data. The FT-IR characteristic frequencies of compounds **1**-**3** as well as the free L^{4-OH} ligand are summarized in Sections 2.2 and are shown in Figure S2. The FT-IR spectra of complexes **1**, **2** and **3** show ν(C=N) stretching frequencies at 1619, 1614 and 1613 cm^{-1}, respectively. The C-O stretching frequencies are assigned at 1267, 1284 and 1284 cm^{-1} for **1-3**, respectively. The O-H stretching frequencies of compounds **1-3** have appeared at 3351, 3423 and 3423 cm^{-1}, respectively, which are completely different from the free L^{4-OH} ligand O-H frequency. The pyridine in-plane ring deformation frequencies of complexes **1-3** are assigned at 642, 639 and 635 cm^{-1}, respectively. Terminal M-X and M-Py stretching frequencies as well as pyridine out of plane ring deformation frequencies are located in the far IR-spectrum, at lower frequencies than could be observed here. The photoluminescence properties of complexes **1-3** are listed in section 2.2. Interestingly, the complexes **2** and **3** have different luminescence properties as for excitation and emission wavelengths. ORTEP drawings of compounds **1-3** which are drawn at 50% ellipsoid probability level are shown in Figure 1 [51]. Selected bond distances and angles are listed in Table 2. In **1** and **2** the complex molecules are unsymmetrical (however some degree of pseudo-symmetry can be found), so the asymmetric part contains one molecule; in **3** the complex is C_2-symmetrical, central Cd ion lies across crystallographic two-fold axis in the space group *Pba*2, and only one ligand molecule and one solvent – methanol molecule is symmetry-independent. The molecular structure of all three compounds shows discrete mononuclear four-coordinate zinc(II) or cadmium(II) units, coordinated by two pyridyl nitrogen atoms of two different $L^{4\text{-OH}}$ ligands and two terminal halide ions. According to the four-coordinate geometry index (τ_4) defined by Houser and his co-workers, within the continuum between square planar (τ_4=0) and tetrahedral (τ_4=1), the coordination geometry around M(II) can be described as tetrahedral (**1**) and trigonal pyramidal (**2** and **3**), with τ_4 values of 0.98, 0.88, 0.73 for compounds **1**, **2**, and **3**, respectively [52]. The dihedral angle between the planes of phenyl and pyridyl rings of free $L^{4\text{-OH}}$ ligand has been reported as 8.84°[53]. For compounds **1-3**, the defined dihedral angle between the aromatic rings of $L^{4\text{-OH}}$ ligand lies between 5.50-52.81º and thus the ligand can adjust itself to meet the requirement of coordination geometry of the metal atom and the optimal inter-atomic distances in the crystal structure, Table S1. The molecular overlay of compounds **2** and **3** and the structural overlay of $L^{4\text{-OH}}$ ligands, which adopt *trans* conformation, in compounds **1-3** and the free $L^{4\text{-OH}}$ ligand [53] are shown in Figure S3. In this regard, Vittal and his co-workers report the crystal structure of $[ZnBr_2(4\text{-styrylpyridine})_2]$ in which Zn(II) is in perfect tetrahedral geometry and the dihedral angle between the two aromatic rings of 4-styrylpyridine ligand is similar to that for compound **1** [54]. In Hg(II) complexes containing substituted styrylpyridine ligand, the two aromatic rings of the corresponding ligand no longer show the large dihedral angle, but instead the two aromatic rings adopt a nearly coplanar geometry [55-57].

In the crystal structure of **1**, adjacent mononuclear units are linked to each other through a combination of π-interactions, namely $_{\text{pyridyl}}\pi\text{-}\pi_{\text{phenyl}}$ stacking (ring centroid to ring centroid distance =3.753 Å), $_{\text{pyridyl}}\text{C-H}\cdot\cdot\pi_{\text{phenyl}}$, $_{\text{phemyl}}\text{C-H}\cdot\cdot\pi_{\text{pyridyl}}$, as well as $_{\text{pyridyl}}\text{C-H}\cdots\text{O}$ non-classical hydrogen bonds in the crystallographic *b*-direction. The overall supramolecular structure results from linking the $[Zn(L^{4\text{-OH}})_2Cl_2]$ units *via* $_{\text{imine}}\text{C-H}\cdots\text{Cl}$, $\text{O-H}\cdots\text{Cl}$ and $\text{C-H}\cdot\pi_{\text{phenyl}}$ interactions in the *ac*-plane, Figure 2. For compounds **2** and **3**, while **3** is a solvate form of **2**, they exhibiting both striking similarities as well as some significant differences in their supramolecular structure. In the crystal structure of **2**, discrete neutral [Cd(L)$_2$I$_2$] units are linked to each other, along the crystallographic *a*-direction, through $_{\text{pyridyl}}\pi$-π_{pyridyl} (ring centroid to ring centroid distance =3.975 Å), $_{\text{pyridyl}}$C-H$\cdots\pi_{\text{phenyl}}$ and I$\cdots\pi_{\text{pyridyl}}$ interactions, Table 4 and Figure 3(a). The O-H···N, $_{\text{phenyl}}$C-H···O [$R_2^2(8)$ graph set notation] and $_{\text{phenyl}}$C-H···I hydrogen bonds link these units in the *bc*-plane to form the three-dimensional (3D) network, Figure 3(b). Analysis of the crystal structure of **3** reveals that the [Cd(L$^{4\text{-OH}}$)$_2$I$_2$] units are stacked on one another *via* $_{\text{imine}}\pi$-π_{phenyl}, $_{\text{imine}}\pi$-π_{pyridyl} (bond centroid to ring centroid distances of 3.503 and 3.555 Å, respectively), and O(lone pair)$\cdots\pi_{\text{phenyl}}$ interactions along the crystallographic *c*-direction, Figure 4(a). The methanol molecules of crystallization link discrete molecular units, in the *ab*-plane, *via* $_{\text{MeOH}}$O–H···N$_{\text{imine}}$ and $_{\text{MeOH}}$C-H···O$_{\text{OH}}$ hydrogen bonds, which is further assisted by $_{\text{imine}}$C-H···I interaction to generate the 3D crystal packing, Table 3, Figure 4(b).

