Electronic Supplementary Information

Positional Isomeric Effect on Structural Variation of Cd(II) Coordination Polymers Based on Flexible Linear/V-Shaped Bipyridyl Benzene Ligands

Lei-Lei Liu,*[a] Cai-Xia Yu,[a] Ya-Ru Li,[a] Jing-Jing Han,[a] Feng-Ji Ma[a] and Lu-Fang Ma*[b]

[a] *College of Chemistry and Chemical Engineering, Anyang Normal University, Anyang 455000, Henan, P. R. China*

[b] *College of Chemistry and Chemical Engineering, Luoyang Normal University, Luoyang 471022, Henan, P. R. China*

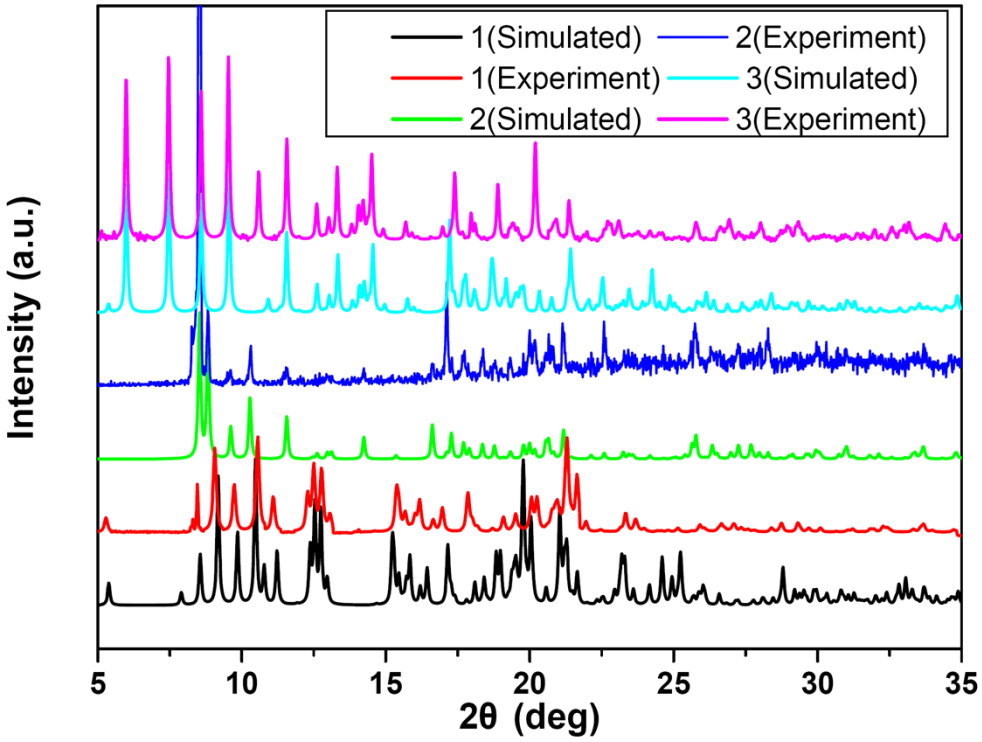


Figure S1. Experimental and simulated PXRD patterns for **1**−**3**. The obtained PXRD signals of the compound **1** had a little shifts comparing with the simulated one maybe due to preferred orientation of the crystals.

