Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

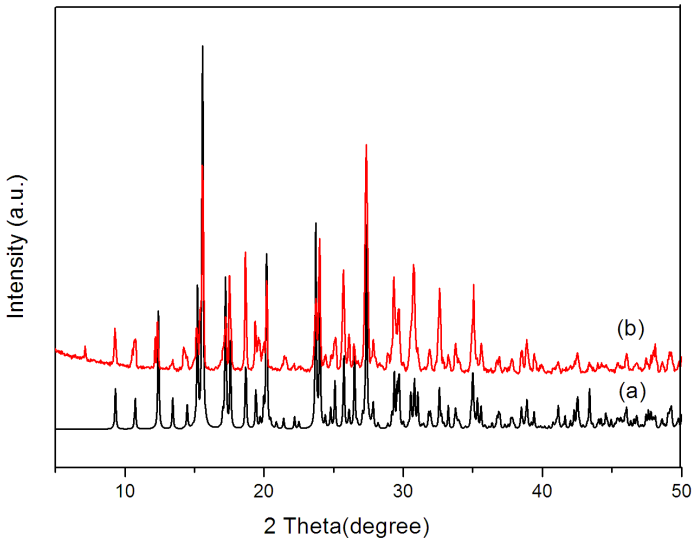

Fig. S1 The PXRD graph for complex **1** ((a) modulated by Mercury; (b) observed.)

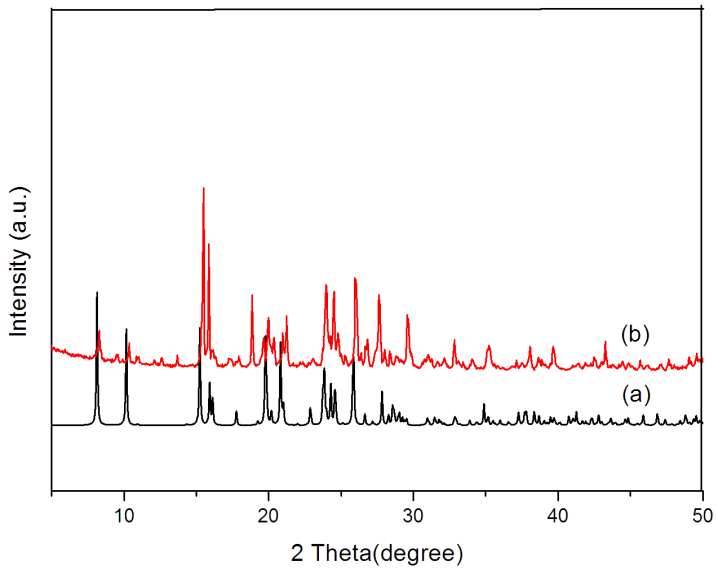

Fig. S2 The PXRD graph for complex **2** ((a) modulated by Mercury; (b) observed.)

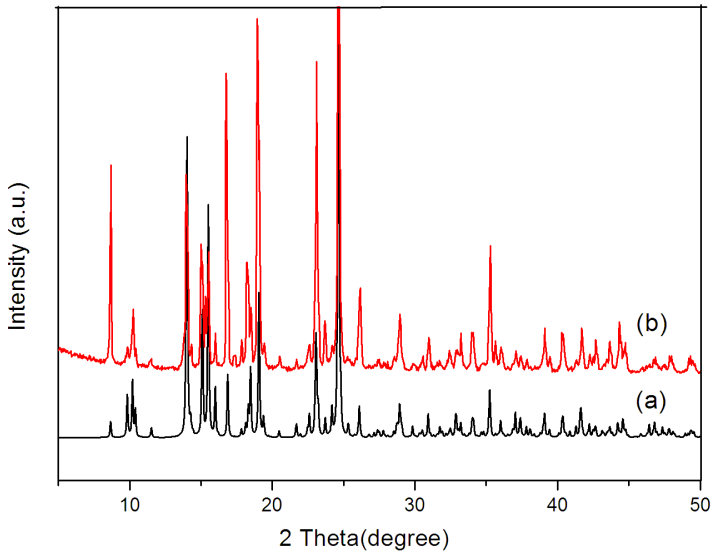

Fig. S3 The PXRD graph for complex **3** ((a) modulated by Mercury; (b) observed.)