A search in the Cambridge Structural Database (CSD) on the coordination compounds based on (4-substituted)-1-(pyridin-4-yl)methanimine ligand returned 13 hits [58]. All of these coordination compounds contain Hg(II) as metal centers that have different molecular structures and supramolecular features, which are listed in Table 5. These results reveal that the variation of **L** ligand *para*-substituents can have a profound effect on the coordination geometry of metal atom as well as supramolecular arrangement of these coordination compounds. In this regard, the [Cd(L$^{4\text{-F}}$)I$_2$] is a 1D coordination polymer with the cadmium atom in a distorted octahedral configuration, while both [Cd(L$^{4\text{-OH}}$)I$_2$] polymorphs are discrete coordination complexes in which the cadmium atoms are found in a trigonal pyramidal environment [59, 60]. Also, the [Hg(L$^{4\text{-OH}}$)Br$_2$] and [Hg(L$^{4\text{-Br}}$)$_2$Br$_2$] are discrete complexes with four-coordinate seesaw geometries for Hg(II) ions, while [Hg(L$^{4\text{-Cl}}$)Br$_2$] and [Hg(L$^{4\text{-F}}$)Br$_2$], [Hg(L$^{4\text{-I}}$)Br$_2$] are all 1D coordination polymers with a four-coordinate seesaw and five-coordinate square pyramid geometries [38, 59]. These differences are also observed for the [Hg(L$^{4\text{-OH/F/Cl/Br/I}}$)$_2$I$_2$] series which the data are presented in Table 5.

3.2 Hirshfeld surface analysis and theoretical calculation

Analysis and calculations of the Hirshfeld surface analysis were carried out to analyze the intermolecular contacts present in the crystal packing of coordination compounds **1-3**. The Hirshfeld surface analysis is a powerful graphical tool for obtaining additional intuition into the intermolecular contacts in crystalline systems [36]. A bar chart of percentage contributions of the different types of intermolecular contacts and the (2D) fingerprint plots of the coordination compounds are shown in Figure 5 and Table S2. The Hirshfeld surface analysis and associated fingerprint plots reveal that the crystal packing of compounds **1-3** is supported by H···H, C-H··π, C-H···X, C-H···O, andπ··π stacking interactions, Figures 5 and S5. The H···Hand C-H··π intermolecular contacts are the most abundant contacts and play important roles in governing the crystal packing and C-H···X (X=Cl, I), C-H···O/O-H···O, andπ··π interactions are the next priorities, respectively. The small contribution from the other interatomic contacts, namely N···π to the Hirshfeld surface of compounds **1-3** listed in Table S2, show negligible influence upon the packing. The large contribution for the van der Waals H···H interactions is typical of organic molecules and is consistent with the presence of CH groups along the ligand backbone [61]. The comparison of the Hirshfeld surfaces of compounds **2** and **3** reveals that in the crystal structure of **2** the C-H··π interaction is dominant to the C-H···I interaction, while this is vice versa for **3**. Hirshfeld surfaces of complexes **1** (a), **2** (b) and **3** (c) are also mapped with shape index (-1.0 (red) and +1.0 (blue)) and curvedness (between -4.0 (red) and +0.4 (blue), Figure S4. Distinctive features can be identified on the left and right-handed sides of shape index and curvedness plots of compounds **1** and **2**, leading to patterns of intermolecular interactions that are different on each side of these two complexes. The pattern of red and blue triangles on the same region of the shape index surface and the presence of a large flat green surface on the curvedness surface indicate the π···π stacking interactions. This feature is observed in all three compounds plots, whereas in the case of compound **3** it is more significant. The C-H··π interactions manifests itself on the shape index plots of compounds **1-3** as large red depression in the surface above the aromatic ring of concave curvature, while C-H donor regions have the opposite curvature. The hydrogen bond dominates the appearance of all these plots, appearing as a pair of sharp spikes with the upper spike (where de >di) corresponds to the hydrogen-bond donor and the lower spike (where de <di) corresponds to the hydrogen-bond acceptor.

The theoretical study is devoted to analyzing the non-covalent interactions that direct the self-assembly of coordination compounds **1-3** in the solid-state, focusing our attention to the C-H···X hydrogen bonding, C-H··π, and π-π stacking interactions. The binding energies obtained from the BLYP-D3 calculation on two relative fragments provide us with an opportunity to evaluate the intermolecular contacts between [$ML^{4\text{-}OH}X_2$] molecular units, Tables 3 and 4. The selected fragments were cut out directly from the CIF file and are shown in Figure S6. The energies of intermolecular interactions are in the range of those found for a series of neutral complexes [32, 46, 62]. The non-classical C-H···X and C-H···O and classical O-H···N hydrogen-bonding energies in compound **2** calculated to be in the range of 3.20-10.20 kcal/mol which is in agreement with the reported values for hydrogen bonding in the crystal structure of molecular solids, Table 3 [63, 64]. Also, the CH··π interaction energy in compound **1** is calculated to be -15.32 kcal/mol, while that of π··π and I··π interactions in compound **2** are -25.50 and -17.47 kcal/mol. Not surprisingly, the interaction energies of dimeric fragments containing several π-interactions and hydrogen bonds in **1** and **3** are larger than that of the fragments in which only one aromatic ring is involved in π-interactions, Tables 3 and 4, Figure S6.

4. Conclusion

Herein, the crystal structures of three new group IIB coordination compounds containing the 4-((pyridin-4-ylmethylene)amino)phenol ligand are reported. The crystal structures of these compounds, as well as the crystal packing of coordination complexes based on (4-substituted)-1-(pyridin-4-yl)methanimine ligand, retrieved from Cambridge Structural Database (CSD), were investigated.

Structural analysis show the tetrahedral (**1**) and trigonal pyramidal (**2** and **3**) coordination geometry around the metal centers in these structures. It has been revealed that the $L^{4\text{-}OH}$ adjusts its conformation to adopt the coordination geometry requirement of the metal atom and the optimal inter-atomic distances in the supramolecular structure. The crystal structure analyses revealed that the main interactions governing the crystal structure are π-π, C-H··π, as well as O-H···N, C-H···X hydrogen bonding interactions. The results reported herein are useful for understanding the coordination chemistry and solid-state structure of group IIB containing Schiff-base ligands.

AUTHOR INFORMATION
Corresponding Authors

Phone: +98-21-85692619 and +98-21-82884416.
E-mail: t.hajiashrafi@alzahra.ac.ir

ACKNOWLEDGMENT.

