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# Supporting Information

# Hydrogen-Bonded 3D network of $d^{10}$-Metal Halide Coordination Polymer Containing *N*-(3-pyridinyl) nicotinamide: Influence of Ligand Conformation, Halide Anions and Solvent

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## Contents

## Experimental

### Mechanochemical method:

Neat grinding of 3-pna (0.04 g, 0.2 mmol) with mercury (II) chloride (0.054 g, 0.2 mmol) manually in a mortar and pestle for about 15 minutes produced a white powder in high yield. Mp 277-279 °C, IR data (KBr pellet, cm-1): 694, 803, 1053, 1121, 1290, 1333, 1427s, 1484, 1534s, 1585, 1604, 1682s, 3332. The same procedure was used for preparation of product between 3-pna and HgBr2 and powder of this compounds was isolated after grinding of 1:1 stoichiometric ratio of starting material after 15 minutes. In the case of obtained powder from reaction between L and HgBr2, Mp 268-270°C, IR data (KBr pellet, cm-1): 691, 798, 1050, 1117, 1289, 1426s, 1484, 1528s, 1590, 1683s, 3347.

### Thermal method:

In this method, mixture of 3-pna (0.04 g, 0.2 mmol) with mercury (II) chloride (0.054 g, 0.2 mmol) was heated in the oven at 110 °C for about 4 h that produced a white powder which was characterized. Mp 279-280 °C, IR data (KBr pellet, cm-1): 697, 807, 1045, 1117, 1298s, 1333, 1427s, 1482, 1537s, 1587, 1681s, 3338. Same process was performed for reaction between L and HgBr2. The resulting powder of this reaction was isolated after heating of ligand and metal salt at 110 °C for about 4 h. In the case of product prepared from reaction between 3-pna and HgBr2, Mp 268-271°C, IR data (KBr pellet, cm-1): 693, 798, 1050, 1118, 1288, 1424s, 1482, 1525s, 1585, 1681s, and 3347.

**TableS1.** Selected bond distances (Å) and angles (°) for **1-4** (M= Cd / Hg, X= halogen)

| **Compound** | | $[HgCl_2(L)]_n$ (1) | $[HgBr_2(L)]_n$ (2) | $[HgI_2(L)]_n$ .meth (3) | $[CdI_2(L)]_n$ (4) |
|---|---|---|---|---|---|
| **Bond distance** | M-X | 2.396(5) | 2.490(2) | 2.635(1) | 2.677(1) |
| | | 2.356(6) | 2.517(2) | 2.633(1) | 2.688(1) |
| | M-N | 2.363(16) | 2.408(14) | 2.500(10) | 2.275(8) |
| | | 2.315(17) [a] | 2.362(14) [b] | 2.446(11) [c] | 2.251(9) [d] |
| **Bond angle** | X-M-X | 140.3(2) | 140.9(6) | 147.1(4) | 127.2(3) |
| | N-M-N | 89.4(6) [a] | 90.3(5) [b] | 78.3(4) [c] | 99.8(3) [d] |
| | X-M-N | 99.4(4) | 107.0(3) | 101.4(3) | 105.7(2) |
| | | 108.5(4) | 100.7(3) | 101.5(3) | 111.5(2) |
| | | 109.3(4) [a] | 108.1(3) [b] | 100.8(3) [c] | 100.3(2) [d] |
| | | 98.5(4) [a] | 98.5 (3) [b] | 106.8(3) [c] | 108.5(2) [d] |

Symmetry codes: [a] 3/2-x, -1/2+y, 3/2-z. [b] 5/2-x, -1/2+y, 3/2-z. [c] 3/2-x, 1/2+y , 3/2-z. [d] 1/2-x, -1/2+y , 1/2-z.

**Table S2.** Aromatic π···π interaction parameters (Å and °) for **1-4**

| **Compound** | $\pi_{py}...\pi_{py}$ | $d_{Cg-Cg}$ | $d_{plane-plane}$ | $\alpha$ | $\gamma,\beta$ | $d_{offset}$ |
|---|---|---|---|---|---|---|
| **L** | $\pi_{py\text{-}C}\cdots\pi_{py\text{-}C}$ [a] | 3.87 | 3.49 | 0.0 | 25.8 | 1.68 |
| | $\pi_{py\text{-}N}\cdots\pi_{py\text{-}N}$ [a] | | | | | |
| **$[HgCl_2(L)]_n$(1)** | $\pi_{py\text{-}C}\cdots\pi_{py\text{-}N}$ [a] | 3.72 | 3.34, 3.44 | 4.6 | 26.3,22.2 | 1.65,1.40 |
| **$[HgBr_2(L)]_n$(2)** | $\pi_{py\text{-}C}\cdots\pi_{py\text{-}N}$ [a] | 3.82 | 3.44, 3.60 | 8.2 | 25.8,19.8 | 1.67,1.29 |
| **$[HgI_2(L)]_n$ .meth(3)** | $\pi_{py\text{-}C}\cdots\pi_{py\text{-}C}$ [b] | 3.54 | 3.37 | 0.0 | 17.8 | 1.09 |
| **$[CdI_2(L)]_n$ (4)** | $\pi_{py\text{-}C}\cdots\pi_{py\text{-}N}$ [a] | 3.89 | 3.60,3.80 | 13.5 | 22.5,12.4 | 1.49,0.84 |

Symmetry codes: [a] -1+x, y, z. [b] 2-x, -y, 1-z.

**Table S3.** Dihedral angles of Py-C, Py-N rings and amide plane in **1-4**

| **Compound** | < Py-C and Amide plane (°) | <Py-N and Amide plane(°) | <Py-N and Py-C(°) |
|---|---|---|---|
| **L** | 19.3(1) | 4.2 (1) | 22.4(8) |
| **$[HgCl_2(L)]_n$(1)** | 29.9(1) | 32.7(1) | 4.6(6) |
| **$[HgBr_2(L)]_n$(2)** | 26.7(7) | 28. 2(9) | 8.2(5) |
| **$[HgI_2(L)]_n$ .meth(3)** | 6.3(8) | 44.2(6) | 38.1(3) |
| **$[CdI_2(L)]_n$ (4)** | 30.3(4) | 31.5(7) | 13.5(3) |

