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Isostructural Mercury Coordination Polymers with Amide Junction: Interplay of Coordination and π - π Stacking

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ABSTRACT. Two coordination polymers $[Hg_2Cl_4L.2(DMF)]_n$, **1** and $[Hg_2Br_4L.2(DMF)]_n$, **2**, where L is the *N,N'*-(1,2-diphenylethane-1,2-diyl)diisonicotinamide ligand have been synthesized and characterized. X-ray single crystal diffraction reveals that both coordination polymers are isostructural and mercury adopts square based pyramid coordination geometry. Our results show that interplay between the coordination of the carbonyl group and $\pi...\pi$ interaction of adjacent pyridine rings leads to the formation of 2D structures.

Introduction

 In the last few decades, crystal engineering of coordination polymers has attracted great attention due to their usage in different areas such as catalysis, materials and nanotechnology.¹ Many factors such as ligand structure,² coordination geometry of metal center,³ counter ions⁴ and experimental conditions⁵ can affect the final structure of coordination polymers. In addition to coordination bonds, various types of intermolecular interactions can extend crystal packing into higher dimensions. The influence of hydrogen bonds on the structure of coordination polymers has been well studied.⁶ Other than the hydrogen bonds, the π - π interactions undoubtedly play important roles in determining the crystal packing and molecular assemblies of the coordination compounds.⁷ It is notable, that unlike hydrogen bonding, π - π interaction is very difficult to control due to the lack of strength and directionality. There are some examples reported in the literature describing the influence of π - π interactions on the structure-directing of coordination compounds.⁸ Other than the π ... π interactions and the hydrogen bonds, the anion... π interaction also plays an important role in determining the crystal packing and molecular assemblies. Anions can influence the final structures either by coordinating directly to the metal centers or by acting as templates through non-covalent interactions which affect the self-assembly process.⁹

In recent years, coordination polymers with organic ligands based on two pyridine moieties as coordination sites and different spacers such as alkyl chain, imine bond and amide functionality have been designed.¹⁰⁻¹² Considering these bispyridyl ligands with amide junction reveals that: (1) two pyridyl groups are a good choice for connecting metal centers,¹³ (2) the amide group may participate in the binding to metal through the oxygen atom of carbonyl moiety,^{14,15} (3) π - π stacking between pyridine rings and also the hydrogen bonding of amide functionality can add extra dimensionality to the resulted structure^{15,16} and (4) due to the low rotational barrier of the amide group, these ligands can possess rotational flexibility and adopt a variety of conformations.^{16c,17} In this regards, reports on the coordination compounds of *N*,*N'*-(1,2-diphenylethane-1,2-diyl)dipyridineamide ligands are rare, with the exception of Moberg and co-workers (monomeric Zr complex)¹⁸, Zhou and co-workers (monomeric

Ni complex)¹⁹ and Williams and co-workers (polymeric Cu complex)²⁰ reports containing the N,N'-(1,2-diphenylethane-1,2-diyl)dipicolinamide ligand.

In continuation of our previous study on the effect of $\pi...\pi$ interaction on the coordination geometry of central metal,²¹ we synthesized the *N*,*N'*-(1,2-diphenylethane-1,2-diyl)diisonicotinamide ligand (L) bearing two pyridines for coordination to the metal center which would facilitate the formation of $\pi..\pi$ stacking which affects the structure of the coordination polymers. For this purpose, two Hg(II) complexes of this ligand, [Hg₂Cl₄L.2(DMF)]_n, **1**, and [Hg₂Br₄L.2(DMF)]_n, **2**, have been prepared by the reaction of equimolar quantities of mercury halides (chloride and bromide), Scheme 1. X-ray diffraction analysis of these coordination polymers gives details about the interplay of coordination and $\pi...\pi$ interaction in their three-dimensional organizations.

Experimental section

Chemicals and instrumentation

All solvents such as methanol, chloroform and pyridine and the chemicals, pyridine-4-carboxylic acid, *meso*-1,2-diphenylethanediamine, triphenyl phosphate and mercuric (II) halides (chloride and bromide) were commercially available (reagent grade) and were purchased from Merck and used without further purification. Infrared spectra (4000–250 cm⁻¹) of solid sample were taken as 1% dispersion in KBr pellets using a BOMEM - MB102 spectrometer. ¹H NMR spectra were recorded on a Bruker AC-300 MHz spectrometer at ambient temperature in (CD₃)₂SO. All chemical shifts are quoted in part per million (ppm) relative to tetramethylsilane. Melting point was obtained by a Bamstead Electrothermal type 9200 melting point apparatus and corrected.

