Supporting Information

Table S1. Selected Atomic Distances (Å) and Bond Angles (°) for complexes 1-6

1			
Zn1—Cl1	2.2016 (16)	Zn2—N9	2.188 (4)
Zn1—Cl2	2.2380 (15)	Zn2—N10	2.034 (4)
Zn1—N5	2.051 (3)	Zn3—Cl3	2.2390 (14)
Zn1—N8	2.106 (4)	Zn3—Cl4	2.1769 (15)
Zn2—O1	1.982 (3)	Zn3—N13	2.048 (4)
Zn2—N1	2.189 (4)	Zn3—N16	2.142 (4)
Zn2—N3	2.031 (4)		
Cl1—Zn1—Cl2	110.72 (6)	N3—Zn2—N9	96.75 (15)
N5—Zn1—Cl1	127.01 (12)	N3—Zn2—N10	142.66 (16)
N5—Zn1—Cl2	112.88 (11)	N9—Zn2—N1	161.03 (15)
N5—Zn1—N8	80.47 (16)	N10—Zn2—N1	94.54 (14)
N8—Zn1—Cl1	106.75 (13)	N10—Zn2—N9	78.02 (15)
N8—Zn1—Cl2	114.90 (13)	Cl4—Zn3—Cl3	116.26 (6)
O1—Zn2—N1	97.02 (14)	N13—Zn3—Cl3	112.60 (12)
O1—Zn2—N3	106.45 (16)	N13—Zn3—Cl4	124.18 (12)
O1—Zn2—N9	101.94 (14)	N13—Zn3—N16	79.90 (15)
O1—Zn2—N10	110.81 (16)	N16—Zn3—Cl3	108.40 (12)
N3—Zn2—N1	78.49 (14)	N16—Zn3—Cl4	107.71 (13)
2 (Symmetry codes: (A) x, $-y+3/2$, $-z+1$; (B) x, y, $-z+1/2$.)			
Zn1—Cl1	2.228 (3)	Zn2—Cl2	2.207 (2)
Zn1—N1	2.273 (4)	Zn2—Cl3	2.201 (2)
Zn1—N2	2.022 (3)	Zn2—N4	2.050 (3)
Cl1—Zn1—N1A	105.60 (11)	N2i—Zn1—N1	93.58 (14)
Cl1—Zn1—N1	105.60 (11)	N2—Zn1—N2A	142.0 (3)
N1—Zn1—N1A	148.8 (2)	Cl3—Zn2—Cl2	114.74 (9)
N2A—Zn1—Cl1	109.02 (13)	N4B—Zn2—Cl2	113.42 (12)
N2—Zn1—Cl1	109.02 (13)	N4—Zn2—Cl2	113.42 (12)
N2A—Zn1—N1A	76.25 (13)	N4B—Zn2—Cl3	114.18 (11)
N2—Zn1—N1A	93.58 (14)	N4—Zn2—Cl3	114.18 (11)
N2—Zn1—N1	76.25 (13)	N4—Zn2—N4B	83.09 (19)
3 (Symmetry codes: (A) y, $-x+y$, $-z$; (B) $x-y$, x, $-z$; (C) $-x+2/3$, $-y+1/3$, $-z+1/3$.)			
Cd1—Cl1A	2.6318 (18)	Cd1—N2	2.200 (4)
Cd1—Cl1	2.5247 (18)	Cd1—N4	2.502 (5)
Cd1—N1B	2.199 (5)	Cd1A—N5C	3.116 (9)
N1B—Cd1—Cl1	92.69 (12)	N2—Cd1—Cl1A	88.03 (12)
N1B—Cd1—Cl1A	95.98 (15)	N2—Cd1—N4	69.03 (16)
N1B—Cd1—N2	150.58 (17)	N4—Cd1—Cl1	100.25 (14)
N1B—Cd1—N4	97.79 (18)	N4—Cd1—Cl1A	153.33 (13)

N2—Cd1—Cl1	115.06 (14)		

4 (Symmetry codes: (A) $y+1/3, -x+y+2/3, -z+2/3$; (B) $x-y+1/3, x-1/3, -z+2/3$.)

