Supporting Information

The Influence of Structural Isomerism on Fluorescence and Organic Dye Selective Adsorption in Two Complexes Based on Flexible Ligands

Wen-Huan Huang*†, Jia-Zhi Li†, Lu-Sha Gao†, Yan-Xin Wang†, Shu-Ya Liu†, Min Jiang†, Tong Liu† and Yao-Yu Wang‡

† College of Chemistry & Chemical Engineering, Shaanxi University of Science & Techology, Xi'an, Shaanxi 710021, China.
‡ Key Laboratory of Synthetic and Natural Functional Molecule Chemistry of Ministry of Education, Department of Chemistry, Northwest University, Xi'an, Shaanxi, 710069, P.R. China.

TABLE OF CONTENTS

c(1) THE SUPPORTING FIGURES

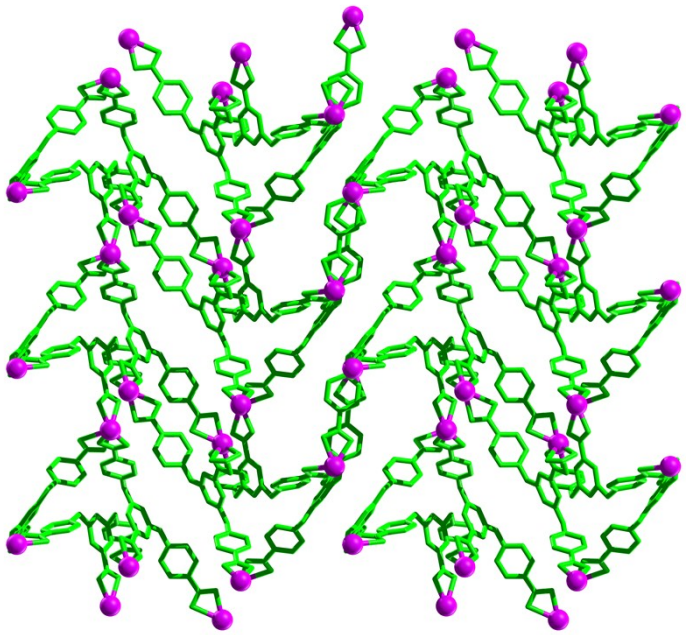

Figure S1. The 3D structure without the bpa linkers of **1** along the *a* axis.

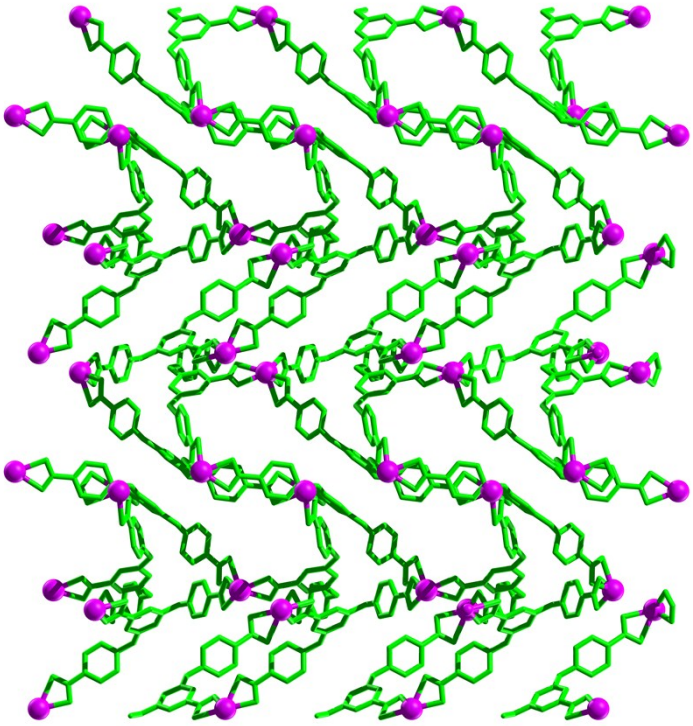

Figure S2. The 3D structure without the bpa linkers of **1** along the *b* axis.