Synthesis of *N*,*N*'-(1, 2-diphenylethane-1, 2-diyl)diisonicotinamide, L

A solution of 5 mmol *meso*-1,2-diphenylethanediamine (1.061 g) in 10 mL pyridine was added to a solution of 10 mmol pyridine-4-carboxylic acid (1.23 g) in 10 mL pyridine. The resulting solution was stirred at 313 K for 20 min then 10 mmol of triphenyl phosphite (2.6 mL) was added dropwise, and the reaction mixture was stirred at 373 K for 5 h and at ambient temperature for 72 h. The resulting yellow solution was added to distilled water, filtered and then washed with diethylether. A light yellow solid resulted with a yield of 60%, mp >270 °C. X-ray quality crystals were obtained by slow solvent evaporation in dimethyl sulfoxide at room temperature. Anal.Calc. for L (C₃₀H₃₄N₄O₄S₂): C, 62.20; H, 5.87; N, 9.68. Found: C, 62.24; H, 5.90; N, 9.73. FT-IR (KBr pellet,cm⁻¹): 3324s, 3062s, 1642s, 1534s, 1406m, 1323s, 758s, 702s. ¹H NMR (DMSO, δ from TMS): 9.1254(s, 1H), 8.6322(d, 2H), 7.6647(d, 2H), 7.4701-7.1929(m, 5H), 75.6691(m, 1H).

Synthesis of [Hg₂Cl₄L.2(DMF)]_n, 1 and [Hg₂Br₄L.2(DMF)]_n, 2.

To a solution of 0.5 mmol of mercury (II) halide (HgX₂, X=Cl and Br) in 3 mL of methanol, a solution of 0.5 mmol of *N*,*N'*-(1,2-diphenylethane-1,2-diyl)diisonicotinamide (ligand L) in mixure of 3 mL of methanol and 3 mL of chloroform was added while stirring. The mixture was heated at 313 K for about 10 min and the resulting sediment was filtered and dried outdoor, it was then, solved in dimethyl foramide solvent. Upon slow evaporation of this solution at room temperature, colorless block crystals for [Hg₂Cl₄L.2(DMF)]_n and [Hg₂Br₄L.2(DMF)]_n complexes, suitable for X-ray analysis were obtained after *ca.* two weeks (yield *ca.* 63% and 71%, mp 260-261 °C and 253-254 °C decompose for [Hg₂Cl₄L.2(DMF)]_n and [Hg₂Br₄L.2(DMF)]_n, respectively). Anal.Calc. for **1** (C₃₂H₃₉Cl₄Hg₂N₆O₄): C, 34.55; H, 3.51; N, 7.56. Found: C, 34.59; H, 3.56; N, 7.60. FT-IR (KBr pellet,cm⁻¹): 3320s, 3065s, 1647s, 1538s, 1403m, 1327s, 758s, 700s. Anal. Calc. for **2** (C₃₂H₃₉Br₄Hg₂N₆O₄): C, 29.78; H, 3.02; N, 6.51. Found: C, 29.83; H, 3.06; N, 6.56. FT-IR (KBr pellet, cm⁻¹): 3318s, 3067s, 1644s, 1541s, 1404m, 1327s, 757s, 699s.

Crystal structure determination of complexes

The x-ray diffraction measurements were made on a STOE IPDS-II diffractometer with graphite monochromated Mo-K α radiation. For N,N'-(1,2-diphenylethane-1,2-diyl)diisonicotinamide, L, a colorless prism crystal with a dimension of $0.37 \times 0.36 \times 0.32$ mm, for $[Hg_2Cl_4L.2(DMF)]_n$, 1, a colorless block crystal with a dimension of $0.40 \times 0.35 \times 0.33$ mm and for [Hg₂Br₄L.2(DMF)]_n, 2, a colorless block crystal with a dimension of $0.21 \times 0.18 \times 0.14$ mm were mounted on a glass fiber and used for data collection. Cell constants and an orientation matrix for data collection were obtained by least-squares refinement of diffraction data from 3010 for L, 5002 for 1 and 3780 for 2 unique reflections. Data were collected at a temperature of 298(2) K to a maximum θ value of 26.00°, 29.21° and 26.00° for L, 1 and 2 and in an a series of ω scans in 1° oscillations and integrated using the Stoe X-AREA²² software package. The numerical absorption coefficient, μ , for Mo-K α radiation are 0.215 mm⁻ ¹ for L, 8.517 mm⁻¹ for $[Hg_2Cl_4L.2(DMF)]_n$ and 12.126 mm⁻¹ for $[Hg_2Br_4L.2(DMF)]_n$. A numerical absorption correction was applied using X-RED and X-SHAPE softwares.²³ Data were corrected for Lorentz and Polarizing effects. The structures were solved by direct methods²⁴ and subsequent different Fourier maps and then refined on F^2 by a full-matrix least-square procedure using anisotropic displacement parameters. All refinements were performed using the X-STEP32 crystallographic software package.²⁵ The crystallographic data and selected bond lengths and bond angles for L, 1 and 2 are listed in Tables 1 and 2.