Cd1—N3C	3.1541 (2)	Cd1—N1	2.246 (6)
I1—Cd1	2.8342 (9)	Cd1—N2B	2.233 (6)
Cd1—I1B	2.9099 (9)	Cd1—N4B	2.476 (7)
I1—Cd1—I1B	100.47 (3)	N2B—Cd1—I1	110.79 (18)
N1—Cd1—I1	96.64 (16)	N2B—Cd1—N1	149.2 (2)
N1—Cd1—I1B	97.13 (18)	N2B—Cd1—N4B	69.4 (2)
N1—Cd1—N4B	93.1 (2)	N4B—Cd1—I1B	156.21 (18)
N2B—Cd1—I1B	91.53 (17)	N4B—Cd1—I1	99.63 (19)

5 (Symmetry codes: (A) $-x+1, -y, -z$; (B) $x, -y+1/2, z-1/2$; (C) $-x+1, y-1/2, -z+1/2$.)

Cd1—Br1A	2.7153 (15)	Cd1—N4B	2.447 (9)
Cd1—Br1	2.6869 (15)	Cd1—N5	2.511 (8)
Cd1—N3	2.348 (8)	Cd1—N6B	2.362 (8)
Cd2—Br2	2.576 (2)	Cd2—N2	2.307 (8)
Cd2—O1	2.6582(5)	Cd2—N7C	2.310 (8)
Cd2—N1	2.400 (9)	Cd2—N8C	2.453 (9)
Br1—Cd1—Br1A	94.52 (5)	Br2—Cd2—H2	164.7
N3—Cd1—Br1	101.5 (2)	N1—Cd2—Br2	92.1 (3)
N3—Cd1—Br1A	92.3 (2)	N1—Cd2—H2	72.7
N3—Cd1—N4B	91.4 (3)	N1—Cd2—N8C	93.5 (3)
N3—Cd1—N5	72.8 (3)	N2—Cd2—Br2	116.4 (2)
N3—Cd1—N6B	158.5 (3)	N2—Cd2—H2	60.5
N4B—Cd1—Br1A	94.3 (2)	N2—Cd2—N1	71.7 (3)
N4B—Cd1—Br1	164.0 (2)	N2—Cd2—N7C	111.4 (3)
N4B—Cd1—N5	79.5 (3)	N2—Cd2—N8C	146.0 (3)
N5—Cd1—Br1A	163.61 (19)	N7C—Cd2—Br2	104.8 (2)
N5—Cd1—Br1	95.2 (2)	N7C—Cd2—H2	89.8
N6B—Cd1—Br1	92.3 (2)	N7C—Cd2—N1	158.1 (4)
N6B—Cd1—Br1A	103.0 (2)	N7C—Cd2—N8C	71.8 (3)
N6B—Cd1—N4B	72.7 (3)	N8C—Cd2—Br2	94.0 (2)
N6B—Cd1—N5	89.7 (3)	N8C—Cd2—H2	86.1

6 (Symmetry codes: (A) $x+1, y, z$; (B) $x-1, y, z$; (C) $-x, -y+2, -z+1$.)

I1—Cd1	3.0994 (12)	I1—Cd2	2.8582 (11)
I2—Cd1	2.9358 (12)	I3—Cd2	3.1055 (14)
I3—Cd1	2.7574 (13)	I4—Cd2	2.8515 (11)
Cd1—I4A	3.0455 (12)	Cd2—I2B	3.0045 (12)
Cd1—N1	2.314 (9)	Cd2—N7C	2.443 (9)
Cd1—N2	2.519 (9)	Cd2—N8C	2.341 (9)
I2—Cd1—I1	90.72 (3)	I1—Cd2—I2B	93.44 (3)
I2—Cd1—I4A	90.42 (3)	I1—Cd2—I3	90.13 (3)
I3—Cd1—I1	92.16 (4)	I2B—Cd2—I3	167.03 (4)
I3—Cd1—I2	93.14 (4)	I4—Cd2—I1	97.17 (4)
I3—Cd1—I4A	99.39 (4)	I4—Cd2—I2B	92.90 (3)