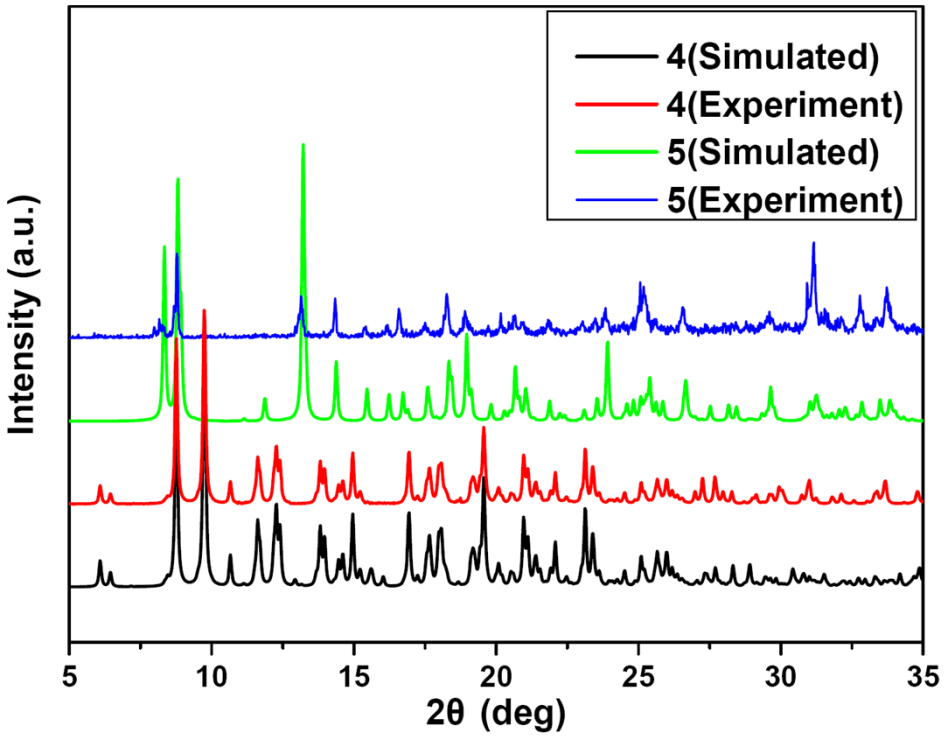


Figure S2. Experimental and simulated PXRD patterns for **4**−**5**.

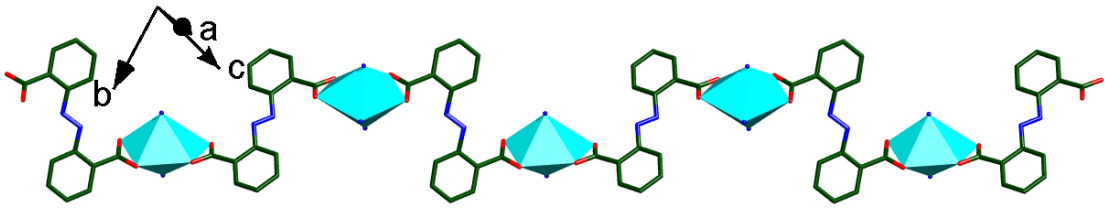
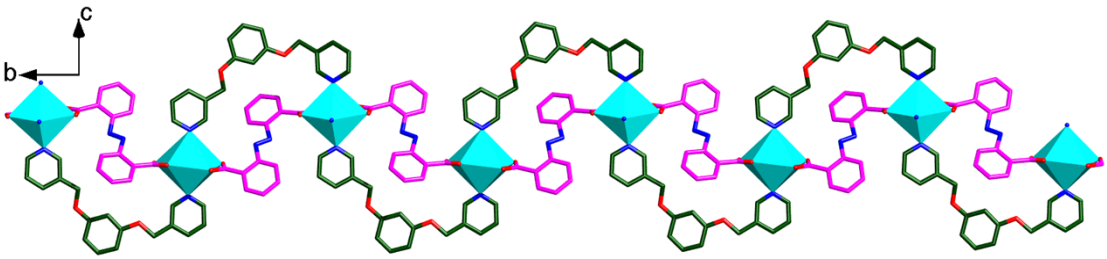
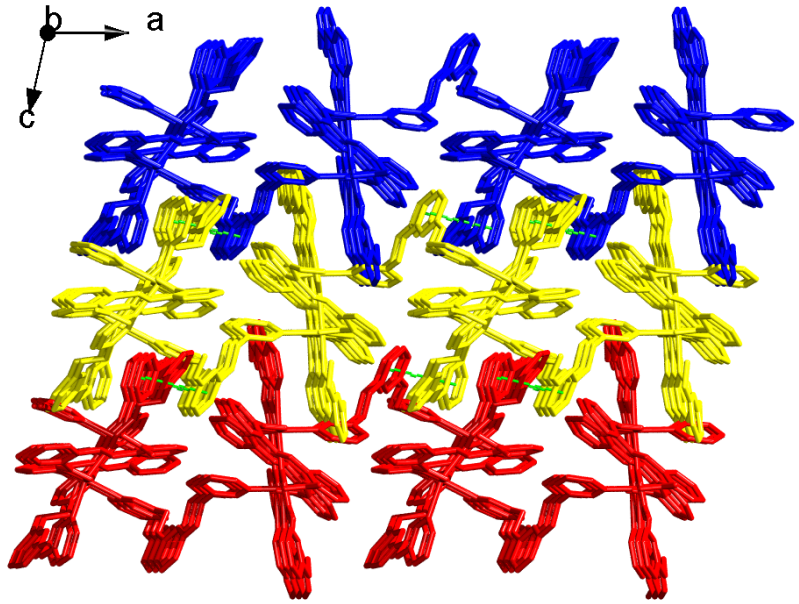