We gratefully acknowledge the financial support from the Research Council of Alzahra University and Science Foundation Ireland (SFI IvP 13/IA/1894)

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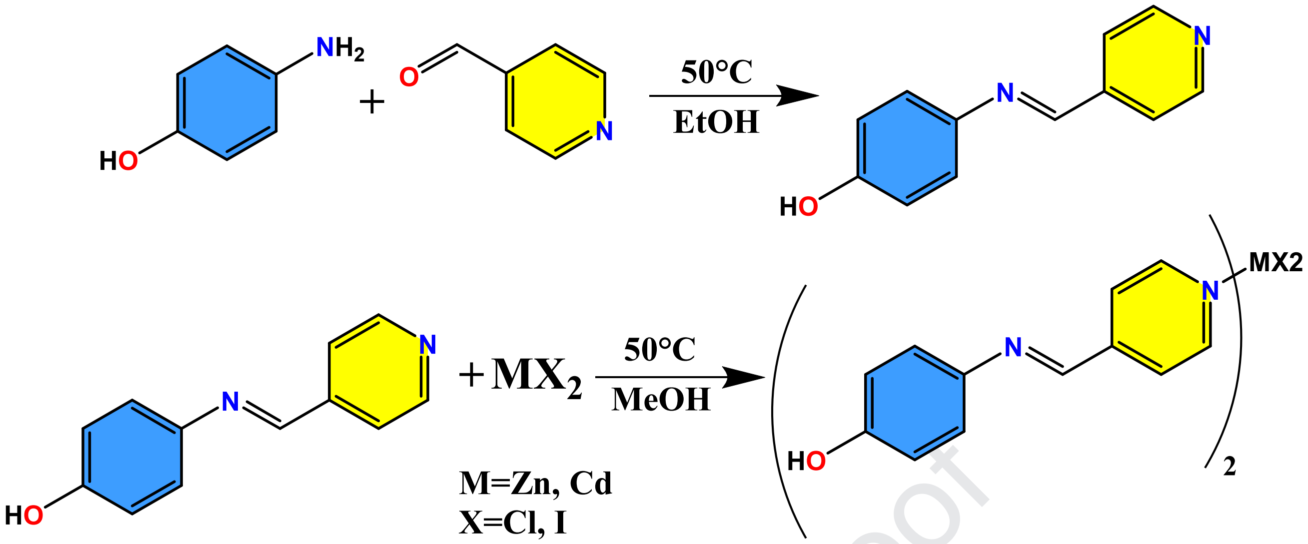


Scheme 1. $L^{4\text{-}OH}$ ligand and coordination complex syntheses

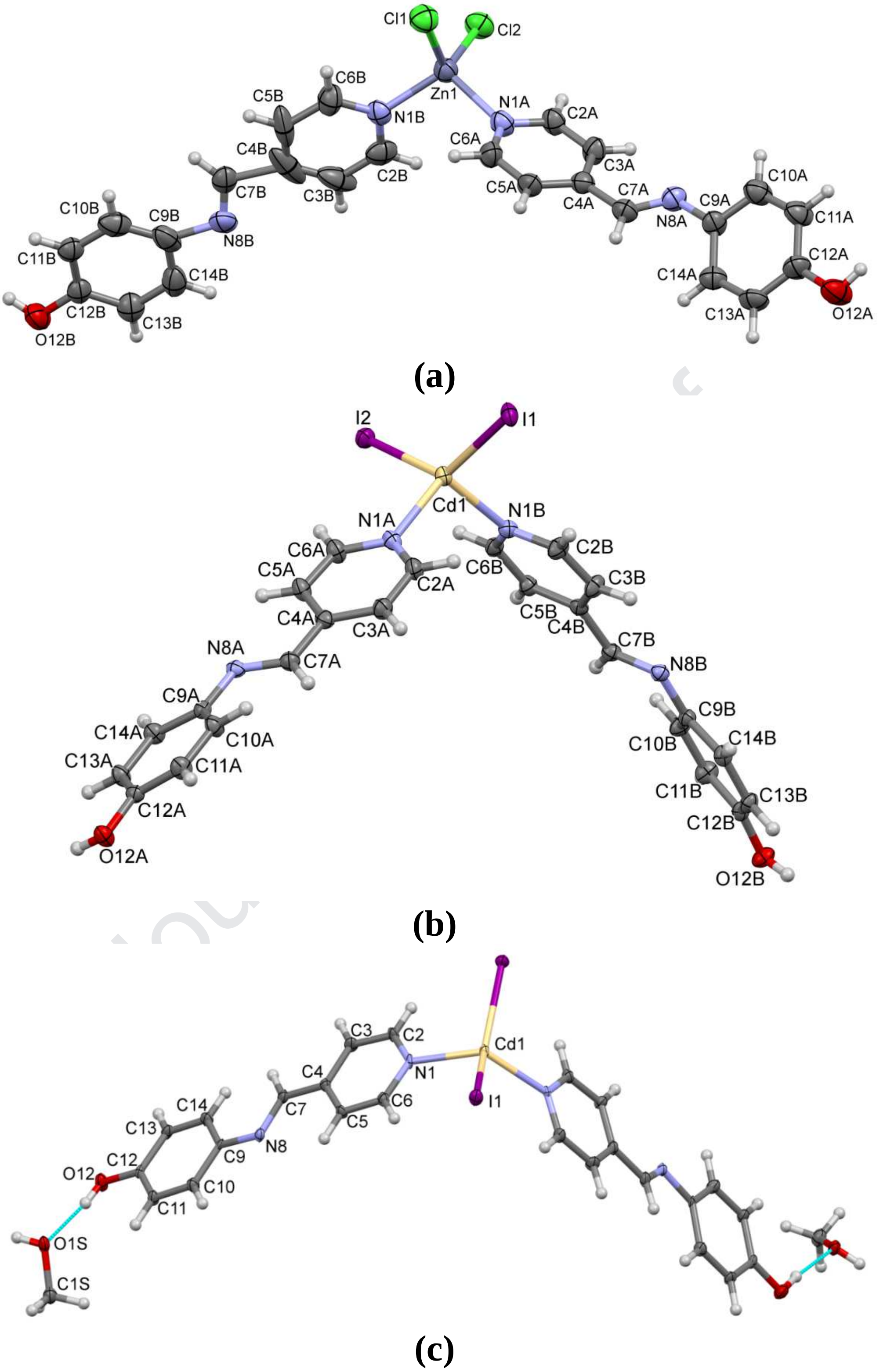


Figure 1. ORTEP diagram of compounds **1** (a), **2** (b), and **3** (c), drawn at 50% probability ellipsoids