I4A—Cd1—I1	168.32 (4)	I4—Cd2—I3	99.03 (4)
N1—Cd1—I1	82.6 (2)	N7C—Cd2—I1	168.4 (2)
N1—Cd1—I2	98.5 (2)	N7C—Cd2—I2B	91.7 (2)
N1—Cd1—I3	167.2 (2)	N7C—Cd2—I3	82.7 (2)
N1—Cd1—I4A	85.7 (2)	N7C—Cd2—I4	93.0 (2)
N1—Cd1—N2	71.4 (3)	N8C—Cd2—I1	100.3 (2)
N2—Cd1—I1	91.7 (2)	N8C—Cd2—I2B	87.1 (2)
N2—Cd1—I2	169.2 (2)	N8C—Cd2—I3	80.0 (2)
N2—Cd1—I3	97.3 (2)	N8C—Cd2—I4	162.5 (2)
N2—Cd1—I4A	85.1 (2)	N8C—Cd2—N7C	69.6 (3)
I2—Cd1—I1	90.72 (3)	I1—Cd2—I2B	93.44 (3)
I2—Cd1—I4A	90.42 (3)	I1—Cd2—I3	90.13 (3)
I3—Cd1—I1	92.16 (4)	I2B—Cd2—I3	167.03 (4)
I3—Cd1—I2	93.14 (4)	I4—Cd2—I1	97.17 (4)
I3—Cd1—I4A	99.39 (4)	I4—Cd2—I2B	92.90 (3)
I4A—Cd1—I1	168.32 (4)	I4—Cd2—I3	99.03 (4)

Table S2 Hydrogen bond lengths and bond angels in complex 1, 5 and 6

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
		1		
O(1)—H(1A)···N(2) #1	0.83 (5)	2.10 (5)	2.871 (6)	155 (5)
O(1)—H(1B)···N(12) #2	0.85 (5)	1.95 (5)	2.766 (6)	161 (5)
N(6)—H(6)···Cl(2) #3	0.87 (4)	2.37 (4)	3.208 (4)	161 (4)
N(15)—H(15)···Cl(3) #4	0.78 (4)	2.44 (5)	3.163 (4)	155 (5)
C(3)—H(3)···Cl(1)#1	0.94 (4)	2.80 (5)	3.478 (6)	131 (4)
Symmetry codes: (#1) −*x*+1, −*y*, −*z*+1; (#2) −*x*+1, −*y*+1, −*z*+1; (#3) −*x*, −*y*, −*z*+1; (#4) −*x*+1, −*y*+1, −*z*+2.				
		5		
O(1)—H(1A)···Br(1) #3	0.85	2.64	3.435 (11)	157
O(1)—H(1B)···N(6) #1	0.85	2.43	3.229 (14)	157
C(12)—H(12)···Br(2) #2	0.93	2.89	3.695 (14)	145
Symmetry codes: (#1) *x*, −*y*+1/2, *z*+1/2; (#2) −*x*+1, *y*+1/2, −*z*+1/2; (#3) −*x*+1, *y*+1/2, −*z*+3/2.				
		6		
N(4)—H(4)···I(4) #1	0.86	2.80	3.611 (10)	158
N(6)—H(6)···I(3)	0.86	2.62	3.454 (9)	163
Symmetry code: (#1) −*x*, −*y*+1, −*z*+1.				