Theoretical Methods.

All calculations have been carried out by means of the GAUSSIAN03 package.²⁶ Calculations between pyridine aromatic rings were performed with the experimental structure as the starting point at the MP2-aug-cc-PVDZ level. The interaction energies were counterpoise corrected for the basis set superposition error (BSSE) with the procedure of Boys and Bernardi.²⁷

Results and Discussion

Synthesis

The combination of **L** with HgX₂ (X=Cl, Br) in 1:1 molar ratio leads to the formation of 2D $[Hg_2Cl_4L.2(DMF)]_n$, **1**, and $[Hg_2Br_4L.2(DMF)]_n$, **2** coordination polymers. Upon slow evaporation of the DMF solution of these complexes, colorless block crystals were obtained after *ca*. two weeks. X-ray diffraction on a single crystal of these complexes demonstrates that they are isostructural compounds and both of them crystallize in the triclinic crystal system with *P*ī space group, Table 1. X-ray powder patterns of compounds **1** and **2** are essentially the same to that simulated from the structure determined by single crystal analysis, see ESI, Fig. S1 and S2. All of the peaks of the two compounds can be indexed to their respective simulated XRD powder patterns, which indicate each of the two compounds is pure phase.

Structural analysis of L, 1 and 2

Based on the comparative direction of the C=O groups, L can adopt *anti-anti-anti* and *anti-syn-anti* conformations, see ESI, Fig. S3. This allows conformational adaptation of L for the generation of different isomers of mercury(II) complexes. To have a better insight into the structural changes of L from free ligand to coordination compounds 1 and 2, we determined its structure by X-ray diffraction study. An ORTEP view of L is shown in Figure 1. The amide N–C and C=O bond distance of 1.337(3) and 1.224(3)Å, respectively, are in normal ranges. As depicted from Figure 1, in the solid state, L adopts an *anti-anti-anti* conformation.

The non-classical C-H...N hydrogen bonds, which are those between C–H pyridine donor and pyridine nitrogen acceptor, form a one dimensional zigzag. These 1D zigzag chains are further linked to generate 2D sheets by head-to-tail dimeric C=O...H-C(pyridine) non-classical classical hydrogen bonds into centrosymmetric $R^2_2(10)$ carbonyl–pyridne synthon, Figure 2a, Table 3. DMSO solvent molecules are

linked adjacent 2D sheets from one side by S=O...H-N(amide) and S=O...H-C(pyridine) classical and non-classical hydrogen bonds and from the other side by the weak intermolecular C=O...H-C(methyl) interactions, Figure 2b, Table 3.