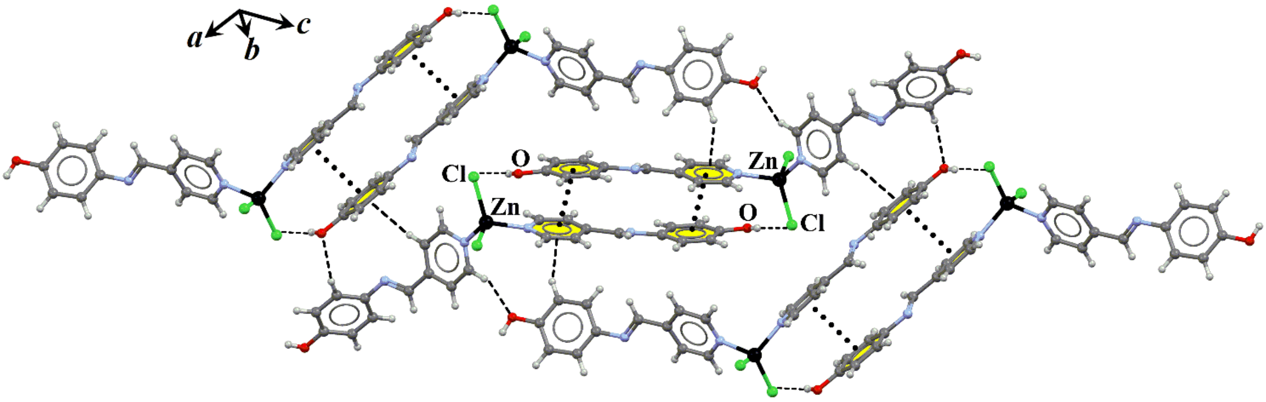


Figure 2. Representation of the crystal packing of compound **1** showing the association of molecular units through a combination of π-π stacking C-H•••π, as well as C-H•••O non-classical hydrogen bonds in the crystallographic *b*-direction. The overall supramolecular structure results from linking the [Zn(L)$_2$Cl$_2$] units *via* C-H•••Cl, O-H•••Cl and C-H•••π interactions in the *ac*-plane.