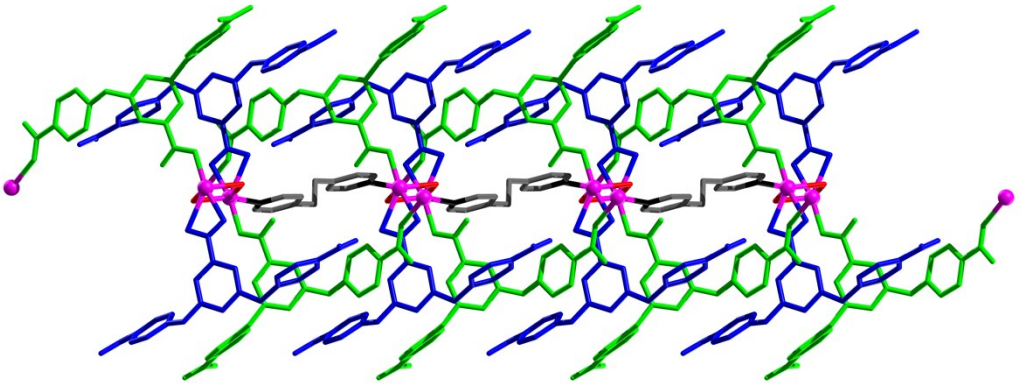

Figure S3. The 2D structure of **2** view along *a* axis.

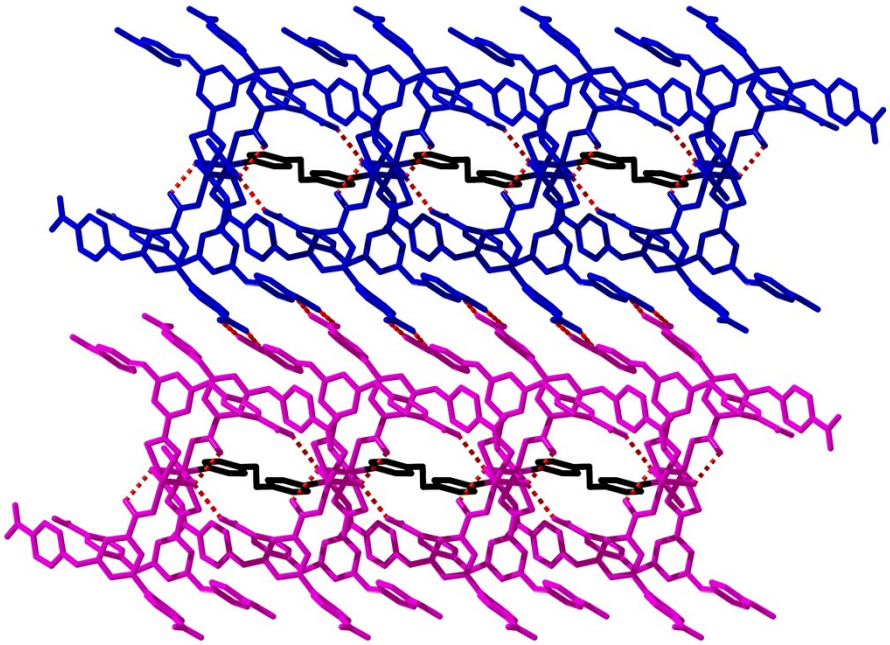

Figure S4. The 3D stacking of **2** along the *a* axis.

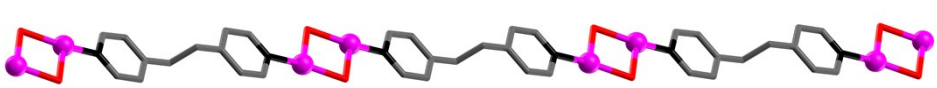

Figure S5. The assembly of bpa linkers in complex **2**.