**TableS4.** Results of Cambridge Structural Database (CSD) analysis of complexes containing 3-pna ligand

| NO. | Refcode | Compounds | Coligand | Conformation 3-pna | Amide Synthon | Guest Mol. | Geometry coordination | Architecture | Ref. |
|---|---|---|---|---|---|---|---|---|---|
| 1 | EVOKUX | [Ni(3-pna)(mip)]·$H_2O$ | H2mip = 5-methylisophthalic acid] | Anti | $D_1^1(2)$ NH…O ($H_2O$) | $H_2O$ | distorted octahedral | 2D networks, ladder-like double chains. | 1 |
| 2 | EVOLAE | [Ni(3-pna)(mip)($H_2O$)]·4$H_2$ | H2mip = 5-methylisophthalic acid] | Anti | $R_2^2(18)$ NH…O (mip) | $H_2O$ | distorted octahedral | 2D, 4-connected grid structure consisting of 1D $[Ni\text{-}3\text{-}pna]_n$ and $[Ni\text{-}mip]_n$ chains. | 1 |
| 3 | EVOLEI | [Cd2(3pna)(mip)2(H2O)]·2H2O | H2mip = 5-methylisophthalic acid] | Anti | $D_1^1(2)$ NH… O ($H_2O$) | $H_2O$ | distorted pentagonal bipyramidal | 3D framework constructed from $Cd_4(COO)_4$ subunits and $\mu^2$-bridging 3-pna. | 1 |
| 4 | EVOLIM | [Cd(3-pna)(mip)]2·3H2O | H2mip = 5-methylisophthalic acid] | Anti | - | $H_2O$ | distorted octahedral | 2D networks, ladder-like double chains | 1 |
| 5 | EVOLOS | [Co(3-pna)(mip)]·H2O | H2mip = 5-methylisophthalic acid] | Anti | $D_1^1(2)$ NH… O ($H_2O$) | $H_2O$ | distorted octahedral | 2D networks, ladder-like double chains. | 1 |
| 6 | AVUBAU | [$Co(NO_3)_2$(3-pna)2]*n* | - | Syn | $C_1^1(4)$ NH… O (3-pna) | - | octahedral | honeycomb-shaped grid | 2 |
| 7 | AVUBEY | [CoBr2(3-pna)2]*n* | - | Syn | - | - | distorted octahedral | Honeycomb-shaped grid. | 2 |
| 8 | BIPCIO | {[Zn(H3-pna)(sip)].1.5H2O}n | metal 5-sulfoisophthalate (sip) | Syn | $D_1^1(2)$ NH… O ($H_2O$) | $H_2O$ | A slightly distorted tetrahedral | 3-connected 1D ladder structure. | 3 |
| 9 | BIPCUA | {[Cd3(3pna)2(sip)2($H_2O$)$_6$].2H2O}n | metal 5-sulfoisophthalate (sip) | Syn | $C_1^1(17)$ NH…O (sip) | $H_2O$ | distorted pentagonal bipyramid/ octahedron | 2D network topology, ladder motifs | 3 |
| 10 | CICSAK | [Cd(D-cam)(3-pna)($H_2O$)$_2$]n | D-camphoric acid (H2D-cam) | Syn | - | - | Octahedral | 1-D coordination polymer chain structure. | 4 |
| 11 | DOLSEE | [Cu(ip)(3-pna)]*n* | ip = isophthalate | Anti | - | - | distorted square pyramidal | (4,4) layered grid structure based on $\{Cu_2(OCO)_2\}$ dimeric units. | 5 |
| 12 | FIGQOD | {[Cu(glu)(3-pna)($H_2O$)].$H_2O$}n | glu = glutarate, | Syn | $D_1^1(2)$ NH… O ($H_2O$) | $H_2O$ | distorted octahedron | Simple (4,4) grid-like layer structure. | 6 |
| 13 | FUHPIJ | {[Cu(adp)(3-pna)].2.5$H_2O$}n | adipic acid (H2adp) | Anti | $D_1^1(2)$ NH… O ($H_2O$) | $H_2O$ | square pyramidal | Dimer-based 3-D network | 7 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 14 | GOBTUO | $[Cu_2(pyro)(pyroH_2)(3pnaH)_2(H_2O)_2]n$ | Pyro = 1,2,4,5-benzenetetracarboxylate | Syn | $C_1^1(10)$ NH… O (pyro) | - | distorted octahedral | 2-D coordination polymer built from $\{Cu_2O_2 (OCO)_2\}$ dimeric units. | 8 |
| 15 | GOCSOI | $\{[Cu(pyro)(3\text{-}pnaH)_2(H_2O)_2].4H_2O\}n$ | Pyro = 1,2,4,5-benzenetetracarboxylate | Anti | $C_1^1(14)$ NH…O (Pyro) | $H_2O$ | distorted octahedral | Simple neutral 1-D chain polymer. | 8 |
| 16 | IMEXAB | $[Zn_2(2,4\text{-}pdc)_2(H_2O)_4(3pna)].3H_2O\}n$ | 2,4-pyridinedicarboxylic acid (2,4-pdcH2) | Anti | $D_1^1(2)$ NH…O ($H_2O$) | $H_2O$ | octahedral | Two-fold parallel interpenetrated herring bone layer net. | 9 |
| 17 | JAFDEC | [Co(L)(ADTZ)]·H2O | H2ADTZ=2,5-(s-acetic acid)dimercapto-1,3,4-thiadiazole] | Anti | $D_1^1(2)$ NH…O ($H_2O$) | $H_2O$ | distorted octahedral geometry | 2D double-layer networks based on 1D $[M\text{-}L]_n$ zigzag chains and 1D $[M\text{-}ADTZ]_{2n}$ double-chains. | 10 |
| 18 | PADLAK | [Cd(L)(ADTZ)]·H2O | H2ADTZ=2,5-(s-acetic acid)dimercapto-1,3,4-thiadiazole] | Anti | $C_1^1(17)$ NH…O (ADTZ) | $H_2O$ | distorted octahedral geometry | 2D double-layer networks based on 1D [M-L]*n* zigzag chains and 1D [M-ADTZ]2*n* double-chains | 10 |
| 19 | PADLEO | [Zn(L)(ADTZ)]·H2O | H2ADTZ=2,5-(s-acetic acid)dimercapto-1,3,4-thiadiazole] | Anti | $D_1^1(2)$ NH…O ($H_2O$) | $H_2O$ | distorted octahedral geometry | 2D double-layer networks based on 1D [M-L]*n* zigzag chains and 1D [M-ADTZ]2*n* double-chains. | 10 |
| 20 | KIJWUX | [Cd(suc)(3-pna)·2.5H2O]n | succinic acid (H2suc) | Syn | $D_1^1(2)$ NH…O ($H_2O$) | $H_2O$ | distorted pentagonal bipyramidal | simple 3-D non-interpenetrated network | 11 |
| 21 | KIJWUX01 | [Cd(suc)(3-pna)·2.5H2O]n | succinic acid (H2suc) | Syn | $D_1^1(2)$ NH…O ($H_2O$) | $H_2O$ | distorted pentagonal bipyramid | simple 3-D non-interpenetrated network | 11 |
| 22 | MOVPUI | $\{[Co(NCS)_2 (3\text{-}pna)_2]n\}$ | - | Anti | - | - | octahedral | 2D sheet composed of a nearly square grid. | 12 |
| 23 | MULQOB | [Co(tpdc)(3-pna)]n | 2,5-thiophenedicarboxylic acid (H2tpdc). | Anti | - | - | distorted trigonal bipyramidal | 2-D layer structure containing $\{Co_2 (OCO)_2\}$ dimers linked by tpdc and 3-pna ligands. | 13 |
| 24 | MULQUH | [Co(D-cam)(3-pna)(H2O)2]n | chiral D-camphorate (D-cam) | Syn | - | - | distorted octahedron | Acentric ribbon coordination polymer motifs. | 13 |
| 25 | MULRAO | [Ni(D-cam)(3-pna)(H2O)2]n | chiral D-camphorate (D-cam) | Syn | - | - | distorted octahedron | Acentric ribbon coordination polymer motifs. | 13 |
| 26 | PORXIF | $\{[Cd(msuc)(3\text{-}pna)]\cdot 2H2O\}n$ | (msuc = 2-methylsuccinate) | Anti | $D_1^1(2)$ NH…O ($H_2O$) | $H_2O$ | distorted pentagonal bipyramidal | Layer motifs that contain {Cd2 (OCO)2} dimeric units, linked into a non-interpenetrated 3D network. | 14 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 27 | PORXOL | [Cd2(dmsuc)2(3-pna)2]·1.5H2O}*n* | (dmsuc = 2,2-dimethylsuccinate) | Anti | $S_1^1(10)$ NH…O (dmsuc) | $H_2O$ | distorted octahedral coordination | 1D [Cd(dmsuc)]$_n$ ribbons containing{$Cd_2O_2$} dimeric units. | 14 |
| 28 | QISYEY | {[Zn2(hmph)2(3-pna)]·H2O}*n* | hmph = homophthalate | Syn | $D_1^1(2)$ NH… O ($H_2O$) | $H_2O$ | distorted square-pyramidal / distorted tetrahedral | (4,4) grid coordination polymer layers. | 15 |
| 29 | QIYHAJ | {[Zn(tere)(3-pna)$_2$ ($H_2O$)$_2$].2$H_2O$}n | potassium terephthalate (K2tere) | Syn | $D_1^1(2)$ NH…O ($H_2O$) | $H_2O$ | octahedral | 1-D coordination polymer chains. | 16 |
| 30 | QIXWUR | {[Zn(tere)(3-pna)] .3$H_2O$}n | potassium terephthalate (K2tere) | Syn | $D_1^1(2)$ NH… O ($H_2O$) | $H_2O$ | pseudo-tetrahedral | 2-D (6,3) hexagonal grid topology | 16 |
| 31 | SIXTUP | [{(CH3COO)(μ–OOCH3)Zn}$_2$( 3-pna )$_2$]n | - | Anti | - | - | slightly distorted trigonal bipyramidal | 1-D zigzag polymeric chain / ladder type architecture. | 17 |
| 32 | SIXVAX | [{($H_2O$)$_2$Zn}( 3-pna )$_4$}$BF_4$]n | - | Syn | $C_1^1(9)$ O…HO(coordinated $H_2O$) | $BF_4$ | slightly distorted octahedral | 2-D nonporous corrugated sheet. | 17 |
| 33 | SIXVEB | [{($Cl$)$_2$Zn}( 3-pna )]n | - | Anti | $R_2^2(14)$ NH…Cl | - | distorted tetrahedral | 1-D zigzag coordination polymeric chain. | 17 |
| 34 | SIXVOL | [{($NO_3$)$_2$Cd( 3-pna )$_2$} .nitrobenzene]n | - | Anti | - | Ph-NO2 | slightly distorted octahedral | 2-D grid architecture 2-D porous sheet. | 17 |
| 35 | VIGYUH | [Cu(t-14cdc)(3-pna)]n | (t-14cdc) = trans1,4-cyclohexanedicarboxylate | Anti | $C_1^1(9)$ NH… O (t-14cdc) | - | Jahn–Teller distorted square pyramidal | Non-interpenetrated 3-D coordination polymer network | 18 |
| 36 | VIPTIY | [{($H_2O$)4Co( 3-pna)$_2$}. fumarate.2$H_2O$]n | - | Syn | $C_1^1(9)$ O…HO(coordinated $H_2O$) | $H_2O$ fumarate | slightly distorted octahedral | 1-D zigzag polymeric chain. | 19 |
| 37 | VIPTOE | [{($H_2O$)3( μ -fumarate)Co( μ -L1)$_2$}.fumarate.2$H_2O$]n | L1= 3-pna | Anti | $D_1^1(2)$ NH… O (fumarate) | $H_2O$ fumarate | slightly distorted octahedral | ladder type 1-D polymeric network. | 19 |
| 38 | WIZMUP | [CuMoO4(3-pna)]*n* | MoO4 | Anti | $R_2^2(18)$ NH…O (MoO4 ) | - | distorted square pyramid/ | 2-D [CuMoO4(3- pna)]*n* coordination polymer | 20 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | distorted tetrahedron | | |
| 39 | WUDGUZ | [Zn(ip)(3-pna)]n | ip= isophthalate | Anti | - | - | distorted trigonal bipyramidal | Dimer-based 3,5-connected layer motif | 21 |
| 40 | WUDHAG | {[Zn(mip)(3-pna)].2H2O}n | mip = 5-methylisophthalate | Syn | $D_1^1(2)$ NH… O ($H_2O$) | $H_2O$ | distorted tetrahedral | 4-connected 1-D ribbon Motif. | 21 |
| 41 | XAFBUD | [{Cd(3-pna )(μ3- SO4)(H2O)}. 2H2O] | - | Anti | $S_1^1(10)$ NH…O (μ3SO4) | $H_2O$ | slightly distorted octahedral | 2D coordination polymer | 22 |
| 42 | XIFJAZ | {[Cd2(adp)(nic)2(3-pna)2] .6H2O}n | H2adp = adipic acid nic = nicotinate | Syn | $D_1^1(2)$ NH…O ($H_2O$) | $H_2O$ | pentagonal bipyramidally | 3-D network 3-D coordination polymer | 23 |