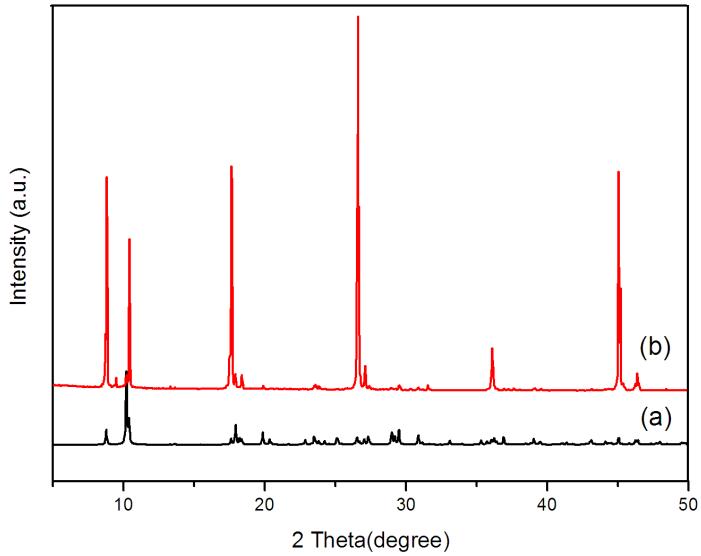

Fig. S4 The PXRD graph for complex **4** ((a) modulated by Mercury; (b) observed.)

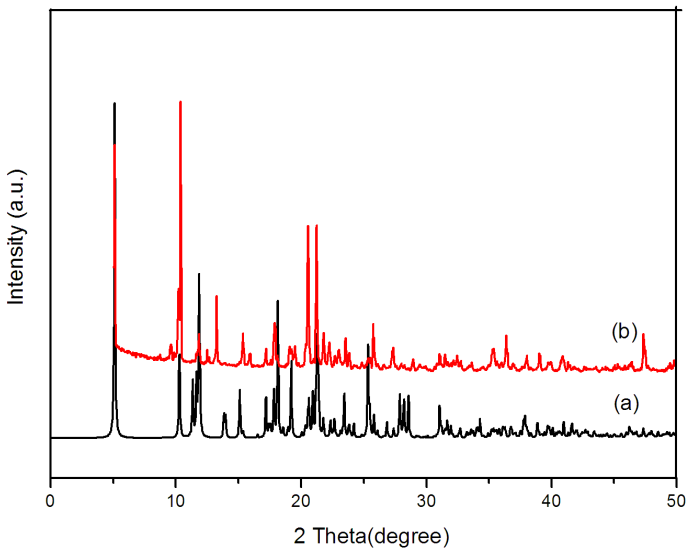

Fig. S5 The PXRD graph for complex **5** ((a) modulated by Mercury; (b) observed.)

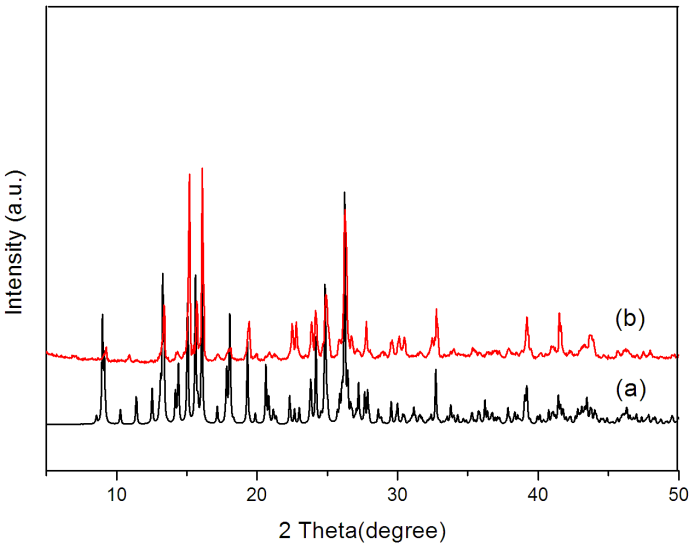

Fig. S6 The PXRD graph for complex **6** ((a) modulated by Mercury; (b) observed.)