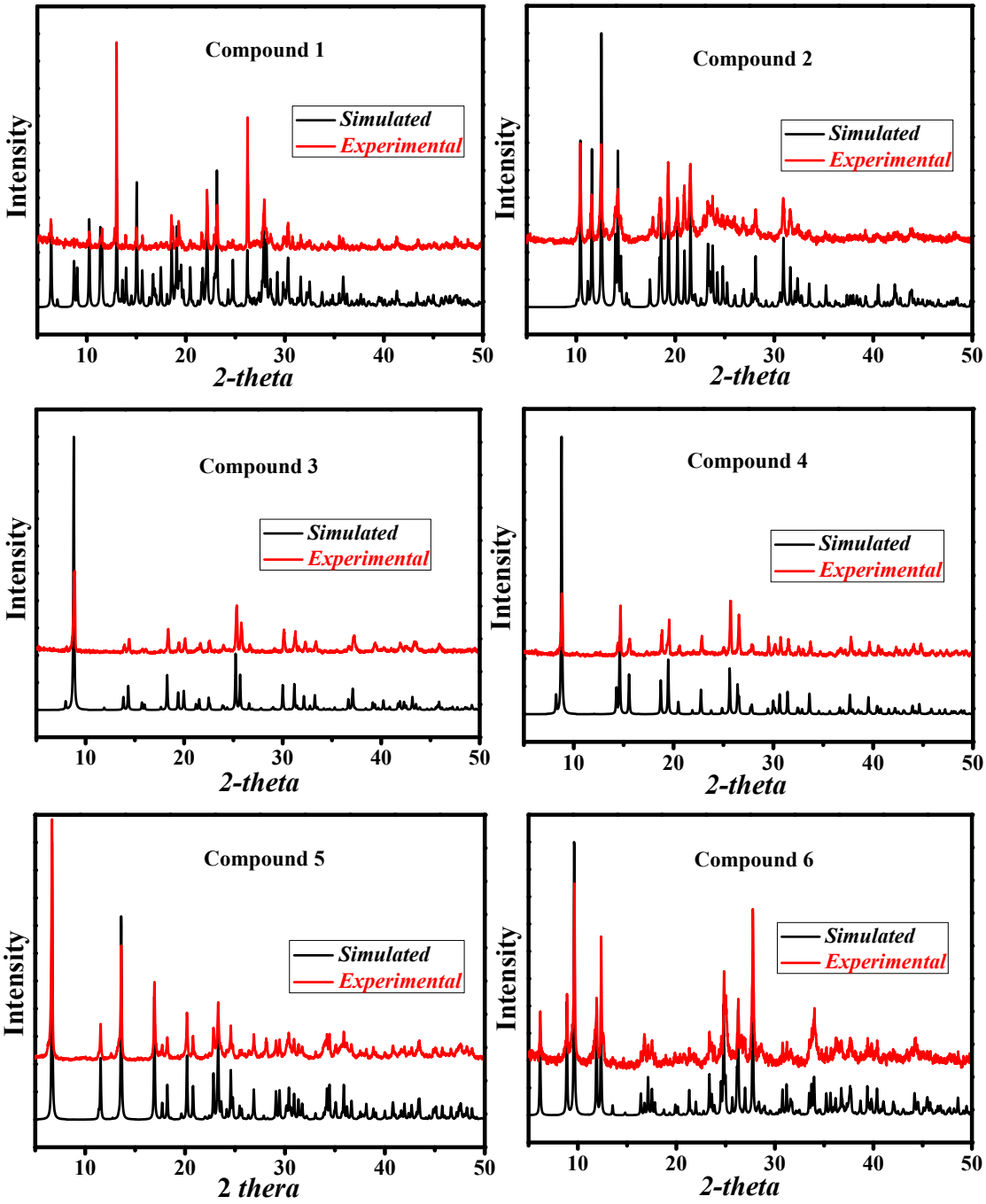
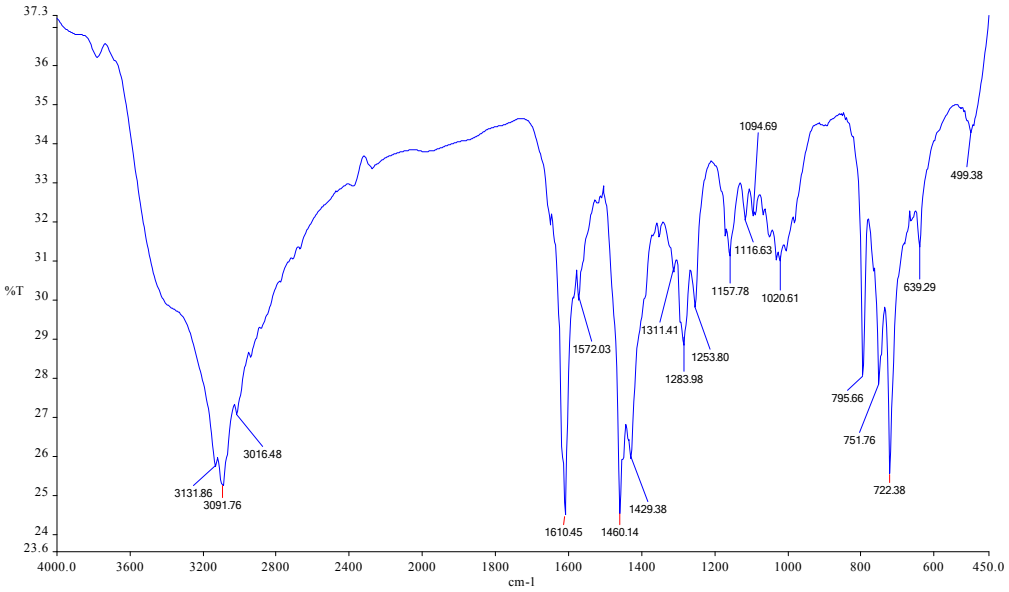