(2) IR RESULTs

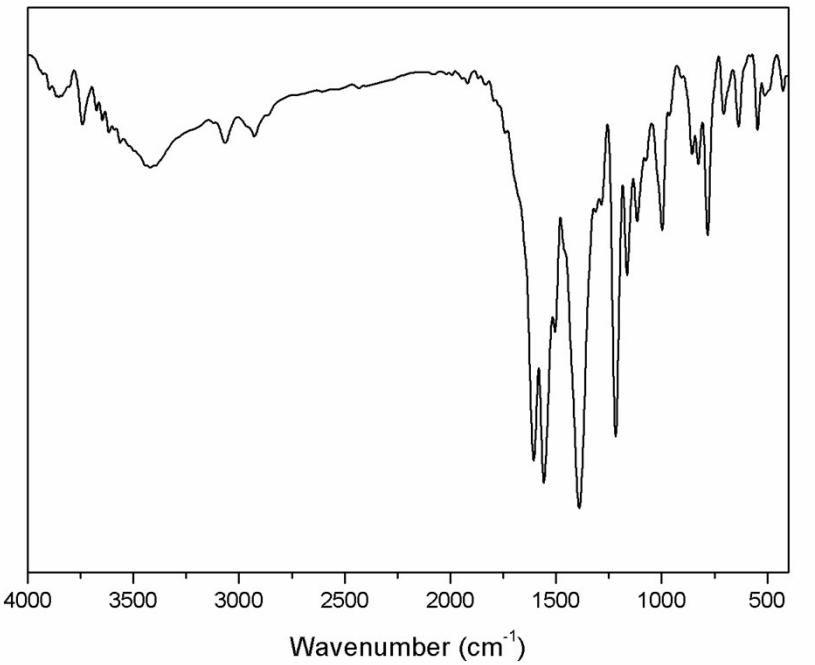

Figure S6. FT-IR spectroscopy of the complex **1.**

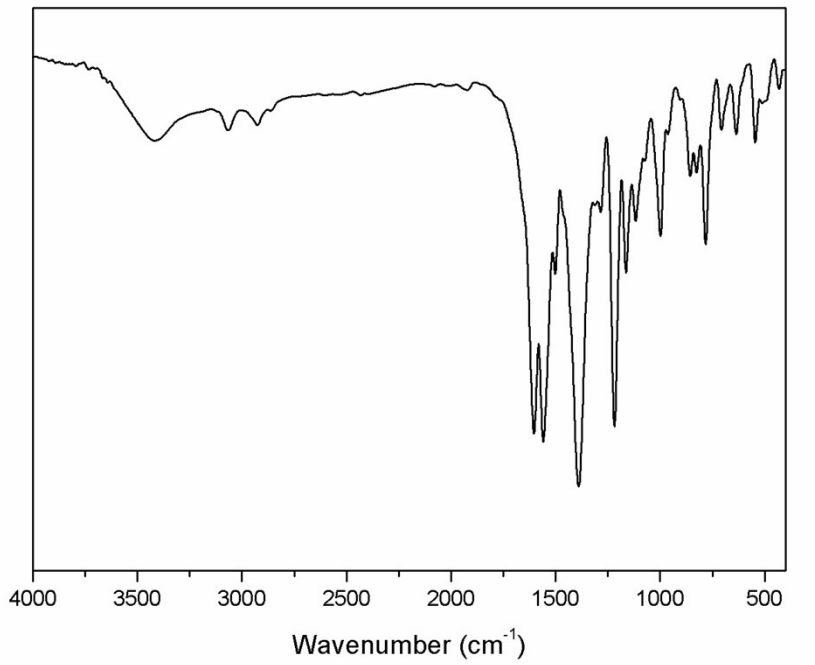

Figure S7. FT-IR spectroscopy of the complex **2**.