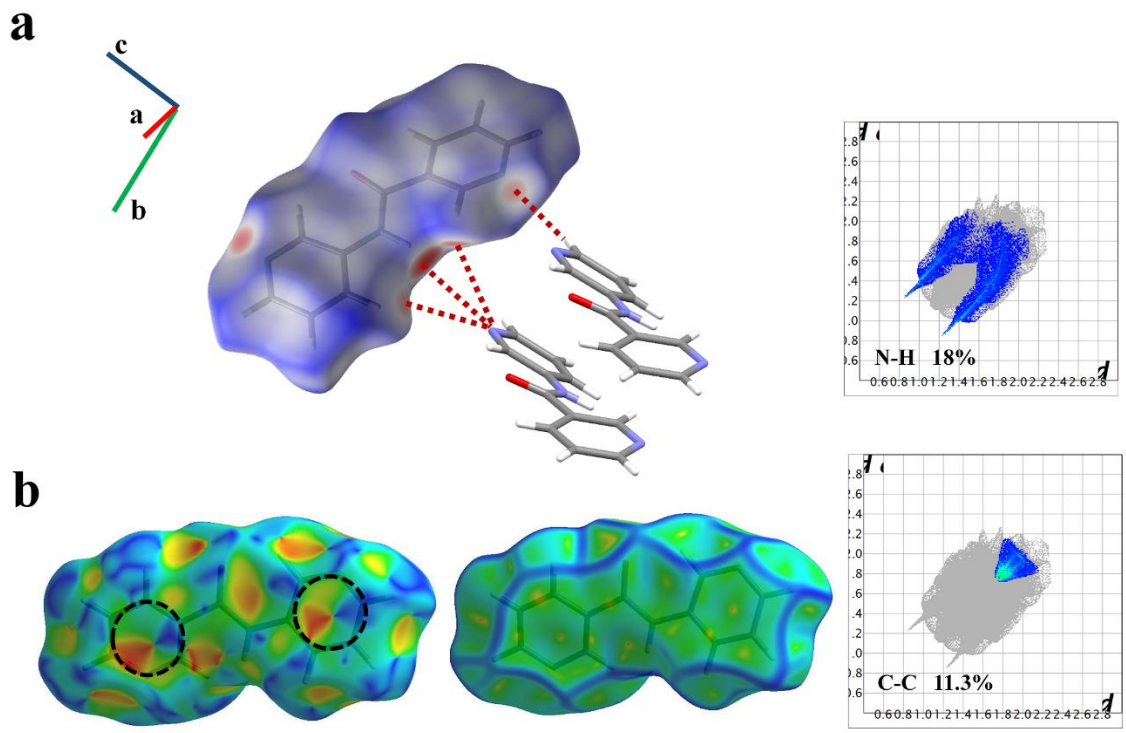


**Fig. S1** Hirshfeld surface mapped with $d_{norm}$ (top, left), decomposed fingerprint plot for compound L (top, right), showing (a) NH···N and CH···N hydrogen bonds and Hirshfeld surfaces mapped with shape index (red and blue triangles has been shown by black circle), curvedness and decomposed finger print plots to C-C contacts (bottom, left to right) showing relative contribution of π···π stacking interactions for compound L.