Fig **S1** Measured and calculated powder X-ray diffraction (PXRD) pattern of **1- 6**.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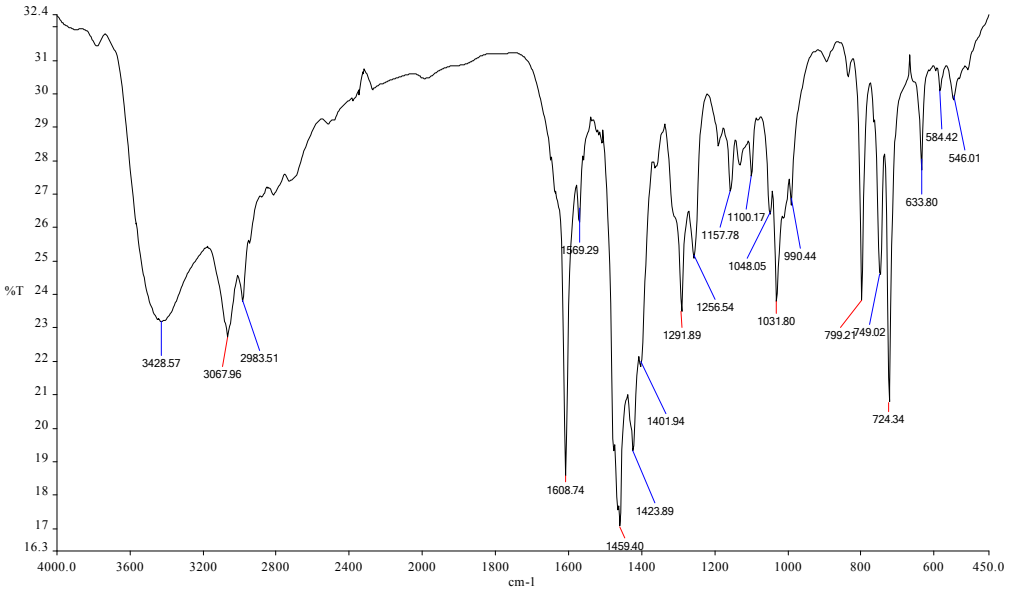