Figure S3. View of the 1D $[CdL]_n$ chain of **3**.

(a)



(b)



(c)

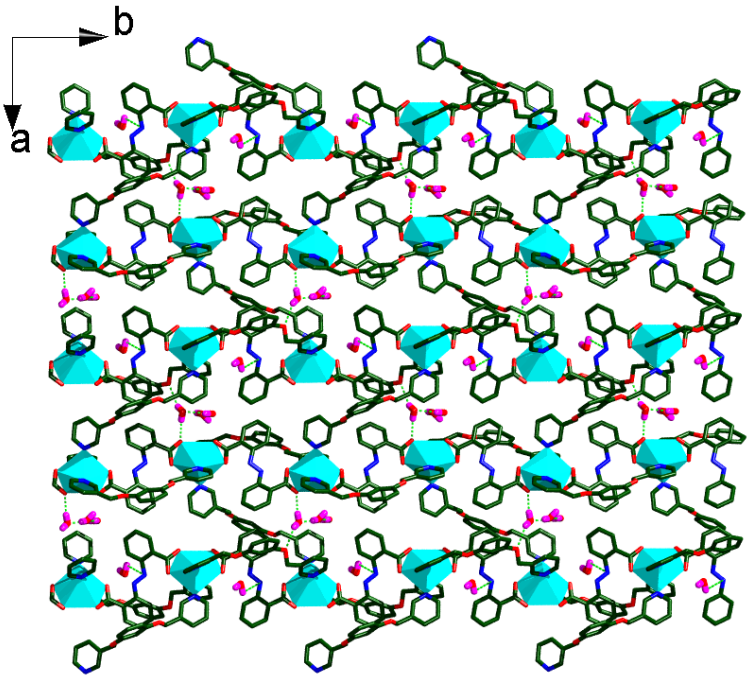


Figure S4. (a) View of the 1D chain of **4** extending along the *b* axis. (b) View of a 3D supramolecular structure in **4** looking down the *b* axis, formed *via* π–π stacking interactions. Green dashed lines represent the π–π interactions. (c) View of a 2D network in **4** extending along the *ab* plane. Green dashed lines represent the hydrogen-bonded interactions.