The coordination ability of L was then tested with mercury(II) halides. Simple reaction between HgX₂ and L in methanol/chloroform afforded well-formed colorless crystals of 1 and 2. The asymmetric unit of 1 and 2 consists of one Hg^{2+} ion, two halogen anions and a half crystallographically independent ligand. As depicted in Figure 3, in these compounds, coordination geometry around the Hg(II) centre in compunds 1 and 2 are square-based pyramid (SBP), Table 2, with trigonality index $(\tau)^{28}$ of 0.016 and 0.023 respectively. In both structures, the plane of square-based pyramid is occupied by three halogen anions (Hg-Cl: 2.319(2), 2.340(2) and 3.051(2) Å and Hg-Br: 2.450(1), 2.464(1) and 3.163(1) Å, Table 2, and carbonyl oxygen atom (Hg-O: 2.726(5) Å and 2.778(5) for 1 and 2 respectively). The appical position in both structures is occupied by a nitrogen atom from the pyridine ring of the L ligand at a normal distance of 2.453(4) and 2.448(5) Å for 1 and 2 respectively. The τ values and geometrical parameters around central metal atoms clearly show, Table 2, that the coordination geometry around Hg(II) is almost perfect SBP in both structures. Examining the crystal structures of 1 and 2 also reveal that L adopts an anti-anti-anti conformation, Figure 3. Reports on the coordination compounds of N,N'-(1,2-diphenylethane-1,2-diyl)dipyridineamide ligands are rare. A few related compounds in the literature are discussed below. Compound [Zr(L^{2-py})(O^tBu)₂]¹⁸ shows a discrete monomeric sixcoordinated Zr complex in which the amide ligand acts as a four-dentate dianion ligand ($L^{2-py} = N, N'$ bis(2-pyridinecarboxamido)-1,2-diphenylethane). Two other coordination sites are occupied by monodentate O^tBu anions. In compound [Ni(L^{2-py})].(C2H5)2O,¹⁹ the metal center is four-coordinted with four-dentate dianion amide ligands. In compound $[Cu(L^{2-py})]^{20}$, the metal center coordinates the four nitrogen donor atoms of amide lagnad, while the carbonyl oxygen atom bridges two adjacent metal centers to generate of a 1D chain motif. It is notable in all of these compounds that L adopts an *anti-syn*anti conformation.

In the crystal packing of these complexes, the adjacent $Hg_2X_2(\mu-X)_2$ moieties are linked by L through N_{pv} to form a one-dimensional, 1D, polymeric chain. The two independent polymeric chains are closely packed through coordination bonds established between the carbonyl group and Hg(II) centre, Figure 4. It is notable that the formation of parallel π - π stacks between the pyridyl rings of adjacent 1D chains influences the C=O-Hg angles. The pyridyl rings of adjacent ligands involved in the *intermolecular* π - π stacking interaction is arranged in such a way that the angle between the plane (containing C-CO-N fragment) normal and O-Hg vector (for geometrical defination see reference 21) reaches about 50.99° and 47.44° in 1 and 2 respectively. A Cambridge Structural Database (with the help of ConQuest version 1.14)²⁹ search about the coordination of ligands which contain isonicotinamide as a portion of their structures was carried out and 326 hits were found. Among these structures only in 15 hits¹⁴ both of the oxygen and nitrogen atoms were coordinated to the transition metal centres and in between them only 1 hit¹⁵ has mercury (II) as its metal center. In these 15 structures additional forces lead to the coordination of carbonyl and pyridine at the same time. These forces involve factors like π ... π stacking interactions, C-H... π intermolecular interactions and chelating effects.¹⁴ In compounds 1 and 2, π ... π stacking interactions between pyridine rings facilitate the coordination of the carbonyl group. It was thought of interest to investigate further, using theoretical methods, the nature of the π ... π stacking interactions in both compounds 1 and 2. Calculations were performed with the experimental structure of the stacked pyridine rings as the starting point at the MP2/aug-cc-PVDZ level. The interaction energy between the two adjacent pyridine rings is 20.3 and 19.8 kJ mol⁻¹ for compounds 1 and 2, respectively. When energetic factors are taken into account, the coordination can be considered as the primary and the aromatic interaction as the secondary effect. Therefore, interplay of coordination of carbonyl group, C=O-Hg, and π ... π stacking of pyridine rings lead to the formation of 2D structures. A simple survey in the CSD shows that the histograms of geometrical parameters of this aromatic interaction such as centroid-to-centroid distance (3.870 and 3.903 Å for 1 and 2, respectively), displacement angle and angle of the pyridine rings are in the normal ranges (see ESI, Fig. S4). The scattergram of centriod-to-

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centriod distances *vs* displacement angles conforms the existence of this interaction, Figure S5. Such π - π interaction effects on the *primary* structure directing coordination geometry around the Hg(II) containing similar ligands with those discussed in this paper has been reported previously in detail by some of us.²¹

As depicted in Figure 4, two different boxes can be defined. In box I, the interchain distance of the neighboring mercury atoms bridged by *different* L ligands through the carbonyl group, are about 7.789(1) and 7.685(1) Å in 1 and 2 respectively. The $\pi...\pi$ interactions between the pyridine rings are shown by red dashed lines in box I. In box II, the distance of neighboring mercury atoms bridged by *one* L ligand through the carbonyl and pyridine group, are about 13.037(2) and 13.142(2) Å in 1 and 2 respectively. Dimethyl formamide molecules are trapped in box II, Figure 4, which is connected through hydrogen bonding interactions between the oxygen atom of DMF molecules and the hydrogen atom of the amide ligand, Table 3.