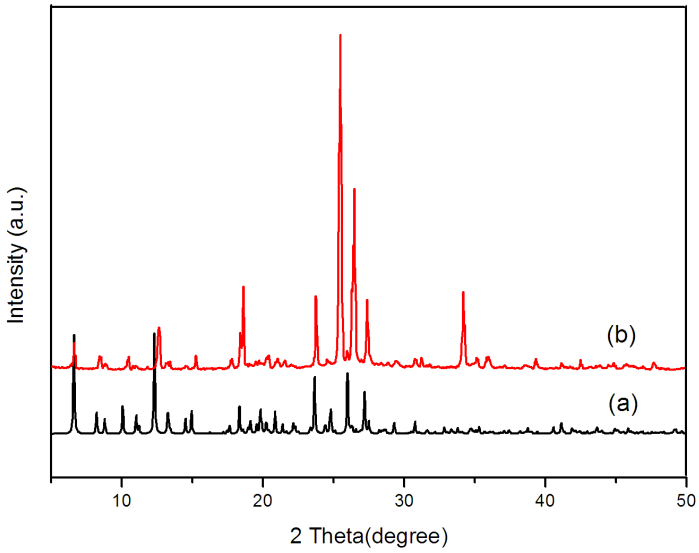

Fig. S7 The PXRD graph for complex **7** ((a) modulated by Mercury; (b) observed.)

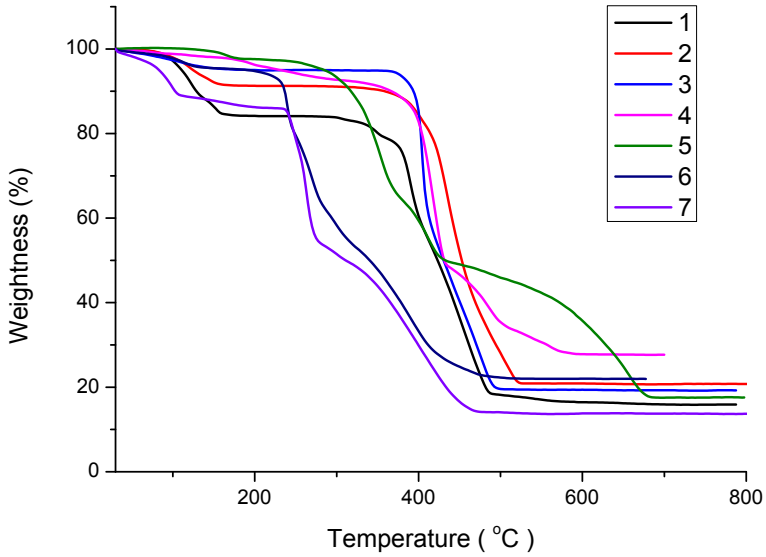

Figure S8 TG curves for complexes **1**-**7**.

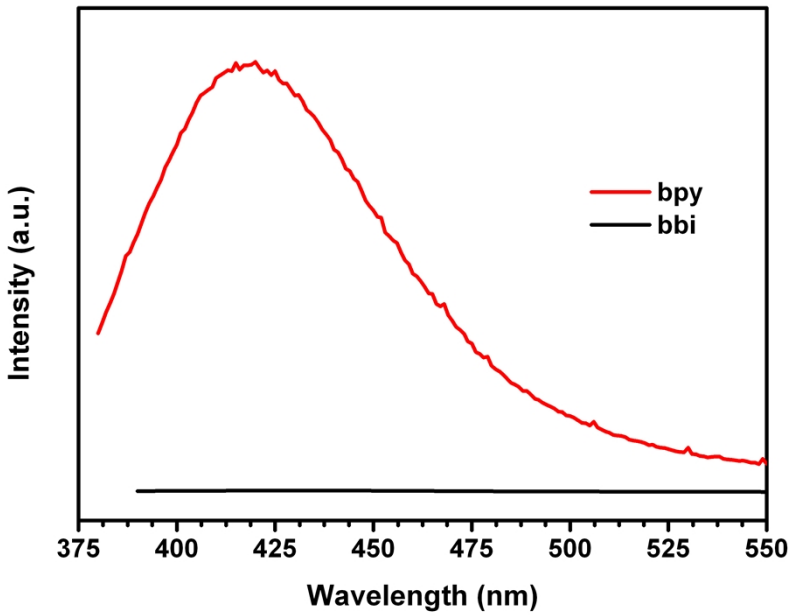

Figure S9 The fluorescent emission spectra of 4,4'-bpy and bbi in solid state at room temperature.