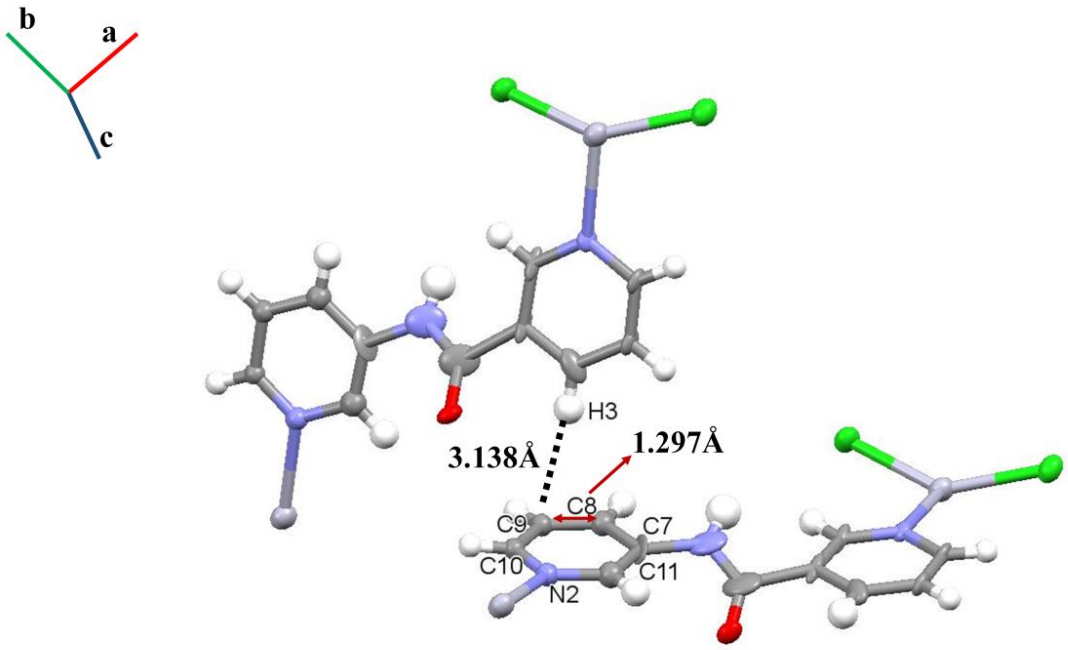


**Fig. S2** Representation of CH…π interaction in compound 1, showing nearest bonds to CH group.

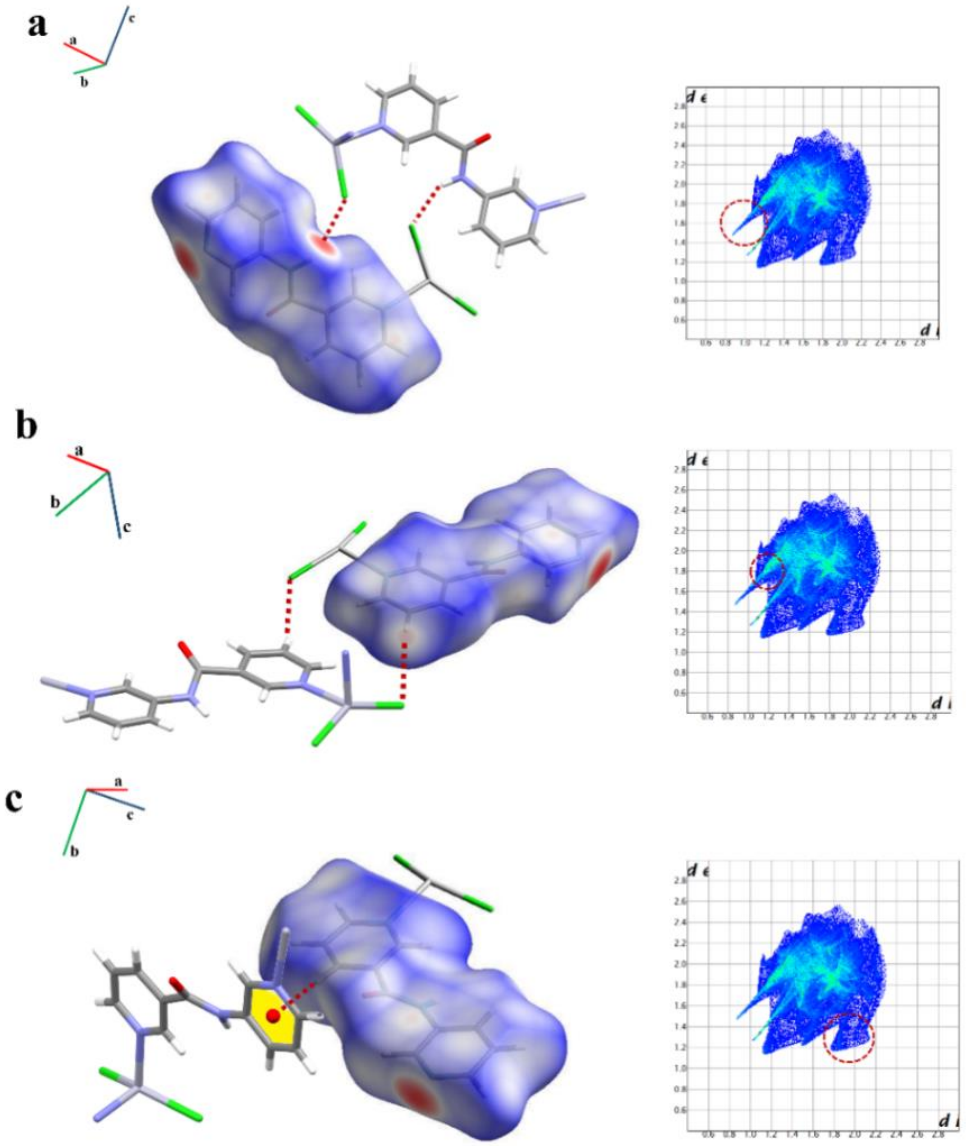


**Fig. S3** Hirshfeld surface mapped with $d_{norm}$ (left) and two-dimensional fingerprint plot for compound 1, showing (a) N-H…Cl, (b) C-H…Cl and (c) CH…π hydrogen bonds.