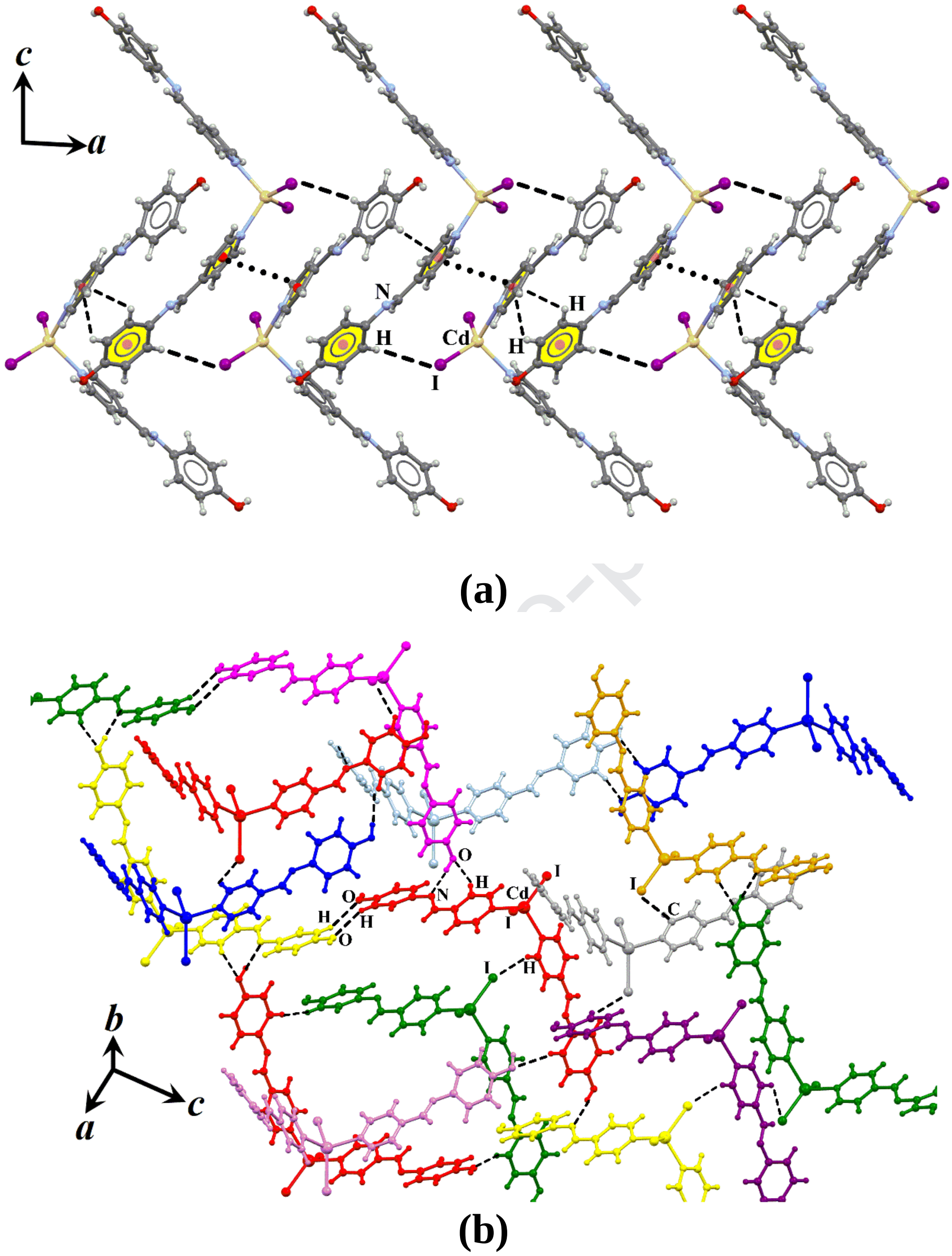
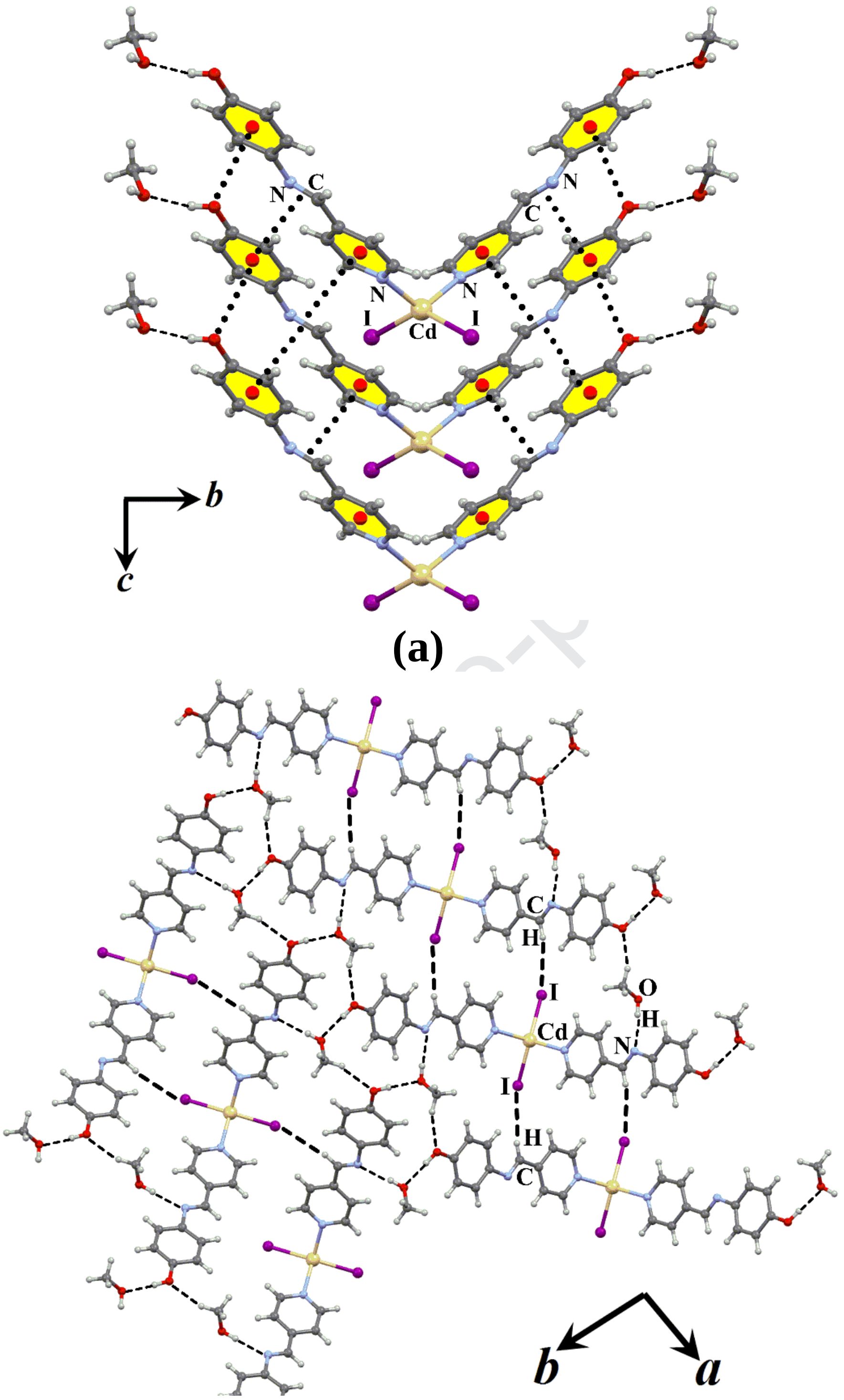


Figure 3. Representation of the crystal packing of compound **2** showing the supramolecular association of discrete molecular units along the crystallographic *a*-direction through π-π stacking, C-H··π and I··π interactions (a) View showing the three-dimensional crystal packing; the O-H···N, $R_2^2(8)$ C-H···O and C-H···I hydrogen bonds link these units in the *bc*-plane (b).



(a)

(b)

Figure 4. Representation of the crystal packing of compound **3** showing the supramolecular association of discrete molecular units ${}_{\text{imine}}\pi$-π_{phenyl}, ${}_{\text{imine}}\pi$-π_{pyridyl}, O(lone pair)$\cdot\cdot\,\pi_{\text{phenyl}}$ interactions along the crystallographic *c*-direction (a) View showing the three-dimensional crystal packing; the methanol molecules of crystallization link discrete molecular units, in the *ab*-plane, via ${}_{\text{MeOH}}$O–H•••N_{imine} and ${}_{\text{MeOH}}$C-H•••O_{OH} hydrogen bonds, which is further assisted by ${}_{\text{imine}}$C-H•••I interaction (b)