Table S1. Crystallographic data for complexes **1**–**7**.

	1	**2**	**3**	**4**	**5**	**6**	**7**
formula	$C_{15}H_{17}NO_{10}Zn$	$C_{15}H_{11}NO_7Zn$	$C_{20}H_{17}N_2O_8Zn$	$C_{15}H_{11}NO_7Cd$	$C_{25}H_{27}N_5O_8Cd$	$C_{25}H_{29}N_3O_{12}Cu$	$C_{27}H_{31}N_3O_{12}Cu$
Mr	436.67	382.62	478.73	429.65	637.92	627.05	653.09
cryst syst	Orthorhombic	Orthorhombic	Monoclinic	Orthorhombic	Triclinic	Triclinic	Triclinic
space group	*Pbca*	Pbca	P21/c	Pbca	P-1	P-1	P-1
a (Å)	14.2707(5)	7.4952(2)	11.7220(4)	17.0363(4)	8.6985(4)	10.1493(5)	10.0801(3)
b (Å)	11.9131(4)	17.4170(5)	15.3650(5)	7.7794(2)	9.4824(6)	11.1061(7)	10.8210(5)
c (Å)	18.9905(6)	21.7353(5)	12.7229(10)	20.1494(5)	17.7549(10)	12.8644(6)	13.4386(6)
α (°)	90	90	90	90	80.703(5)	109.643(5)	95.194(4)
β (°)	90	90	119.424(4)	90	77.485(5)	101.237(4)	92.144(3)
γ (°)	90	90	90	90	65.302(5)	94.591(5)	92.391(3)
V / Å^3	3228.54(8)	2837.41(13)	1995.92(18)	2670.44(11)	1294.72(12)	1322.76(12)	1457.30(10)
Z	8	8	4	8	2	2	2
*D*c / g·cm^{-3}	1.797	1.791	1.593	2.137	1.636	1.574	1.488
F(000)	1792	1552	980	1696	648	650	678
reflns collected	6912	6784	8032	6841	9754	9902	10878
independent reflns	2837	2498	3507	2349	4569	4655	5109
R_{int}	0.0372	0.0236	0.0298	0.0273	0.0399	0.0468	0.0309
GOF on F^2	0.999	1.026	0.999	1.089	1.031	1.013	1.058
R_1, wR_2[$I>2\sigma(I)$]	0.0399, 0.0789	0.0314, 0.0715	0.0463, 0.1070	0.0304, 0.0683	0.0374, 0.0730	0.0497, 0.1017	0.1000, 0.2718
R_1, wR_2(all data)	0.0662, 0.0869	0.0391, 0.0746	0.0648, 0.1185	0.0407, 0.0720	0.0484, 0.0764	0.0734, 0.1095	0.0892, 0.2601

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

Table S2. Selected bond distances and angles for complexes **1**–**7**.