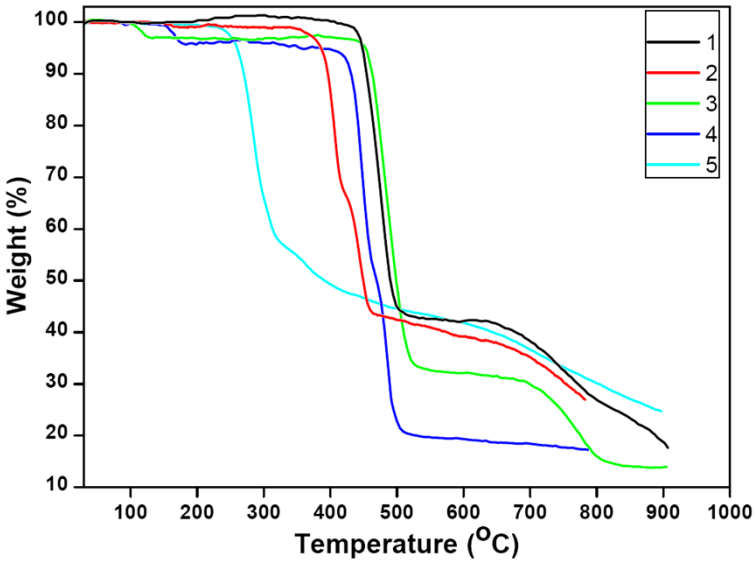


Figure S5. The TGA curves for **1**−**5**.