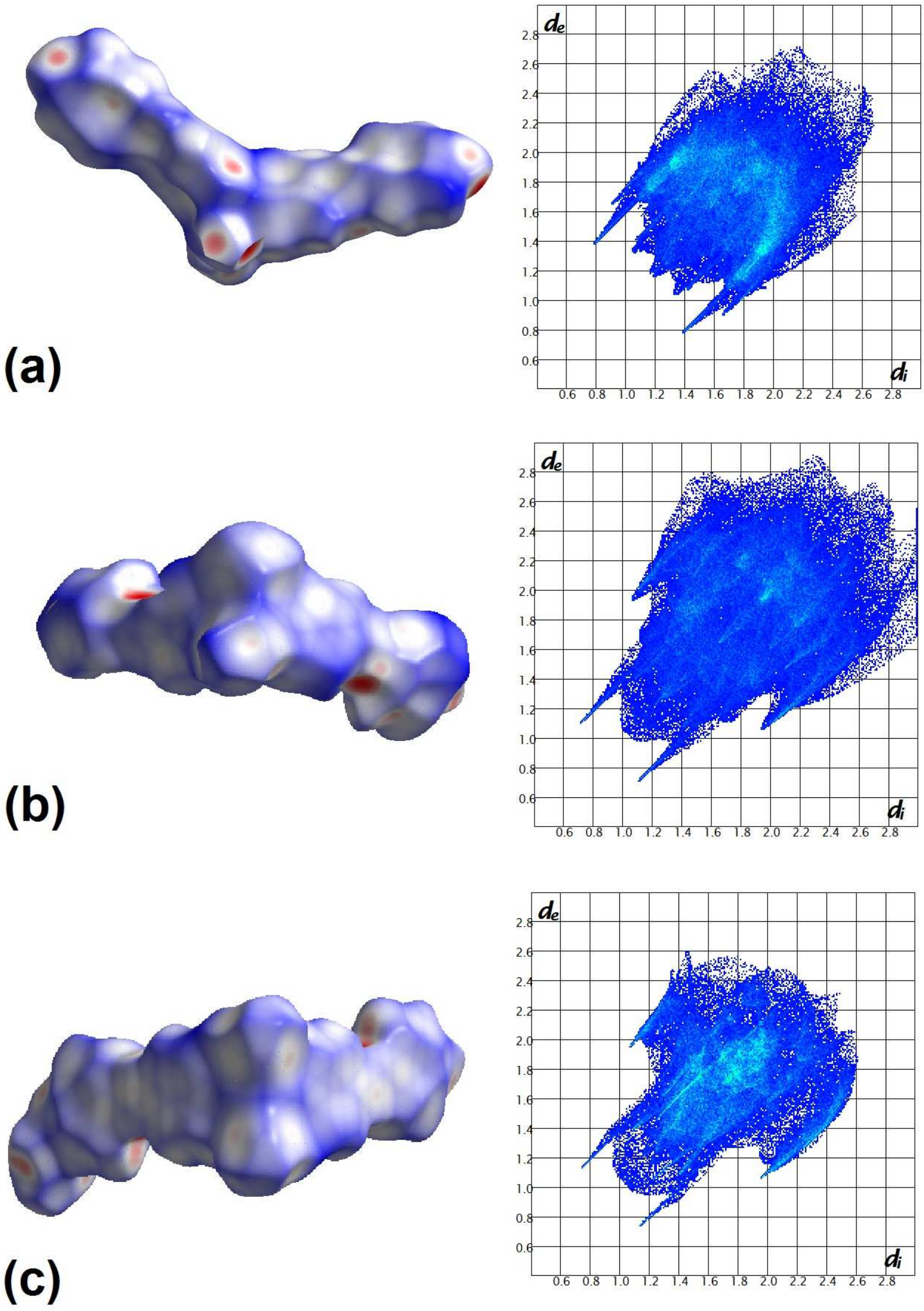


Figure 5. Hirshfeld surface area and two-dimensional fingerprint plots of complexes 1 (a), 2 (b) and 3 (c).

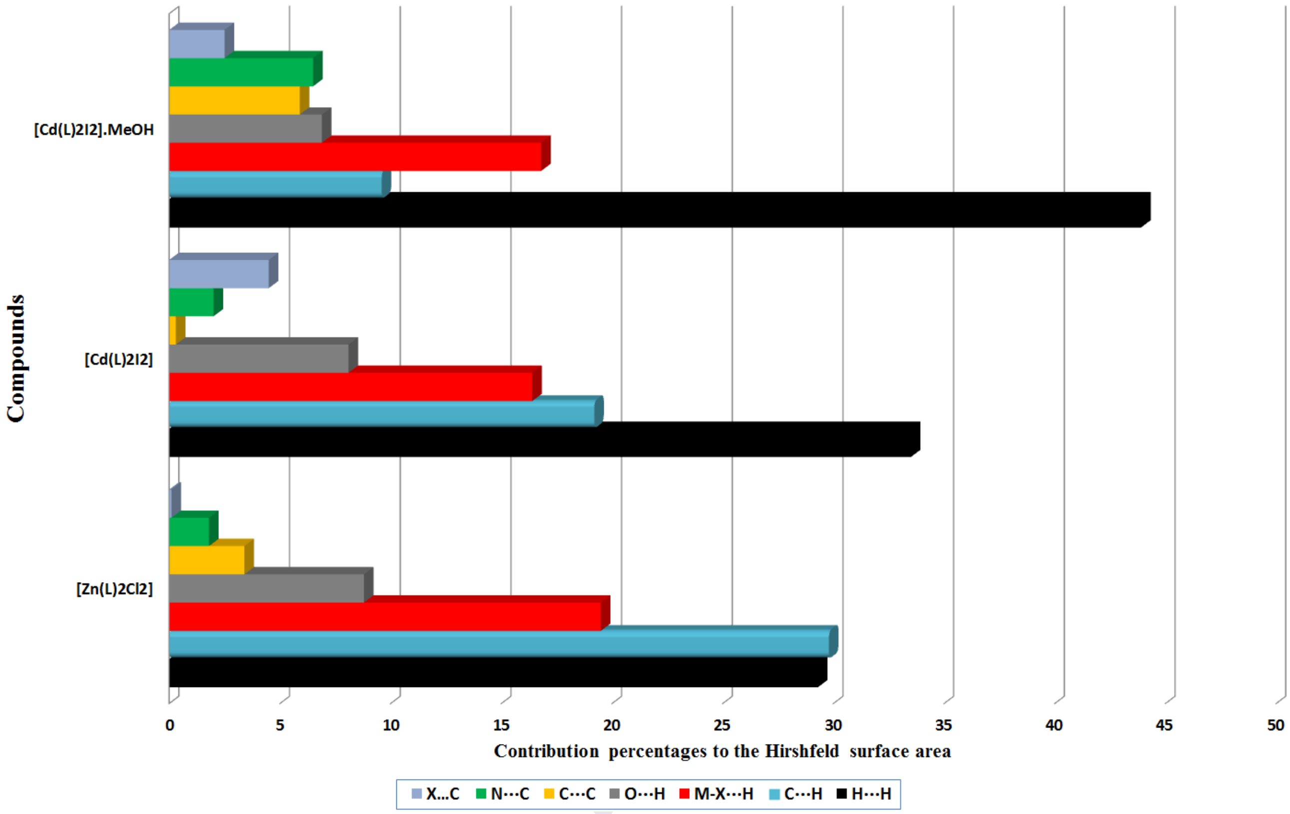


Figure 6. Horizontal bar chart showing the relative contributions of different intermolecular interactions to the Hirshfeld surface areas in compounds **1–3**.