			1		
Zn(1)–O(6)#1	1.995(2)	Zn(1)–O(2W)	2.049(3)	Zn(1)–O(1)	2.081(3)
Zn(1)-O(3W)	2.116(3)	Zn(1)–O(1W)	2.157(3)	Zn(1)–O(2)	2.418(3)
O(6)#1-Zn(1)-O(2W)	111.75(11)	O(6)#1-Zn(1)-O(1)	142.24(11)	O(2W)-Zn(1)-O(1)	104.61(11)
O(6)#1-Zn(1)-O(3W)	92.58(11)	O(2W)-Zn(1)-O(3W)	88.97(11)	O(1)-Zn(1)-O(3W)	98.02(11)
O(6)#1-Zn(1)-O(1W)	81.67(10)	O(2W)-Zn(1)-O(1W)	87.13(11)	O(1)-Zn(1)-O(1W)	90.49(10)
			2		
Zn(1)-O(6)#1	1.9389(19)	Zn(1)-O(1)	1.9452(18)	Zn(1)-O(3)#2	1.9713(19)
Zn(1)-O(4)#3	1.9911(19)	O(4)-Zn(1)#4	1.9911(18)	O(6)-Zn(1)#5	1.9389(19)
O(3)-Zn(1)#2	1.9713(19)				
O(6)#1-Zn(1)-O(1)	128.31(9)	O(6)#1-Zn(1)-O(3)#2	116.79(9)	O(1)-Zn(1)-O(3)#2	94.27(9)
O(6)#1-Zn(1)-O(4)#3	105.13(8)	O(1)-Zn(1)-O(4)#3	108.15(8)	O(3)#2-Zn(1)-O(4)#3	101.02(8)
			3		
Zn(1)-O(1)	1.940(3)	Zn(1)-O(4)#1	1.944(3)	Zn(1)-O(6)#2	1.951(3)
Zn(1)-N(2)	2.045(3)	O(4)-Zn(1)#3	1.944(3)	O(6)-Zn(1)#4	1.951(3)
O(1)-Zn(1)-O(4)#1	120.60(14)	O(1)-Zn(1)-O(6)#2	111.83(15)	O(4)#1-Zn(1)-O(6)#2	99.81(3)
O(1)-Zn(1)-N(2)	99.52(13)	O(4)#1-Zn(1)-N(2)	114.19(13)	O(6)#2-Zn(1)-N(2)	111.32(13)
			4		
Cd(1)-O(3)#1	2.242(3)	Cd(1)-O(2)#2	2.269(3)	Cd(1)-O(1)	2.308(3)
Cd(1)-O(6)#3	2.344(3)	Cd(1)-O(4)#4	2.362(3)	Cd(1)-O(5)#5	2.373(3)
O(2)-Cd(1)#6	2.269(3)	O(3)-Cd(1)#1	2.242(3)	O(4)-Cd(1)#7	2.362(3)
O(5)-Cd(1)#8	2.373(3)	O(6)-Cd(1)#9	2.344(3)		
O(3)#1-Cd(1)-O(1)	83.85(10)	O(2)#2-Cd(1)-O(1)	153.53(10)	O(3)#1-Cd(1)-O(6)#3	164.34(11)
O(2)#2-Cd(1)-O(6)#3	77.72(11)	O(1)-Cd(1)-O(6)#3	81.32(10)	O(3)#1-Cd(1)-O(4)#4	83.38(10)
O(2)#2-Cd(1)-O(4)#4	81.79(10)	O(1)-Cd(1)-O(4)#4	86.41(10)	O(6)#3-Cd(1)-O(4)#4	100.61(11)
O(3)#1-Cd(1)-O(5)#5	88.23(11)	O(2)#2-Cd(1)-O(5)#5	110.00(11)	O(1)-Cd(1)-O(5)#5	83.95(10)
O(6)#3-Cd(1)-O(5)#5	85.25(11)	O(4)#4-Cd(1)-O(5)#5	167.84(11)		
			5		
Cd(2)-O(2)	2.270(2)	Cd(2)-O(3)#1	2.271(2)	Cd(2)-N(3)	2.281(3)
Cd(2)-N(5)#2	2.294(3)	Cd(2)-O(1W)	2.378(2)	N(5)-Cd(2)#3	2.294(3)
O(3)-Cd(2)#4	2.271(2)				
O(2)-Cd(2)-O(3)#1	112.03(8)	O(2)-Cd(2)-N(3)	93.19(10)	O(3)#1-Cd(2)-N(3)	103.84(10)
O(2)-Cd(2)-N(5)#2	100.15(9)	O(3)#1-Cd(2)-N(5)#2	142.95(10)	N(3)-Cd(2)-N(5)#2	91.80(10)
O(2)-Cd(2)-O(1W)	84.62(9)	O(3)#1-Cd(2)-O(1W)	81.94(9)	N(3)-Cd(2)-O(1W)	174.21(9)
N(5)#2-Cd(2)-O(1W)	83.33(9)				
			6		
N(2)-Cu(1)#1	2.001(3)	Cu(1)-N(2)#2	2.001(3)	Cu(1)-O(1)	2.015(2)
Cu(1)-N(1)	2.015(3)	Cu(1)-O(3)#3	2.135(2)	Cu(1)-O(1W)	2.258(3)
O(3)-Cu(1)#4	2.135(2)				
N(2)#2-Cu(1)-O(1)	92.50(11)	N(2)#2-Cu(1)-N(1)	176.01(11)	O(1)-Cu(1)-N(1)	90.48(11)
N(2)#2-Cu(1)-O(3)#3	89.24(10)	O(1)-Cu(1)-O(3)#3	149.05(10)	N(1)-Cu(1)-O(3)#3	86.84(10)
N(2)#2-Cu(1)-O(1W)	89.66(11)	O(1)-Cu(1)-O(1W)	118.29(10)	N(1)-Cu(1)-O(1W)	91.27(11)
O(3)#3-Cu(1)-O(1W)	92.60(9)				
			7		
Cu(1)-O(2)#1	1.944(2)	Cu(1)-O(4)#2	1.996(2)	Cu(1)-N(2)	2.023(3)
Cu(1)-N(3)#3	2.037(3)	Cu(1)-O(1)	2.303(3)	O(2)-Cu(1)#1	1.944(2)
O(4)-Cu(1)#2	1.996(2)	N(3)-Cu(1)#4	2.037(3)		
O(2)#1-Cu(1)-N(2)	92.44(12)	O(4)#2-Cu(1)-N(2)	90.69(11)	O(2)#1-Cu(1)-N(3)#3	86.69(12)
O(4)#2-Cu(1)-N(3)#3	90.52(12)	N(2)-Cu(1)-N(3)#3	178.73(12)	O(2)#1-Cu(1)-O(1)	124.73(11)
O(4)#2-Cu(1)-O(1)	83.30(10)	N(2)-Cu(1)-O(1)	90.16(12)	N(3)#3-Cu(1)-O(1)	89.58(12)