(3) PXRD and TGA RESULTs

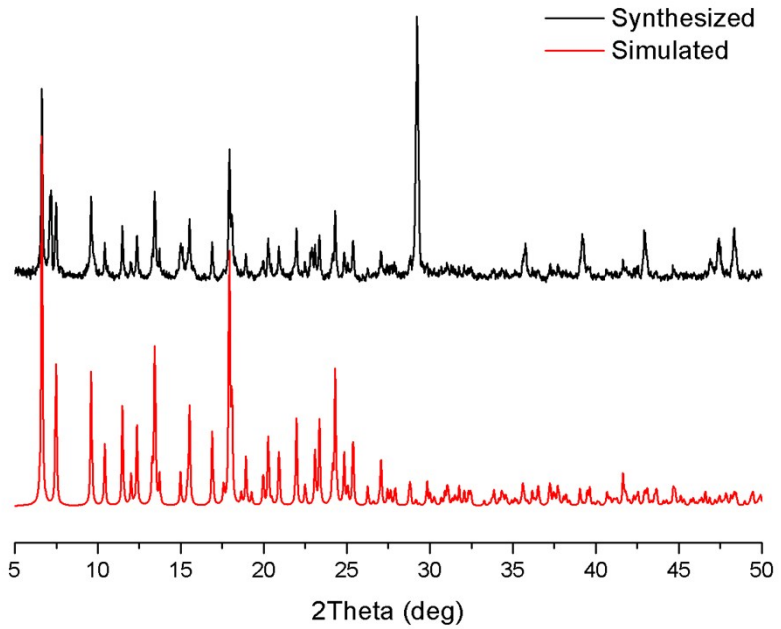

Figure S8. The PXRD result of **1**.