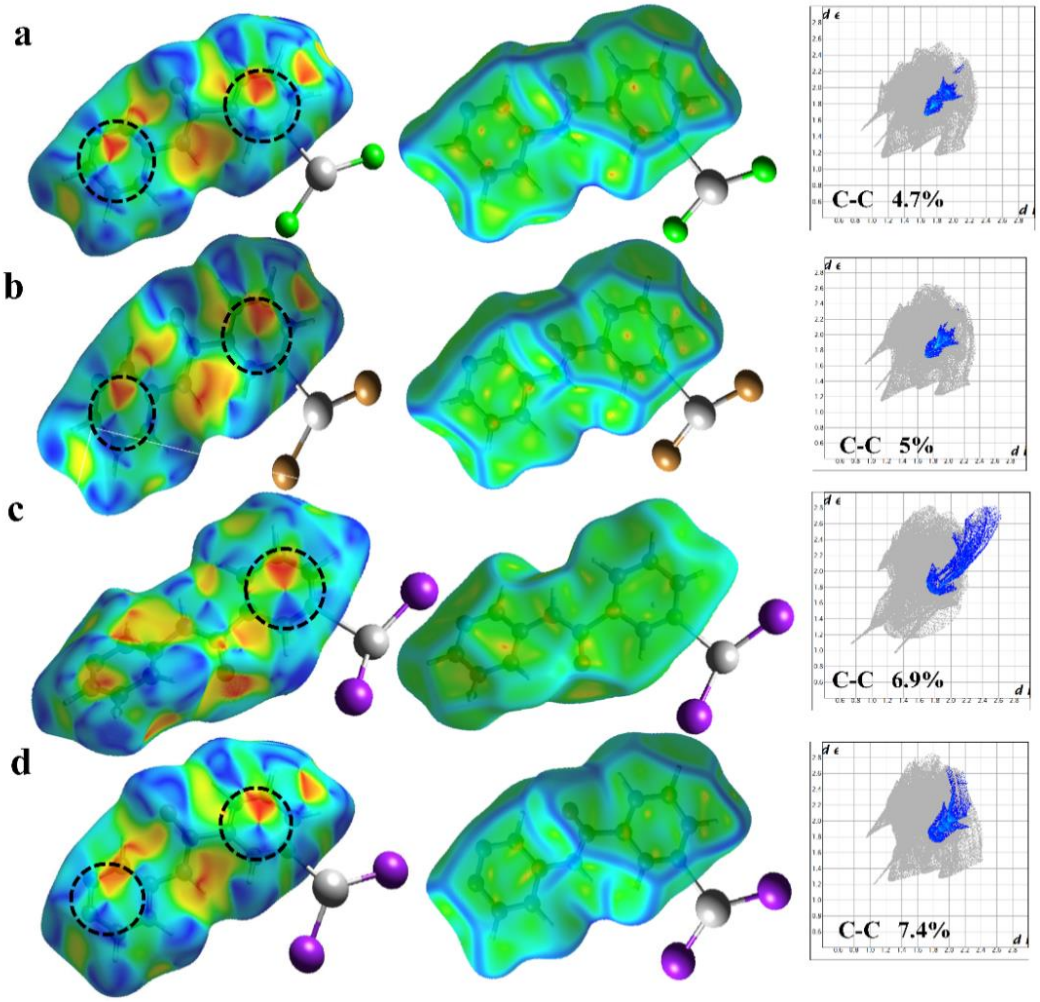


**Fig. S4** Hirshfeld surfaces mapped with shape index (red and blue triangles has been shown by black circle), curvedness and decomposed finger print plots to C-C contacts showing relative contribution of π···π stacking interactions for compound 1(a), 2(b),3(c) and4(d) (left to right).