Symmetry code: **1**: #1 −*x*+3/2, −*y*, *z*−1/2; #2 −*x*+3/2, −*y*, *z*+1/2. **2**: #1 −*x*+1, *y*+1/2, −*z*+3/2; #2 −*x*, −*y*+2, −*z*+2; #3 −*x*+1/2, *y*+1/2, *z*; #4 −*x*+1/2, *y*−1/2, *z*; #5 −*x*+1, *y*−1/2, −*z*+3/2. **3**: #1 −*x*+1, *y*+1/2, −*z*+3/2; #2 *x*+1, *y*, *z*+1; #3 −*x*+1, *y*−1/2, −*z*+3/2; #4 *x*−1, *y*, *z*−1; #5 −*x*+2, −*y*+2, −*z*+1. **4**: #1 −*x*+2, −*y*+2, −*z*+2; #2 −*x*+5/2, *y*+1/2, *z*; #3 *x*+1/2, *y*+1, −*z*+3/2; #4 *x*+1/2, −*y*+3/2, −*z*+2; #5 −*x*+2, *y*+3/2, −*z*+3/2; #6 −*x*+5/2, *y*−1/2, *z*; #7 *x*−1/2, −*y*+3/2, −*z*+2; #8 −*x*+2, *y*−3/2, −*z*+3/2; #9 *x*−1/2, *y*−1, −*z*+3/2. **5**: #1 *x*−1, *y*+1, *z*; #2 *x*, *y*−1, *z*; #3 *x*, *y*+1, *z*; #4 *x*+1, *y*−1, *z*. **6**: #1 *x*, *y*−1, *z*, #2 *x*, *y*+1, *z*, #3 *x*−1, *y*, *z*, #4 *x*+1, *y*, *z*. **7**: #1 −*x*, −*y*+1, −*z*; #2 −*x*+1, −*y*+1, −*z*; #3 *x*, *y*, *z*−1; #4 *x*, *y*, *z*+1.