Table 1. Structural data and refinement parameters for compounds **1-3**.

	1	**2**	**3**
formula	$C_{24}H_{20}Zn\,Cl_2N_4O_2$	$C_{24}H_{20}CdI_2N_4O_2$	$C_{26}H_{28}CdI_2N_4\,O_4$
fw	532.71	762.6	826.72
λ/Å	0.71073	0.71073	0.71073
T/K	130(1)	100(1)	100(1)
crystal system	Monoclinic	Monoclinic	Orthorhombic
space group	*P2₁/n*	*I2/a*	*Pba2*
a/Å	9.3689(6)	10.5408(3)	9.1610(13)
b/Å	12.9152(7)	19.3211(4)	32.257(4)
c/Å	19.1424(13)	25.6456(7)	4.7290(7)
α/°	90	90	90
β/°	93.373(6)	91.511(2)	90
γ/°	90	90	90
V/Å^3	2312.2(2)	5221.2(2)	1397.4(3)
D_{calc}/Mg.m^{-3}	1.530	1.940	1.965
Z	4	8	2
μ (mm^{-1})	3.847	3.229	3.029
F(000)	1088	2896	796
2θ (˚)	65.5	50.0	55.1
R (int)	0.2152	0.0264	0.0604
GOOF	0.968	1.052	1.131
$R_1{}^a(I>2\sigma(I))$	0.0641	0.0174	0.0284
$wR_2{}^b(I>2\sigma(I))$	0.1249	0.0389	0.0678
CCDC No.	1993550	1993551	1993552

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b] $wR_2 = [\Sigma(w(F_o^2 - F_c^2)^2)/\Sigma w(F_o^2)2]^{½}$.

Table 2. Selected bond distances (Å) and angles (°) for complexes **1-3**.

		Complex		
		1	**2**	**3**
Bond distance	M1-N1A	2.032(4)	2.293(2)	2.290(1)
	M1-N1B	2.019(4)	2.283(2)	2.290(1)
	M1-X1	2.234(2)	2.6932(5)	2.7304(2)
	M1-X2	2.228(2)	2.7117(6)	2.7304(2)
Bond angle	N1A-M1-N1B	107.5(2)	107.19(6)	119.8(1)
	X1-M1-X2	114.75(7)	129.33(2)	137.48(1)
	N1A-M1-X1	107.1(1)	105.77(5)	99.4(2)
	N1A-M1-X2	108.1(1)	104.00(5)	101.5(1)
	N1B-M1-X1	106.1(1)	105.18(5)	99.4(2)
	N1B-M1-X2	112.9(1)	103.87(5)	101.5(1)

Table 3. Selected hydrogen bond geometries for coordination compounds **1-3**

Compound	D-H···A	d(D-H)/Å	d(H···A)/Å	d(D···A)/Å	<D-H···A/°	Binding Energy (kcal/mol)	Sym. Code
1	O12A-H12A···Cl1	0.840	2.331(1)	3.127(5)	158.1(1)	-29.75[I]	-x,1-y,1-z
	O12B-H12B···Cl2	0.840	2.312(1)	3.135(4)	167.2(1)	-33.78[II]	2-x,1-y,-z
	C7B-H7B···Cl1	0.950	2.916(1)	3.85(2)	169.0(1)	-20.25	1-x,1-y,-z
	C10B-H10B···Cl1	0.95	3.145(3)	4.022(7)	154.5(2)		1-x,1-y,-z
	C10A-H10A···O12B	0.950	2.618(2)	3.538(8)	162.9(1)		1.5-x, -½+y,½-z
	C6A-H6A···O12A	0.950	2.453(2)	3.083(8)	123.7(2)		½+x, ½-y,-½+z
2	O12A-H12A···N8B	0.840	1.990(1)	2.828(2)	175.0(1)	-10.20	½+x, ½+y,-½+z
	O12B-H12B···N8A	0.840	1.964(2)	2.803(2)	177.7(2)		½+x,-½+y,½+z
	C13A-H13A···N8B	0.950	2.651(2)	3.363(3)	132.1(1)		½+x, ½+y,-½+z
	C13A-H13A···I1	0.950	3.1065(1)	3.837(2)	135.0(2)	-7.32	1-x, ½+y,½-z
	C11A-H11A···O12A	0.950	2.618(3)	3.522(3)	159.1(2)		2-x,1-y,-z
	C14A-H14A···O12B	0.950	2.716(2)	3.327(3)	122.6(2)		-½+x,½+y,-½+z
	C14B-H14B···O12A	0.950	2.696(3)	3.286(3)	120.9(1)		2-x,-½+y,½-z
	C11A-H11A···O15A	0.950	2.511(1)	3.404(3)	156.7(1)	-3.20	-½+x,½+y,-½+z
	C3B-H3B···O12A	0.950	2.712(3)	3.571(3)	150.8(1)		-½+x,-½+y,½+z
3	O1S-H1S···N8	0.840	2.012(1)	2.848(6)	172.5(1)	-5.34	½+x, ½-y,½+z
	O12-H12···O1S	0.840	1.841(3)	2.677(6)	172.9(2)		x,y,z
	C11-H11···O12	0.950	2.579(3)	3.314(8)	134.4(1)		-½+x,½-y,z
	C7-H7···I1	0.950	3.1568(2)	4.064(6)	160.3(1)		1-x,1-y,1-z
	C5-H5···O1S	0.950	2.423(1)	3.341(7)	162.5(1)		½+x,½-y,1+z
	C10-H10···O1S	0.950	2.585(1)	3.354(8)	138.2(1)		½+x,½-y,1+z

[I] The dimer binding energy connected to each other via two C11A-H11A··$\pi_{\text{pyridyl(N1A-C6A)}}$ and two O112A-H12A···Cl1···Cl1 interactions.

[II] The dimer binding energy connected to each other via two ${}_{\text{(N1B-C6B)pyridyl}}\pi\cdot\cdot\pi_{\text{phenyl(C9B-C14B)}}$ and two O12B-H12B···Cl2 interactions.