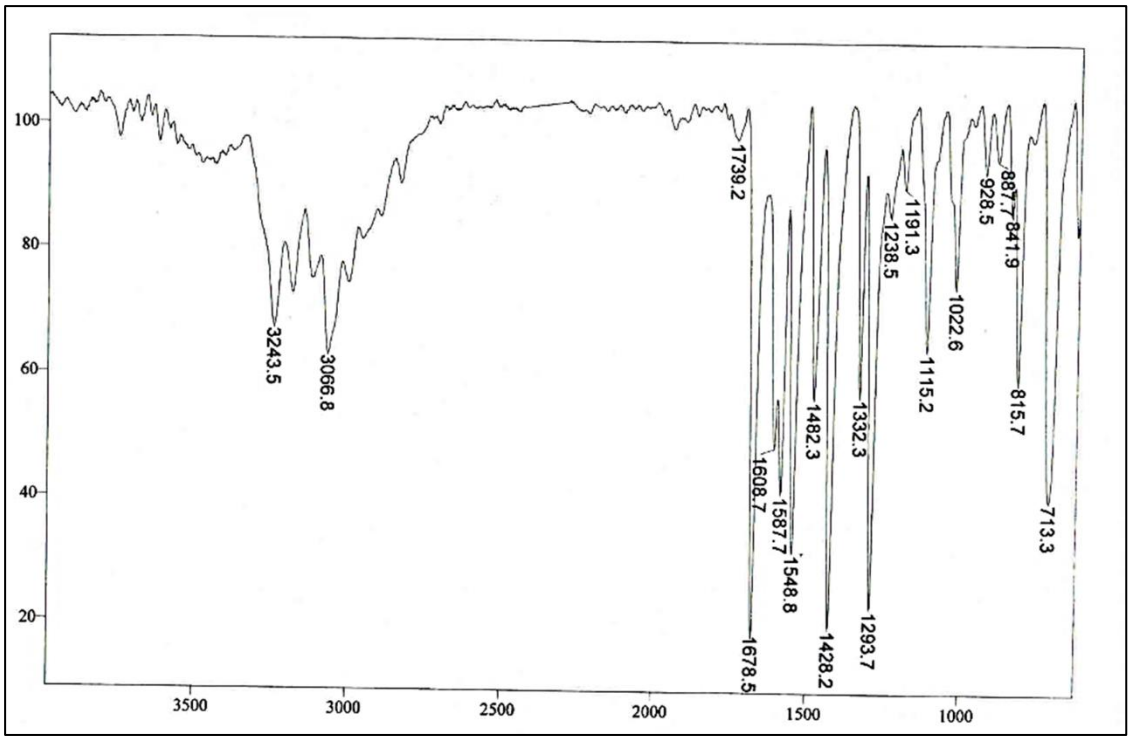


**Fig. S5** IR Spectrum of ligand

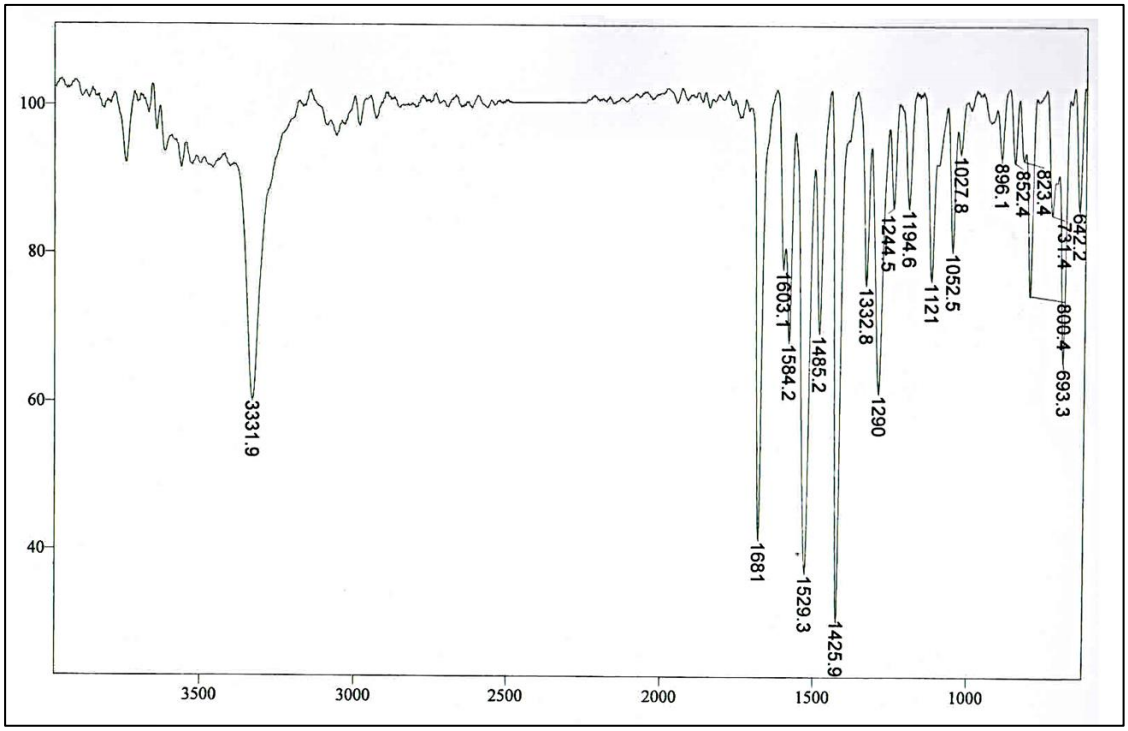


**Fig. S6** IR Spectrum of compound 1 (solution-method)

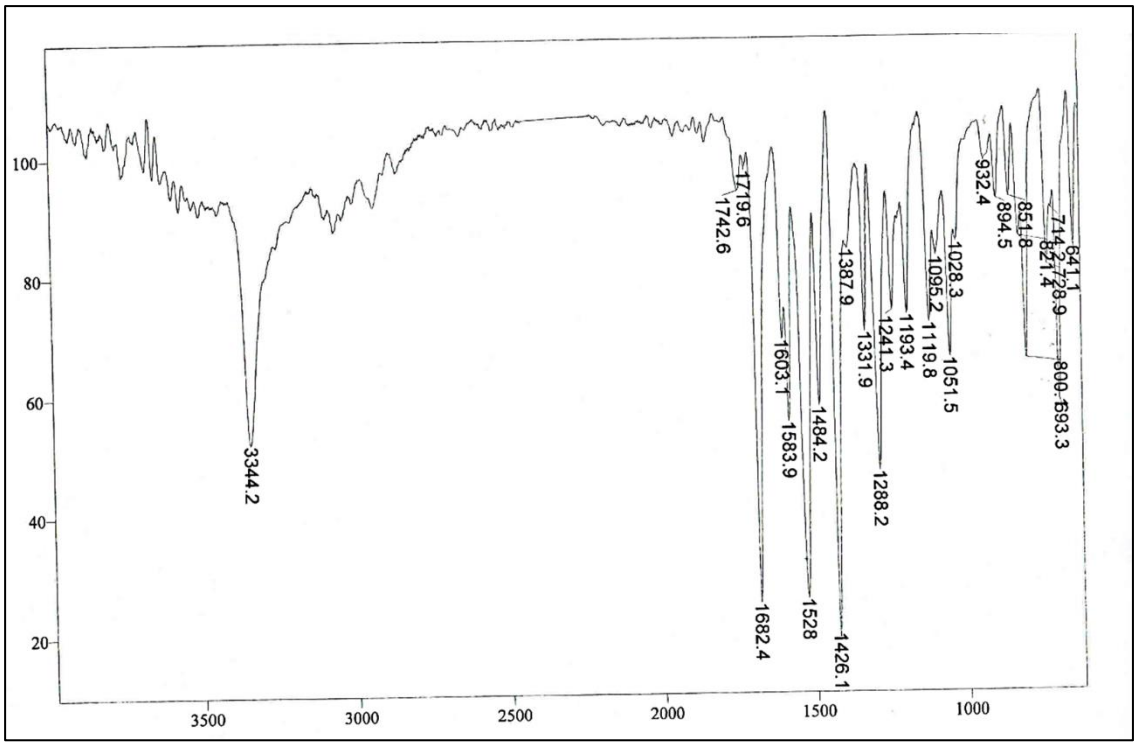


**Fig. S7** IR Spectrum of compound 2 (solution-method)

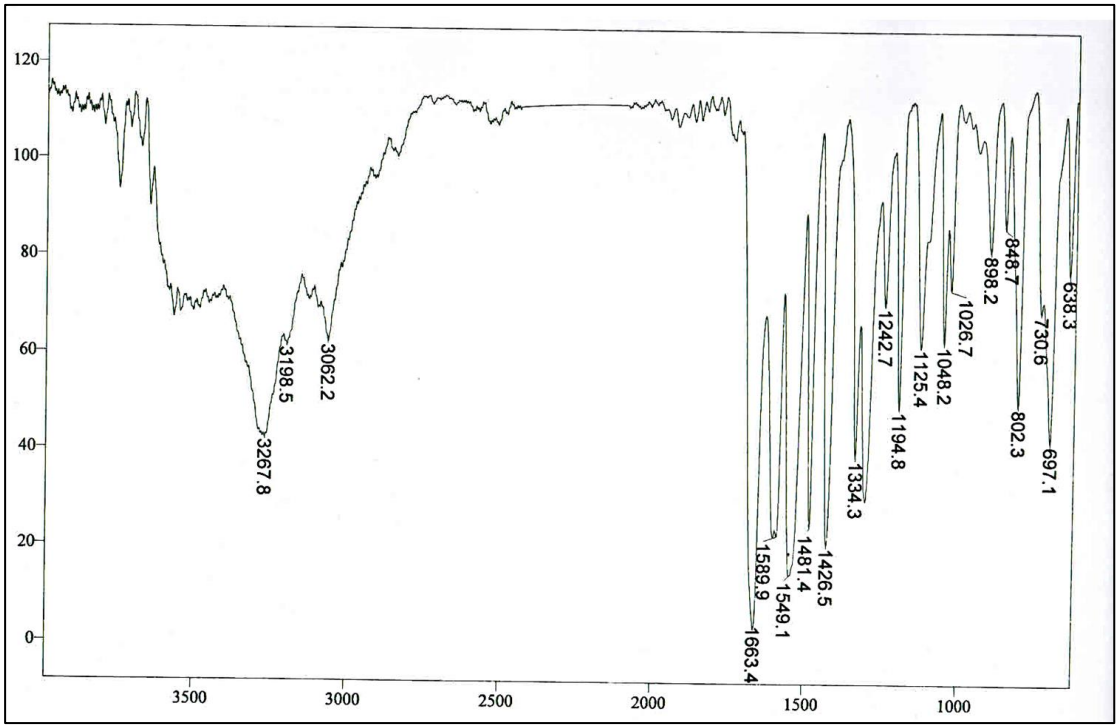


**Fig. S8** IR Spectrum of compound 3 (solution-method)

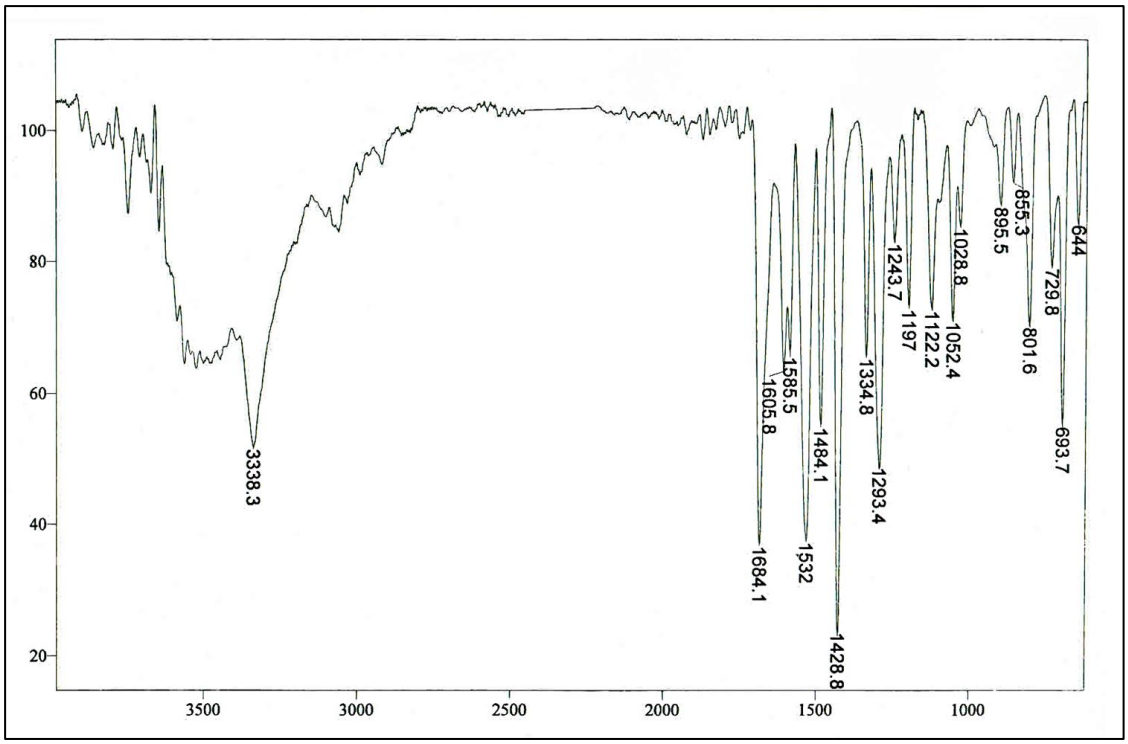


**Fig. S9** IR Spectrum of compound 4 (solution-method)

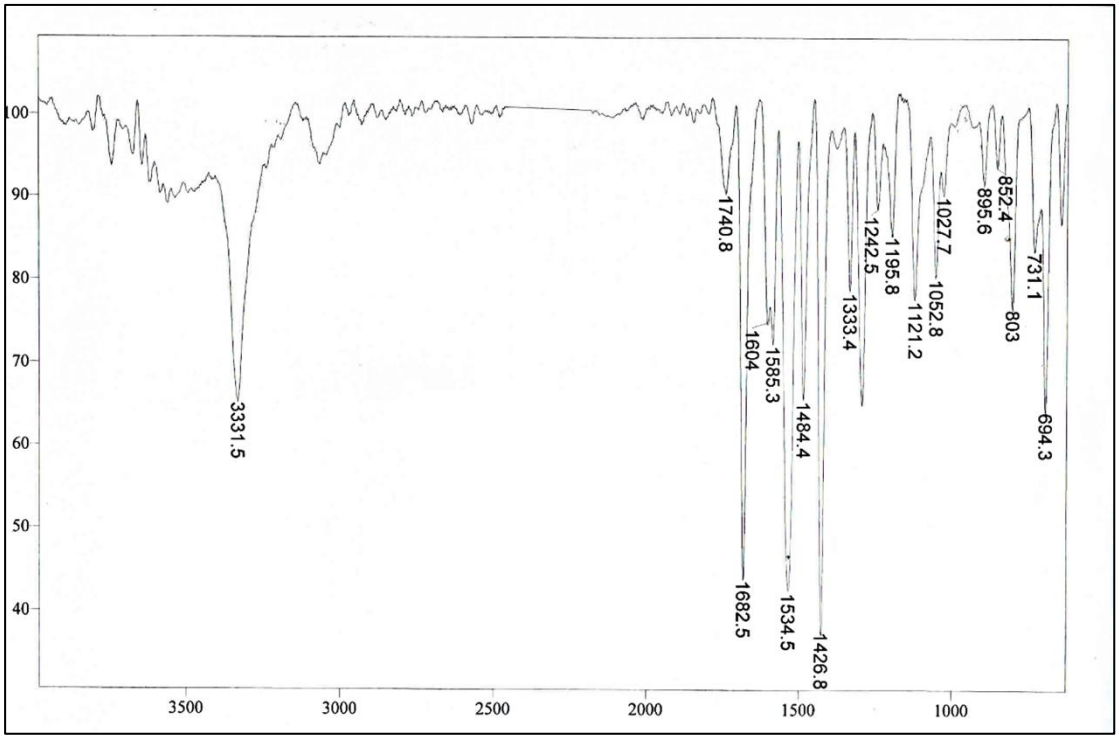


**Fig. S10** IR Spectrum of compound 1 (Grinding method)

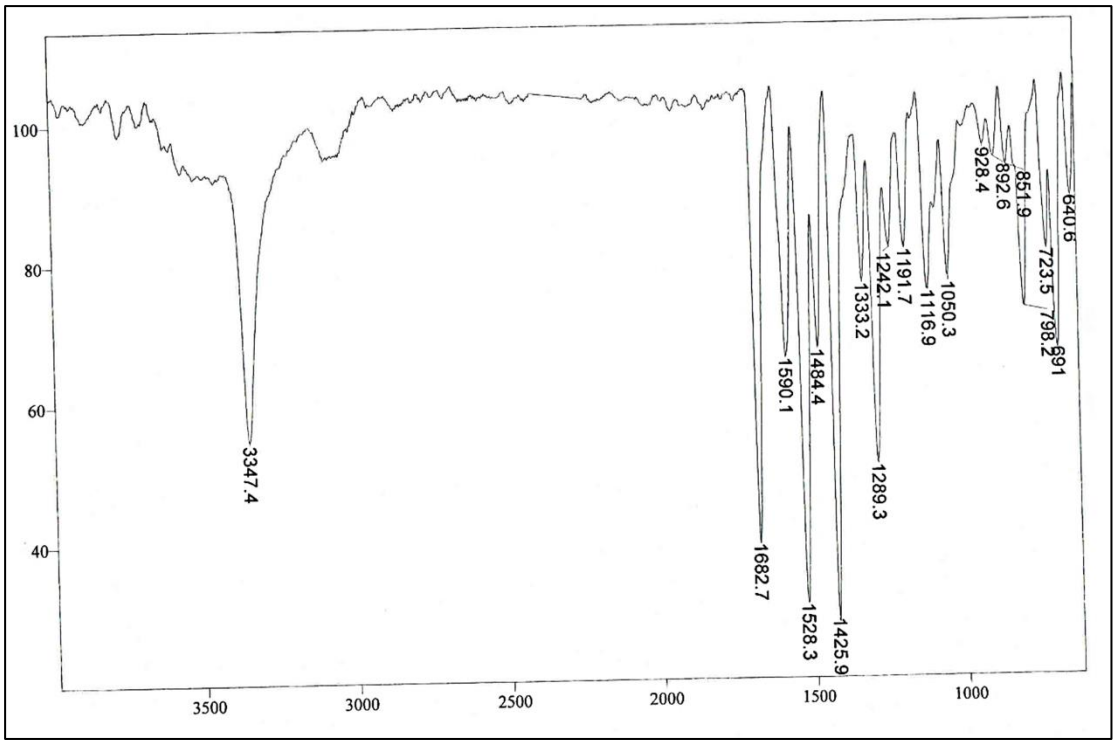


**Fig. S11** IR Spectrum of compound 2 (Grinding method)

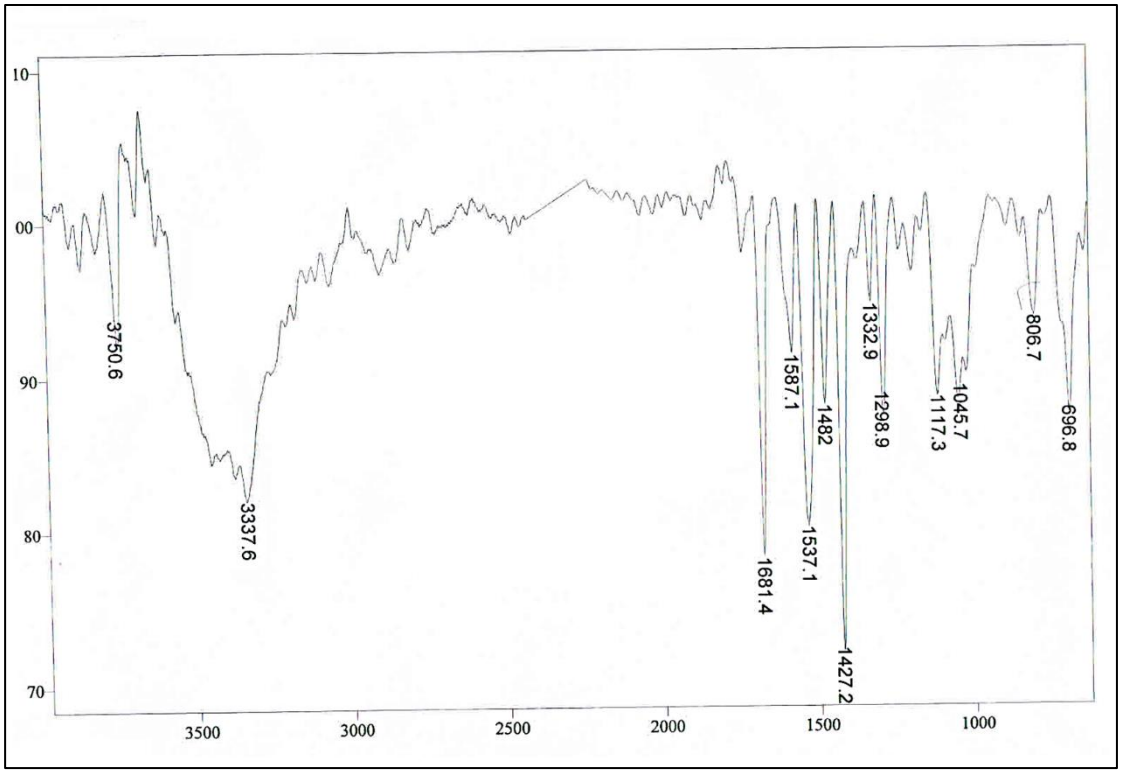


**Fig. S12** IR Spectrum of compound 1 (Thermal method)

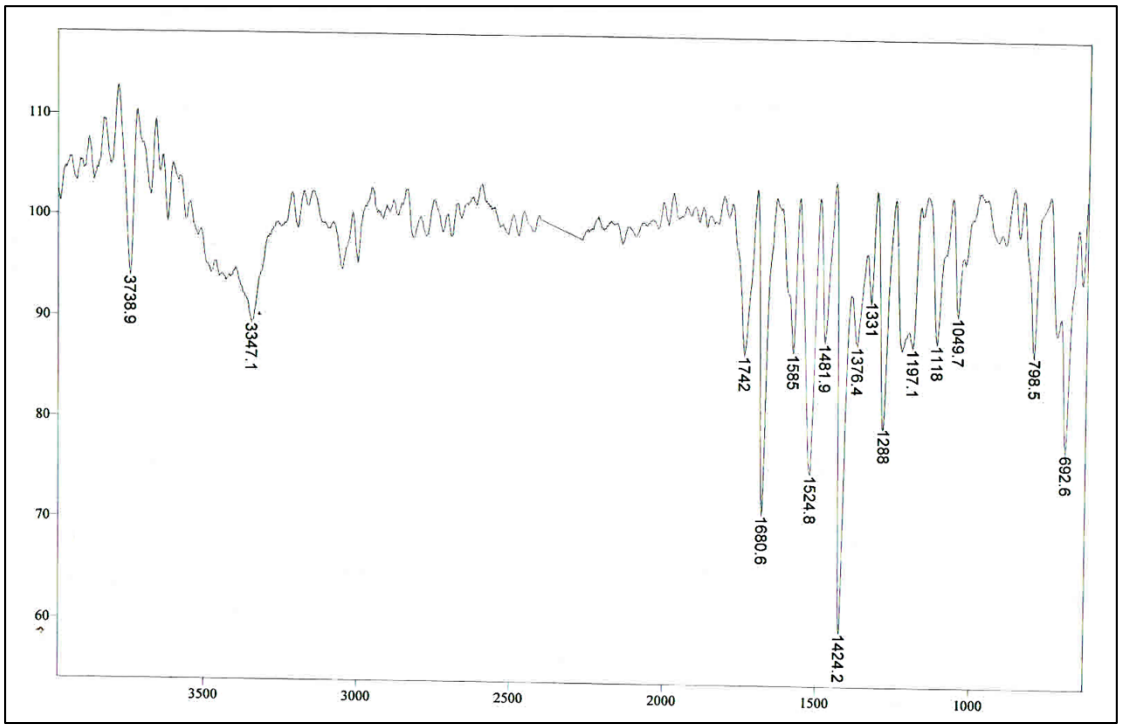


**Fig. S13** IR Spectrum of compound 2 (Thermal method)

## References

(1) Wang, X. L.; Xiong, Y.; Liu, G. C.; Lin, H. Yan.; Sha, X. T.; Shao, J. Y. *Polyhedron.* **2016**, 119, 590-596.