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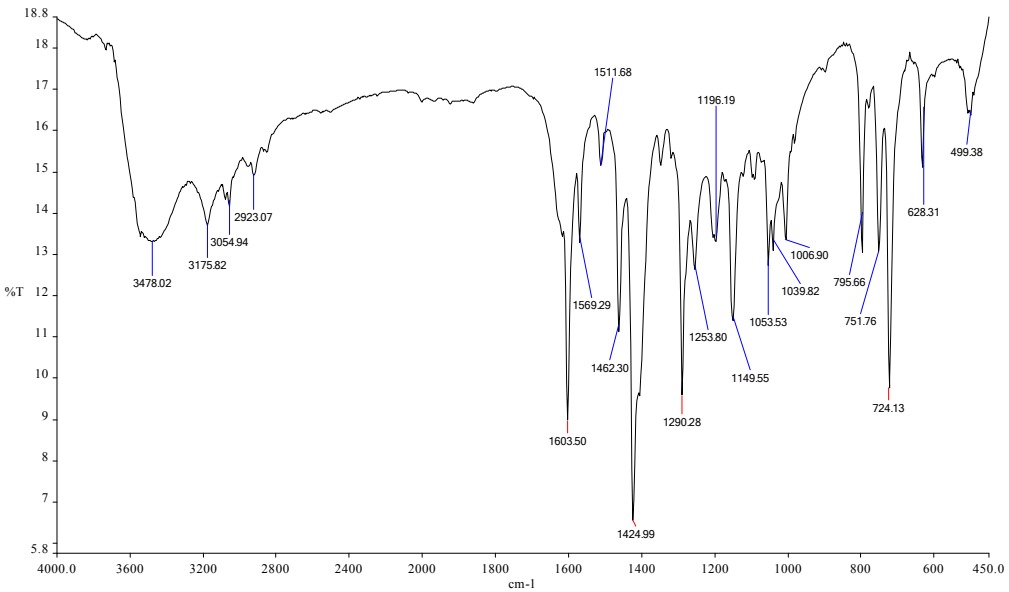
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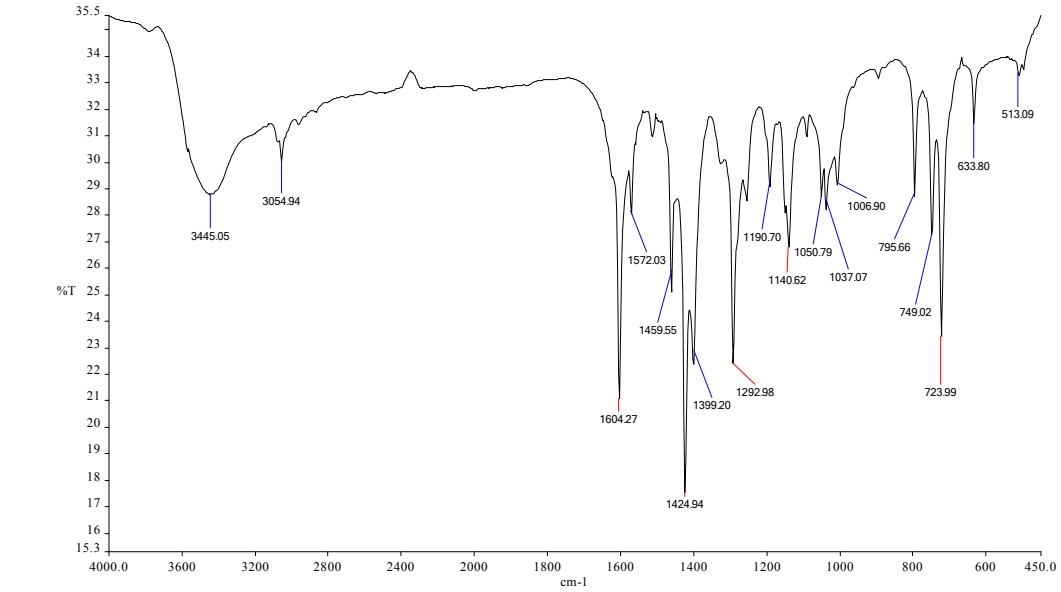