Table 4. π-interactions for compounds **1-3**

Compound	Interaction	C-H/atom··π	π··π				Binding energy (kcal/mol)	Sym. code
			$d_{\text{cg-cg}}$ (Å)	Offset angle (˚)	plane to plane angle (˚)	d_{offset} (Å)		
1	C11A-H11A··$\pi_{\text{pyridyl(N1A-C6A)}}$	2.834(1)	-	-	-	-	-29.75[I]	-x,1-y,1-z
	C2B-H2B··$\pi_{\text{phenyl(C9A-C14A)}}$	2.638(1)					-15.32	-x,1-y,1-z
	C3A-H3A··$\pi_{\text{phenyl(C9B-C14B)}}$	2.817(2)						2-x,1-y,-z
	C13A-H13A··$\pi_{\text{pyridyl(N1B-C6B)}}$	2.922(3)						½+x,½-y,-½+z
	${}_{\text{(N1B-C6B)pyridyl}}\pi\cdot\cdot\pi_{\text{phenyl(C9B-C14B)}}$	-	3.753(2)	19.58	5.88	1.25	-33.78[II]	2-x,1-y,-z
2	${}_{\text{(N1B-C6B)pyridyl}}\pi\cdot\cdot\pi_{\text{pyridyl(N1B-C6B)}}$	-	3.975(2)	18.39	24.45	1.28	-25.50	½-x,y,1-z
	C3B-H3B··$\pi_{\text{phenyl(C9B-C14B)}}$	3.161(1)						1.5-x,y,1-z
	I··$\pi_{\text{pyridyl(N1B-C6B)}}$	3.875(2)					-17.47	-½+x,1-y,z
3	O(lone pair)··π_{phenyl}	3.488(2)	-	-	-	-		x,y,-1+z
	${}_{\text{imine}}\pi\cdot\cdot\pi_{\text{phenyl(N1-C6)}}$	3.497(2)	-	-	-	-	-36.32[III]	x,y,-1+z
	${}_{\text{imine}}\pi\cdot\cdot\pi_{\text{phenyl(C9-C14)}}$	3.355(1)	-	-	-	-		x,y,-1+z

[I] The dimer binding energy connected to each other via two ${}_{\text{(N3-C18)pyridyl}}\pi\cdot\cdot\pi_{\text{phenyl(C20-C25)}}$ and two C15-H13···Cl3 interactions.

[II] The dimer binding energy connected to each other via two ${}_{\text{(N2-C13)pyridyl}}\pi\cdot\cdot\pi_{\text{phenyl(C2-C7)}}$ and two C8-H8···I1 interactions.

[III] The dimer binding energy connected to each other via two sets of ${}_{\text{imine}}\pi\cdot\cdot\pi_{\text{phenyl(N1-C6)}}$, ${}_{\text{imine}}\pi\cdot\cdot\pi_{\text{phenyl(C9-C14)}}$ and O(lone pair)··π interactions.

Table 5. Molecular features of coordination compounds containing (4-substituted)-1-(pyridin-4-yl)methanimine ligand

Ref Code	**Space group**	**Metal atom coordination geometry**	**Molecular structure**	**Reference**
-	$I2/a$	4-coordinate tetrahedral	Discrete coordination complex	This work
-	$P2_1/a$	4-coordinate trigonal pyramidal	Discrete coordination complex	This work
-	$Pba2$	4-coordinate trigonal pyramidal	Discrete coordination complex	This work
KOWWEB	$I2/a$	6-coordnate octahedral	1D coordination polymer	[38]
KOWWIF	$Pba2$	4-coordinate seesaw	Discrete coordination complex	[38]
KOWWOL	$Pba2$	4-coordinate seesaw	Discrete coordination complex	[38]
ZUNSUY	$P2_1/c$	6-coordnate octahedral	1D coordination polymer	[60]
HOYLIS	$P\bar{1}$	5-coordinate square pyramidal	1D coordination polymer	[59]
HOYLOY	$P2_12_12_1$	4-coordinate seesaw	1D coordination polymer	[59]
HOYLUE	$Fdd2$	4-coordinate seesaw	Discrete coordination complex	[59]
HOYMAL	$P2_1/c$	5-coordinate square pyramidal	1D coordination polymer	[59]
HOYMEP	$Fdd2$	4-coordinate seesaw	1D coordination polymer	[59]
HOYMIT	$P2_12_12_1$	4-coordinate seesaw	1D coordination polymer	[59]
HOYMOZ	$Pna2_1$	4-coordinate seesaw	1D coordination polymer	[59]
HOYMUF	$P2_1/c$	4-coordinate seesaw	1D coordination polymer	[59]
ZUNTAF	$C2/c$	6-coordnate octahedral	1D coordination polymer	[59]

- Group IIB complexes containing Schiff-base ligands were synthesized.
- The molecular structure and crystal packing of these compounds were investigated.
- The crystal packing was governed by π-stacking and non-classical hydrogen bonds.

CRediT authorship contribution statement

Taraneh Hajiashrafi: Writing - original draft, review & editing, Software

Shiva Salehi: acquisition of data, analysis and/or interpretation of data

Maciej Kubicki: acquisition of data

Keith J. Flanagan: acquisition of data

Mathias O. Senge: revising the manuscript

Author declaration

1. Conflict of Interest

☒No conflict of interest exists.

We wish to confirm that there are no known conflicts of interest associated with this publication and there has been no significant financial support for this work that could have influenced its outcome.

2. Funding

☒Funding was received for this work.

All of the sources of funding for the work described in this publication are acknowledged below:

We gratefully acknowledge the financial support from the Research Council of Alzahra University- Science Foundation Ireland

☒We confirm that the manuscript has been read and approved by all named authors.

☒We confirm that the order of authors listed in the manuscript has been approved by all named authors.

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Graphical abstract (synopsis):

Zn(II) and Cd(II) coordination compounds containing 4-((pyridin-4-ylmethylene)amino)phenol ligands were synthesized and then characterized using spectroscopic techniques and single crystal X-ray crystallography. The molecular structure and crystal packing of these complexes, as well as the packing of related compounds, were investigated using geometrical, Hirshfeld surface analyses, and theoretical calculations. The supramolecular architecture of these coordination complexes is governed by a combination of π•••π stacking, C-H•••π, O-H•••N, and C-H•••X hydrogen bonding interactions. This study provides further insight into the understanding of the coordination chemistry of group IIB containing Schiff-base ligand and the role of weak non-covalent interactions in the solid-state structure of coordination compounds.