(2) Uemura, K.; Kitagawa, S.; Fukui, K.; Saito, K. *J. Am. Chem. Soc.* **2004**, 126, 3817-3828.

(3) Kraft, P. E.; Mizzi, J. E.; LaDuca, R. L. *Inorg. Chim. Acta*. **2014**, 409, 449-457.

(4) Wilson, J. A.; LaDuca, R. L. *Inorg. Chim. Acta*. **2013**, 403, 136-141.

(5) ODonovan, M. E.; Porta, A. R.; Torres Salgado, M. D.; LaDuca, R. L. *Z. Anorg. Allg. Chem*. **2014**, 640, 2113-2122.

(6) Uebler, J. W.; Pochodylo, A. L.; LaDuca, R. L. *Inorg. Chim. Acta*. **2013**, 405, 31-42.

(7) Pochodylo, A. L.; Wilson, J. A.; Uebler, J. W.; Qiblawi, S. H.; LaDuca, R. L. *Inorg. Chim. Acta*. **2014**, 423, 298-306.

(8) Mizzi, J. E.; LaDuca, R. L. *Inorg. Chim. Acta*. **2014**, 411, 188-198.

(9) Wudkewych, M. J.; LaDuca, R. L. *J. Mol.Struct.* **2016**, 1120, 156-162.

(10) Wang X.; Chunhua, G.; Yun, Q.; Guocheng, L.; Juwen, Z. *Chem. Res. Chin. Univ*. **2014**, 30, 709-714.

(11) Uebler, J. W.; Pochodylo, A. L.; Staples, R. J.; LaDuca, R. L. *Cryst. Growth Des.* **2013**, 13, 2220-2232.

(12) Uemura, K.; Kitagawa, S.; Kondo, M.; Fukui, K.; Kitaura, R.; Chang, H. C.; Mizutani, T. *Chem. Eur. J.* **2002**, 8, 3586-3600.