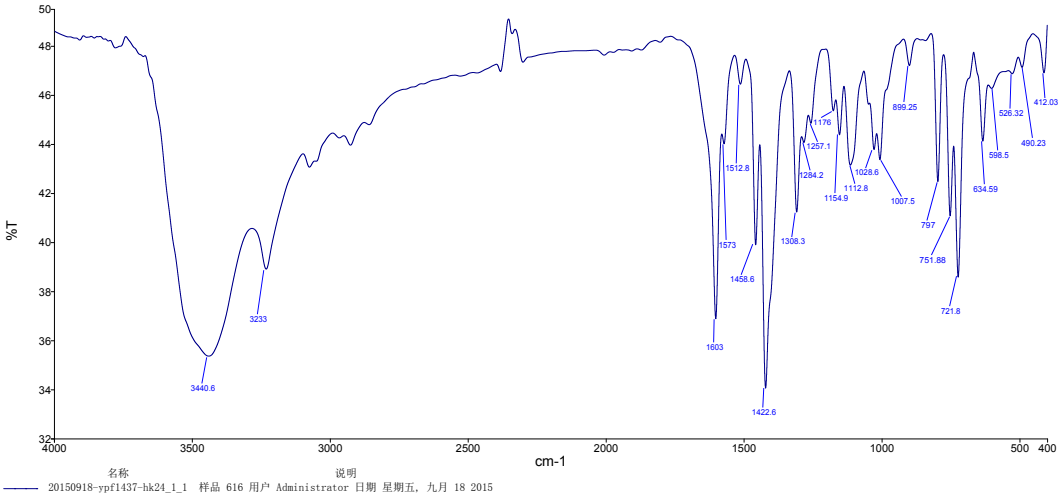

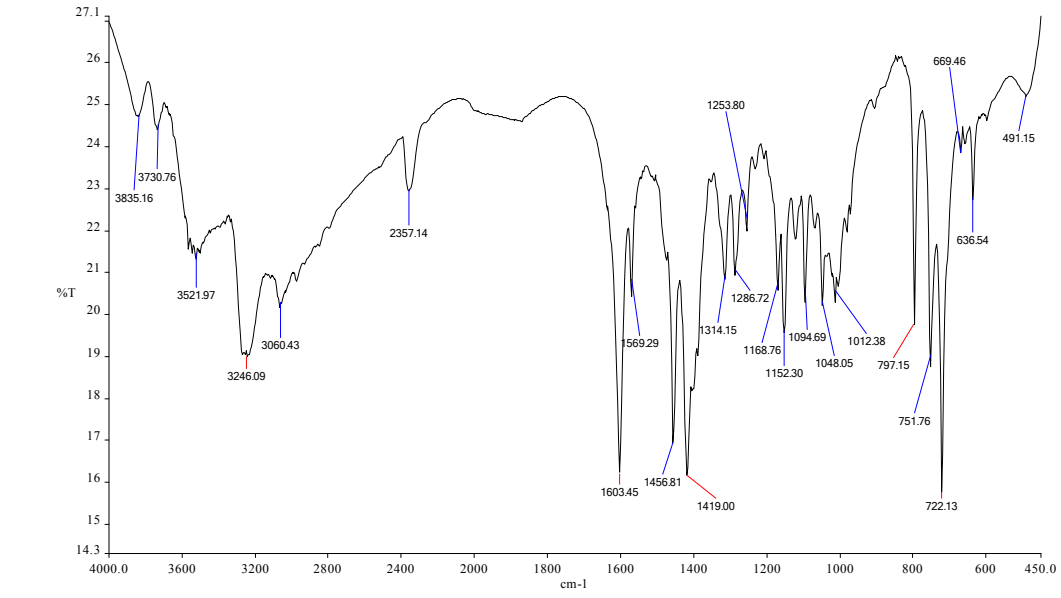

Fig **S2** The IR curves for complexes **1- 6**.