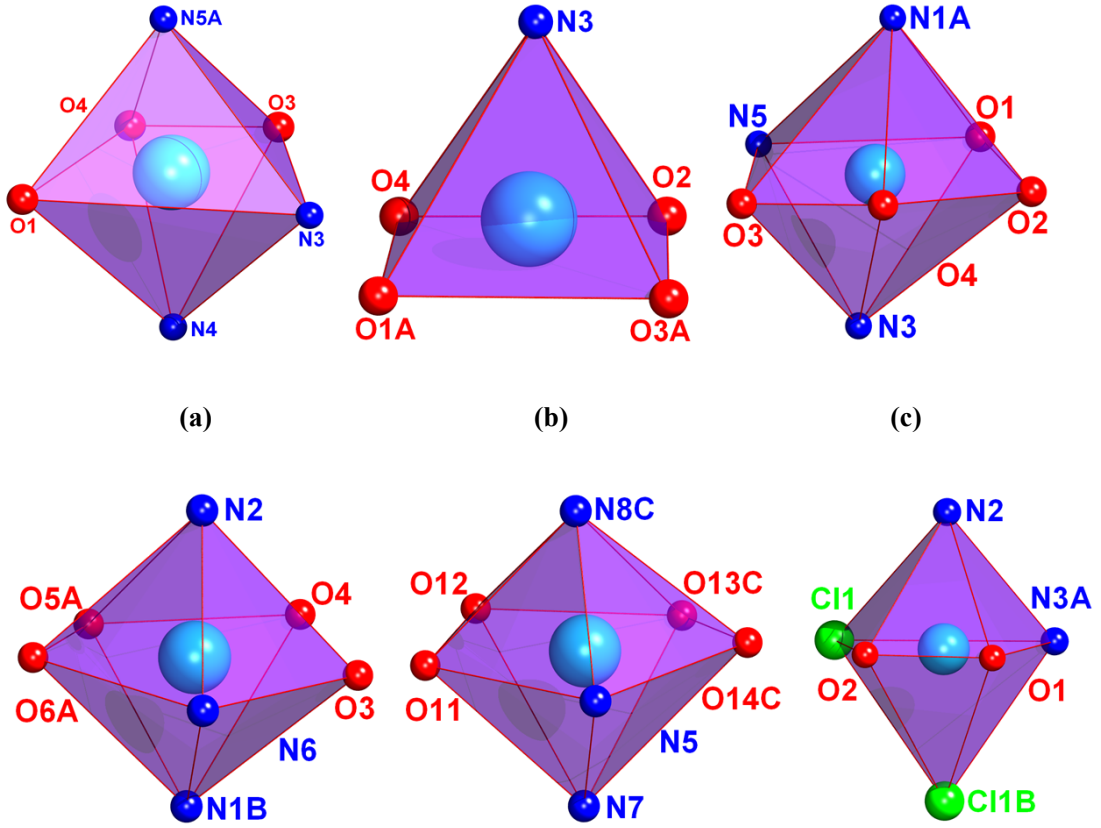


Figure S6. (a) CdN_3O_3 polyhedron showing the coordination geometry of Cd(II) atom in **1**. Symmetry codes: (A) $x + 1, -y + 3/2, z + 1/2$. (b) $CdNO_4$ polyhedron showing the coordination geometry of Cd(II) atom in **2**. Symmetry codes: (A) $-x + 1, -y + 1, -z + 1$. (c) CdN_3O_4 polyhedron showing the coordination geometry of Cd(II) atom in **3**. Symmetry codes: (A) $-x + 1, -y + 2, -z + 2$. (d-e) CdN_3O_4 polyhedron showing the coordination geometry of Cd(II) atoms in **4**. Symmetry codes: A: $-x + 1, y - 1/2, -z + 3/2$; B: $-x + 1, y + 1/2, -z + 3/2$; C: $-x + 2, y - 1/2, -z + 3/2$. (f) $CdCl_2N_2O_2$ polyhedron showing the coordination geometry of Cd(II) atom in **5**. Symmetry codes: A: $-x + 1, -y + 1, -z + 1$; B: $-x, -y + 1, -z + 1$.

Table S1. Selected angles (°) for **1**−**5**[a].

Compound **1**			
O(1)−Cd(1)−N(5A)	91.87(12)	O(1)−Cd(1)−O(3)	149.20(12)
N(5A)−Cd(1)−O(3)	89.16(11)	O(1)−Cd(1)−N(4)	86.22(12)
N(5A)−Cd(1)−N(4)	177.78(11)	O(3)−Cd(1)−N(4)	91.91(11)
O(1)−Cd(1)−N(3)	125.55(12)	N(5A)−Cd(1)−N(3)	97.67(11)
O(3)−Cd(1)−N(3)	84.70(10)	N(4)−Cd(1)−N(3)	84.38(12)
O(1)−Cd(1)−O(4)	95.37(11)	N(5A)−Cd(1)−O(4)	90.70(10)
O(3)−Cd(1)−O(4)	53.83(9)	N(4)−Cd(1)−O(4)	88.36(10)
N(3)−Cd(1)−O(4)	137.63(10)		
Compound **2**			
O(3A)−Cd(1)−O(1)	97.79(7)	O(3A)−Cd(1)−N(3)	114.57(6)
O(1)−Cd(1)−N(3)	116.47(7)	O(3A)−Cd(1)−O(2A)	84.01(7)
O(1)−Cd(1)−O(2A)	153.28(6)	N(3)−Cd(1)−O(2A)	86.15(7)
O(3A)−Cd(1)−O(4)	152.95(6)	O(1)−Cd(1)−O(4)	82.65(6)
N(3)−Cd(1)−O(4)	88.66(6)	O(2A)−Cd(1)−O(4)	83.98(7)
Compound **3**			
O(4)−Cd(1)−O(2)	85.91(8)	O(4)−Cd(1)−N(5)	135.53(8)
O(2)−Cd(1)−N(5)	138.55(8)	O(4)−Cd(1)−N(6A)	88.04(9)
O(2)−Cd(1)−N(6A)	89.65(9)	N(5)−Cd(1)−N(6A)	92.40(9)
O(4)−Cd(1)−N(3)	100.57(9)	O(2)−Cd(1)−N(3)	90.14(9)
N(5)−Cd(1)−N(3)	82.07(9)	N(6A)−Cd(1)−N(3)	171.34(8)

O(4)−Cd(1)−O(1)	138.42(8)	O(2)−Cd(1)−O(1)	53.57(8)
N(5)−Cd(1)−O(1)	85.57(8)	N(6A)−Cd(1)−O(1)	83.34(9)
N(3)−Cd(1)−O(1)	89.58(9)	O(4)−Cd(1)−O(3)	52.00(8)
O(2)−Cd(1)−O(3)	137.14(8)	N(5)−Cd(1)−O(3)	83.80(8)
N(6A)−Cd(1)−O(3)	95.81(9)	N(3)−Cd(1)−O(3)	90.23(9)
O(1)−Cd(1)−O(3)	169.29(7)		