Phenyl groups in both complexes are in the *trans* position. This *trans* conformation is due to anion... π interactions between phenyl rings and bridged halogen among two metal centres, Figure 5. Over the past decade, the importance of lone-pair... π interaction has been recognized as a highly directional supramolecular interaction.³⁰ This interaction forms between an electron-deficient π ring system and an electron-rich atom such as a halogen atom. Figure S6 shows geometrical parameters which determine the strenght of this interaction. A CSD search reveals that all parameters for determining these interactions are in the normal range³¹ and phenyl groups are in the *trans* position.

The decomposition behaviour of compounds **1** and **2** was investigated in static air atmosphere from ambient to 600 °C, Figures S7 and S8 respectively. The thermogravimetric analyses reveal that both compounds have identical decomposition patterns. As can be seen from the thermograms, **1** and **2** are stable up to 243 and 250 °C respectively, when the hydrogen bonds between DMF and ligand are broken and consequently the loss of DMF molecules takes place. The experimental mass loss of 13.5% and 11.7% for **1** and **2** respectively, is in consistant with the calculated values of 13.2% and 11.3% for

elemination DMF solvent molecules. At 275-363 °C for **1** and 280-383 °C for **2**, both compounds will be decomposed.

Conclusions

In summary, we have illustrated that 1D coordination polymeric chains further extend into 2D networks *via* cooperation of coordination bonds along with $\pi...\pi$ interactions. Hence weak non-covalent interactions seem to play a significant role in the formation of crystal packing and stabilizing of the supramolecular structures. The results also demonstrate that the flexibility of the ligand enables the formation of higher dimensional structures.

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SUPPORTING INFORMATION PARAGRAPH. Electronic Supplementary Information (ESI) available: [Figures S1–S5 show conformations of L and diagrams of CSD searches. CCDC reference numbers for L, 1 and 2 are 875332, 875330 and 875331, respectively]. These materials are free of charge *via* Internet at http://pubs.acs.org.

Scheme 1. Schematic representation of portions of the structure of the 2D isostructural coordination networks formed between L and HgX₂ (X=Cl, Br). DMF solvent molecules are omitted for clarity. Different colors show different 1D chains.

Figure 1. The ORTEP diagram of N,N'-(1,2-diphenylethane-1,2-diyl)diisonicotinamide ligand, L. Ellipsoids are drawn at 30% probability level. Sulfur atom in DMSO solvent is split into two partial atoms with 50% occupancies. Symmetry code; i) 1-x, -y, 2-z.

Figure 2. (a) A representation of part of the unit cell contents of L shows generation of 2D sheets by cooperation of C-H...N and C-H...O=C non-classical classical hydrogen bonds and (b) a side view representation of L showing the presence of S=O...H-N and S=O...H-C classical and non-classical hydrogen bonds between adjacent 2D sheets. DMSO solvent molecules are shown in ball and stick. Different colors show different adjacent molecules in (a) or different adjacent 2D sheets in (b).

Figure 3. Portion of the structure of coordination polymers formed between L and HgX₂, showing coordination geometry around centeral metal. Symmetry codes; i) 2–x, 1-y, 1-z, ii) 1-x, 1-y, 1-z, iii) -x, 2-y, -z.

Figure 4. Portion of **1** and **2** which are generated through interplay of Hg–O=C coordination bonds and π ... π interaction of pyridine moieties to form 2D network. In box I, π - π stacking interactions are shown by dashed red lines. In box II, DMF solvent molecules are shown by ball and stick style and packed *via* hydrogen bonding which are displayed by dashed blue lines. All hydrogen atoms except those involved in hydrogen bonds are omitted for clarity.

Figure 5. Anion... π interactions in crystal packing of $[Hg_2Cl_4L.2(DMF)]_n$ and $[Hg_2Br_4L.2(DMF)]_n$. The interactions of anion...centroid and separating distance of phenyl ring are shown by dashed lines.

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Scheme 1.



Figure 1.



(a)



(b)

Figure 2.

Crystal Growth & Design



Figure 3.



Figure 4.