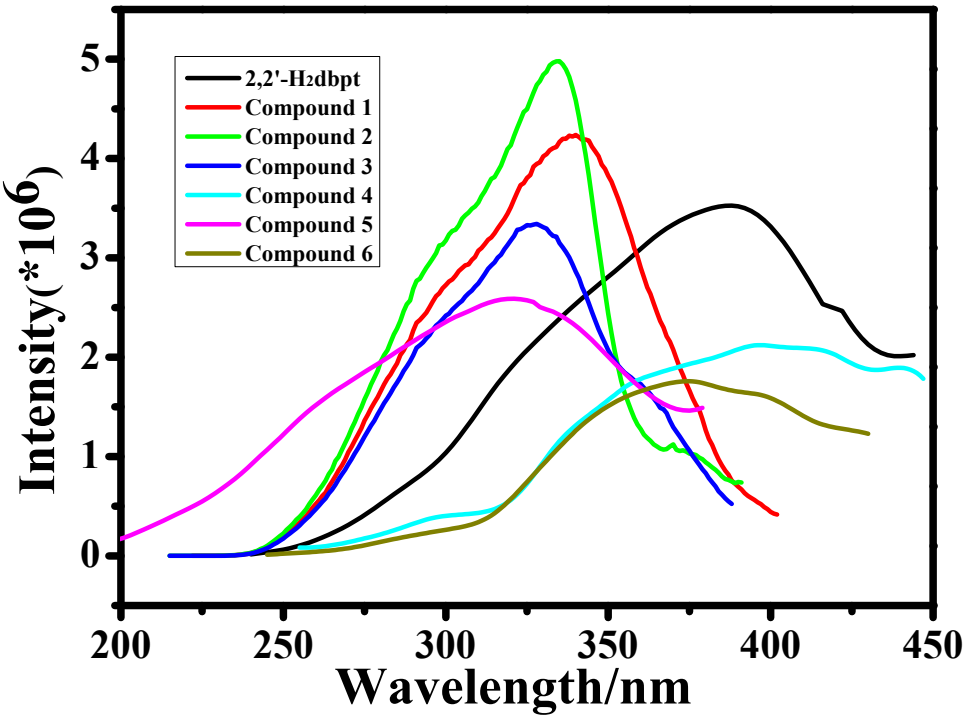

Fig S3 The excited band of **1-6** as well as the free ligand 2,2′- H_2dbpt.

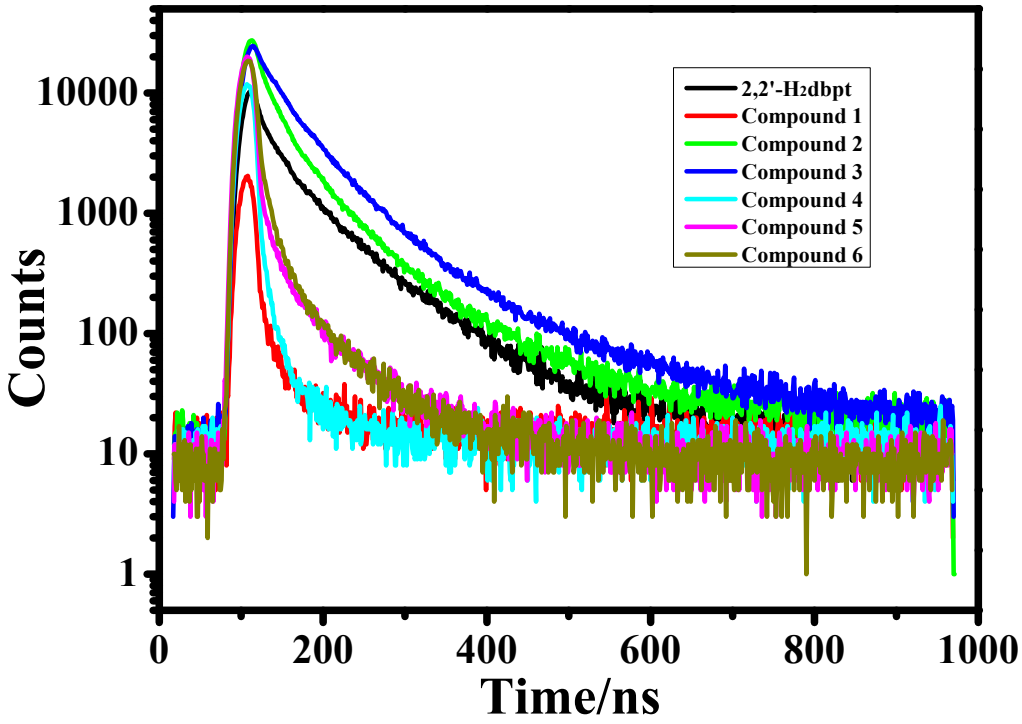

Fig S4 Luminescence decay curves for complexes **1-6** and 2,2′- H_2dbpt.