Compound **4**

O(5A)−Cd(1)−N(6)	140.45(9)	O(5A)−Cd(1)−O(4)	84.52(9)
N(6)−Cd(1)−O(4)	135.01(9)	O(5A)−Cd(1)−N(1B)	84.95(10)
N(6)−Cd(1)−N(1B)	91.27(11)	O(4)−Cd(1)−N(1B)	92.34(11)
O(5A)−Cd(1)−N(2)	96.63(9)	N(6)−Cd(1)−N(2)	86.42(10)
O(4)−Cd(1)−N(2)	89.53(10)	N(1B)−Cd(1)−N(2)	177.66(10)
O(5A)−Cd(1)−O(6A)	54.22(8)	N(6)−Cd(1)−O(6A)	86.46(9)
O(4)−Cd(1)−O(6A)	138.38(9)	N(1B)−Cd(1)−O(6A)	89.47(9)
N(2)−Cd(1)−O(6A)	90.07(9)	O(5A)−Cd(1)−O(3)	136.93(9)
N(6)−Cd(1)−O(3)	82.04(9)	O(4)−Cd(1)−O(3)	53.30(9)
N(1B)−Cd(1)−O(3)	88.18(9)	N(2)−Cd(1)−O(3)	91.82(9)
O(6A)−Cd(1)−O(3)	168.21(9)	O(13C)−Cd(2)−N(7)	95.77(10)
O(13C)−Cd(2)−N(8C)	101.30(9)	N(7)−Cd(2)−N(8C)	160.73(10)
O(13C)−Cd(2)−O(12)	82.57(9)	N(7)−Cd(2)−O(12)	97.98(10)
N(8C)−Cd(2)−O(12)	93.07(10)	O(13C)−Cd(2)−N(5)	137.23(9)
N(7)−Cd(2)−N(5)	81.69(11)	N(8C)−Cd(2)−N(5)	79.72(10)
O(12)−Cd(2)−N(5)	140.18(9)	O(13C)−Cd(2)−O(11)	135.53(8)

N(7)−Cd(2)−O(11)	85.45(9)	N(8C)−Cd(2)−O(11)	88.56(9)
O(12)−Cd(2)−O(11)	53.44(8)	N(5)−Cd(2)−O(11)	87.05(9)
O(13C)−Cd(2)−O(14C)	53.96(8)	N(7)−Cd(2)−O(14C)	93.92(10)
N(8C)−Cd(2)−O(14C)	88.99(9)	O(12)−Cd(2)−O(14C)	135.89(9)
N(5)−Cd(2)−O(14C)	83.49(9)	O(11)−Cd(2)−O(14C)	170.51(8)
Compound **5**			
N(3A)−Cd(1)−O(1)	103.01(7)	N(3A)−Cd(1)−N(2)	88.93(7)
O(1)−Cd(1)−N(2)	87.51(7)	N(3A)−Cd(1)−O(2)	158.32(6)
O(1)−Cd(1)−O(2)	55.42(6)	N(2)−Cd(1)−O(2)	88.02(7)
N(3A)−Cd(1)−Cl(1)	103.21(5)	O(1)−Cd(1)−Cl(1)	153.76(5)
N(2)−Cd(1)−Cl(1)	91.69(6)	O(2)−Cd(1)−Cl(1)	98.33(4)
N(3A)−Cd(1)−Cl(1B)	88.70(6)	O(1)−Cd(1)−Cl(1B)	93.46(5)
N(2)−Cd(1)−Cl(1B)	177.59(5)	O(2)−Cd(1)−Cl(1B)	94.35(5)
Cl(1)−Cd(1)−Cl(1B)	88.42(4)		

[a] Symmetry codes for **1**: A: $x + 1, y, z + 1$; Symmetry codes for **2**: A: $-x + 1, -y + 1, -z + 1$; Symmetry codes for **3**: A: $-x + 1, -y + 2, -z + 2$; Symmetry codes for **4**: A: $-x + 1, y - 1/2, -z + 3/2$; B: $-x + 1, y + 1/2, -z + 3/2$; C: $-x + 2, y - 1/2, -z + 3/2$; Symmetry codes for **5**: A: $-x + 1, -y + 1, -z + 1$; B: $-x, -y + 1, -z + 1$.