(13) Torres Salgado, M. D.; Bouchey, C. J.; Wilson, J. A.; LaDuca, R. L. *J. Coord. Chem.* **2015**, 68, 2029-2040.

(14) Spies, H. J.; LaDuca**,** R. L.; *Z. Anorg. Allg. Chem.* **2014**, 640, 1930-1936.

(15) Murray, N. H.; Farnum, G. A.; LaDuca, R. L.; Z. *Anorg. Allg. Chem.* **2013**, 639, 2162-2170.

(16) Goldsworthy, J. S.; Staples, R. J.; LaDuca, R. L. *J. Mol. Struct.* **2014**, 1062, 116-124.

(17) Kumar, D. K.; Das, A.; Dastidar, P. *CrystEngComm*. **2007**, 9, 548-555.

(18) Qiblawi, S. H.; Pochodylo, A. L.; LaDuca, R. L. *CrystEngComm*. **2013**, 15, 8979-8988.

(19) Kumar, D. K.; Das, A.; Dastidar, P. *CrystEngComm*. **2007**, 9, 895-901.

(20) Qiblawi, S. H.; LaDuca, R. L. *Inorg. Chim. Acta*. **2014**, 413, 115.120.

(21) Kraft, P. E.; Weingartz, A. L.; LaDuca, R. L. *Inorg. Chim. Acta*. **2015**, 432, 283-288.

(22) Banerjee, S.; Adarsh, N. N.; Dastidar, P. *Eur. J .Inorg. Chem.* **2010**, 24, 3770-3779.

(23) Wilson, J. A.; Uebler, J. W.; LaDuca, R. L. *CrystEngComm*. **2013**, 15, 5218-5225.