	L	1	2
furmula	$C_{30}H_{34}N_4O_4S_2$	$C_{32}H_{39}Cl_4Hg_2N_6O_4$	$C_{32}H_{39}Br_4Hg_2N_6O_4$
fw	578.75	1111.64	1289.44
λ/Å	0.71073	0.71073	0.71073
<i>T</i> /°C	25	25	25
cryst. system	monoclinic	triclinic	triclinic
space group	$P2_{1}/n$	Pī	Pī
a/Å	10.1703(10)	9.8707(8)	9.9706(11)
b/Å	14.5624(19)	10.2064(8)	10.2954(12)
c/Å	10.7222(10)	11.1344(9)	11.2168(13)
α/°	90.0	72.266(6)	71.308(9)
βI°	105.410(7)	87.9069(7)	87.893(9)
γ/°	90.0	62.061(6)	63.152(8)
V/Å ³	1530.9(3)	936.34(13)	965.15(19)
$D_{\rm calc}/{\rm Mg.m^{-3}}$	1.255	1.972	2.218
Ζ	2	1	1
μ (mm ⁻¹)	0.215	8.517	12.126
<i>F</i> (000)	612	530	602
2θ (°)	52.00	58.42	52.00
<i>R</i> (int)	0.0578	0.0986	0.0450
GOOF	1.109	1.097	1.196
$R_1^a(I>2\sigma(I))$	0.0624	0.0466	0.0360
$w R_2^{b}(I > 2\sigma(I))$	0.1298	0.1108	0.0958

 Table 1. Crystal Data and Structural Refinement for Compounds L, 1 and 2

^a $R_1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|, {}^{b}wR_2 = [\Sigma (w(F_o^2 - F_c^2)^2) / \Sigma w(F_o^2)^2]^{1/2}$

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Table 2. Bond lengths [Å] and angles [°] around mercury (II) for $[Hg_2Cl_4L.2(DMF)]_n$, 1, and $[Hg_2Br_4L.2(DMF)]_n$, 2.

		Complex	
		1	2
Bond distance	Hg1-X1	2.340(2)	2.464(1)
	Hg1-X1 ^a	3.051(2)	3.163(1)
	Hg1-X2	2.319(2)	2.450(1)
	Hg1-O1 ^b	2.453(4)	2.778(5)
	Hg1-N1	2.453(4)	2.448(5)
Bond angle	X1-Hg1-X2	164.35(8)	162.64(3)
	X1-Hg1-X1 ^a	85.19(6)	87.86(3)
	X1-Hg1-O1 ^b	81.79(11)	80.83(11)
	X2-Hg1-O1 ^b	95.17(11)	93.16(11)
	X1-Hg1-N1	96.53(12)	97.76(12)
	X2-Hg1-N1	99.12(12)	99.48(12)
	N1-Hg1-O1 ^b	89.2(5)	103.3(2)
	Hg1-Õ1=C6 ^b	50.99	47.44

Symmetry codes; (a) 2–x, 1-y, 1-z, (b) 1-x, 1-y, 1-z.

Compound	D-H…A	d(D-H)	d(H···A)	$d(D \cdots A)$	<(DHA)	Symmetry code
Ligand, L	C2-H2N1	0.930	2.690	3.435(5)	138.0	-x, -y, 3-z
	C1-H1O1	0.930	2.450	3.357(3)	166.0	-x, -y, 2-z
	С3-Н3О2	0.930	2.530	3.404(3)	157.0	1-x, -y, 2-z
	C14-H14CO1	0.960	2.550	3.488(3)	166.0	-1/2x, 1/2+y, 3/2-z
	C15-H15BO1	0.960	2.629	3.488(5)	149.0	-1/2x, 1/2+y, 3/2-z
	N2-H2O2	0.86	2.000	2.851(3)	168	x, y, 1+z
$[Hg_2Cl_4L.2(DMF)]_n, 1$	N2-H2BO2	0.860	2.000	2.821(10)	158	-
$[Hg_2Br_4L.2(DMF)]_n$, 2	N2-H2BO2	0.860	2.050	2.839(11)	153	-

Table 3. Hydrogen bonding parameters (Å and °) for L, $[Hg_2Cl_4L.2(DMF)]_n$, 1 and $[Hg_2Br_4L.2(DMF)]_n$, 2.



Two coordination polymers $[Hg_2Cl_4L.2(DMF)]_n$ and $[Hg_2Br_4L.2(DMF)]_n$ where L is N,N'-(1,2-diphenylethane-1,2-diyl) diisonicotinamide ligand have been synthesized and characterized. Our results show that interplay between the coordination of carbonyl group and $\pi...\pi$ interaction of adjacent pyridine rings lead to the formation of 2D structures.