Table S2. Selected dihedral angles (°) for **1**−**5**[a].

Compound **1**			
Cg1−Cg2	30.715	Cg1−Cg3	40.166
Cg4−Cg5	61.167	Cg4−Cg5A	61.167

Cg1 is the C30-C35 benzene ring; Cg2 is the N5/C37-C41 pyridine ring; Cg3 is the N4/C24-C28 pyridine ring; Cg4 is the C21-C23/C21A-C23A benzene ring; Cg5 is the N3/C15-C19 pyridine ring; Cg5A is the N3A/C15A-C19A pyridine ring.

Compound **2**			
Cg6−Cg7	46.217	Cg6−Cg7A	46.217

Cg6 is the C21-C23/C21A-C23A benzene ring; Cg7 is the N3/C15-C19 pyridine ring; Cg7A is the N3A/C15A-C19A pyridine ring.

Compound **3**			
Cg8−Cg9	89.220	Cg8−Cg10	13.191
Cg12−Cg11	74.683	Cg12−Cg13	59.872

Cg8 is the C39-C44 benzene ring; Cg9 is the N5/C33-C37 pyridine ring; Cg10 is the N6/C46-C50 pyridine ring; Cg11 is the N3/C15-C19 pyridine ring; Cg12 is the C21-C26 benzene ring; Cg13 is the N4/C28-C32 pyridine ring.

Compound **4**			
Cg14−Cg15	89.788	Cg14−Cg16	82.081
Cg17−Cg18	25.608	Cg17−Cg19	8.667

Cg14 is the C39-C44 benzene ring; Cg15 is the N5/C33-C37 pyridine ring; Cg16 is the N6/C46-C50 pyridine ring; Cg17 is the C7-C12 benzene ring; Cg18 is the N2/C14-C18 pyridine ring; Cg19 is the N1/C1-C5 pyridine ring.

Compound **5**			
Cg20−Cg21	77.160	Cg20−Cg22	20.199

Cg20 is the C14-C19 benzene ring; Cg21 is the N3/C21-C25 pyridine ring; Cg22 is the N2/C8-C12 pyridine ring;

[a] Symmetry codes for **1**: A: $-x, -y, -z+2$; Symmetry codes for **2**: A: $-x, -y+1, -z+2$.

Table S3. Selected torsion angles (°) for **1**−**5**.

Compound **1**			
C(18)−C(20)−O(5)−C(21)	−155.9(3)	C(27)−C(29)−O(6)−C(30)	−173.7(4)
C(37)−C(36)−O(7)−C(33)	−179.5(4)		
Compound **2**			
C(19)−C(20)−O(5)−C(21)	−175.71(17)		
Compound **3**			
C(46)−C(45)−O(8)−C(43)	173.5(2)	C(35)−C(38)−O(7)−C(39)	−178.2(3)
C(17)−C(20)−O(5)−C(21)	−171.0(3)	C(28)−C(27)−O(6)−C(25)	176.6(3)
Compound **4**			
C(4)−C(6)−O(1)−C(7)	159.0(3)	C(14)−C(13)−O(2)−C(11)	−170.6(3)
C(36)−C(38)−O(7)−C(39)	179.1(3)	C(46)−C(45)−O(8)−C(43)	−172.9(3)
C(54)−C(56)−O(9)−C(57)	178.1(3)	C(64)−C(63)−O(10)−C(61)	−172.6(3)
Compound **5**			
C(11)−C(13)−O(3)−C(14)	−167.26(19)	C(21)−C(20)−O(4)−C(19)	−177.6(2)