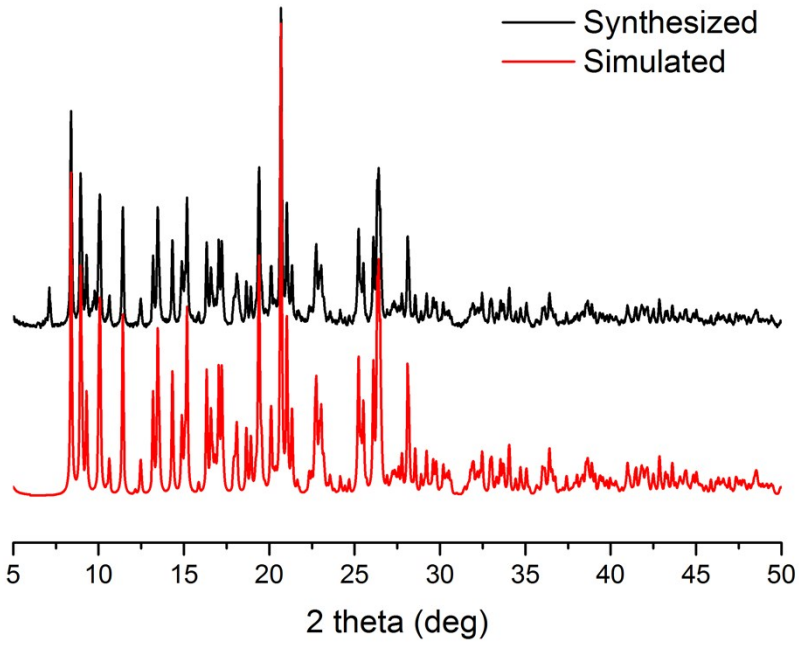

Figure S9. The PXRD result of **2.**

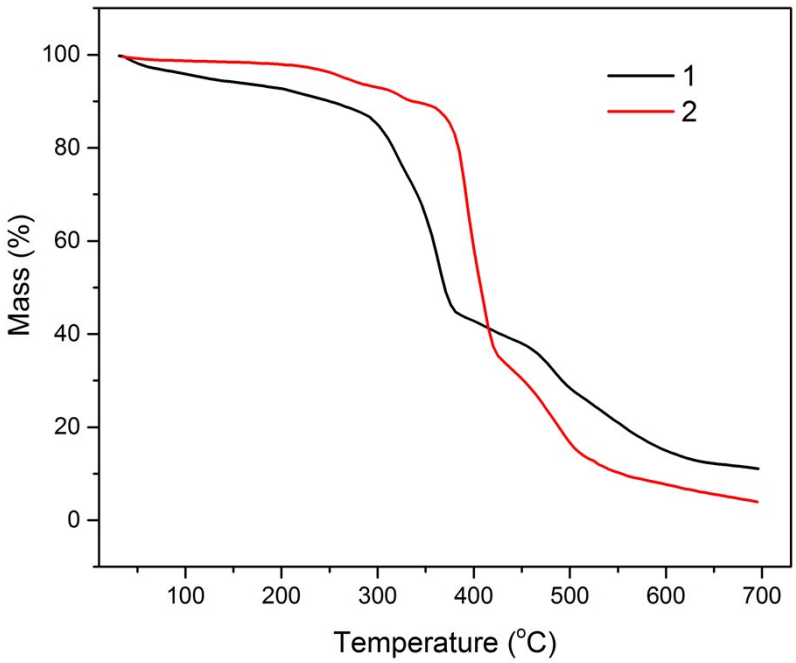

Figure S10. TGA curves of complex **1-2**.

(4) LUMINESCENCE SENSING FIGURES

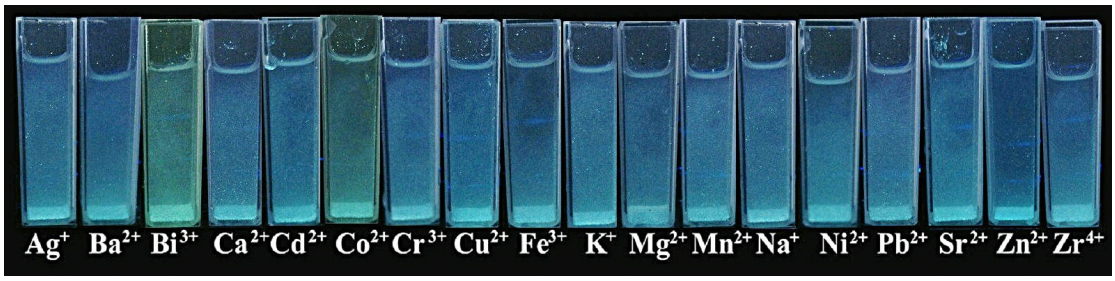

Figure S11. The visual fluorescence of complexes **1** after the addition of various metal cations.

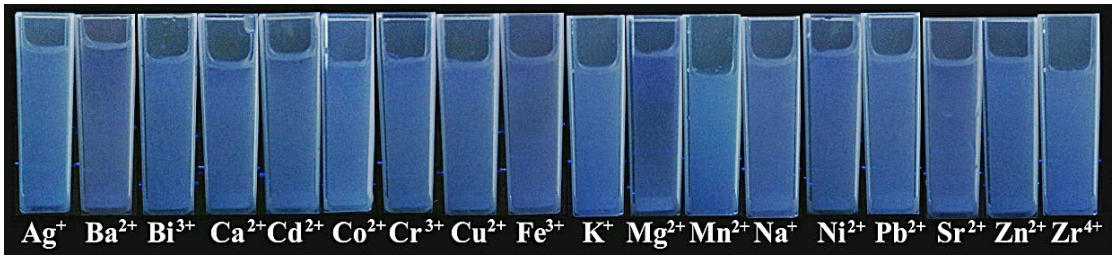

Figure S12. The visual fluorescence of complexes **2** after the addition of various metal cations.

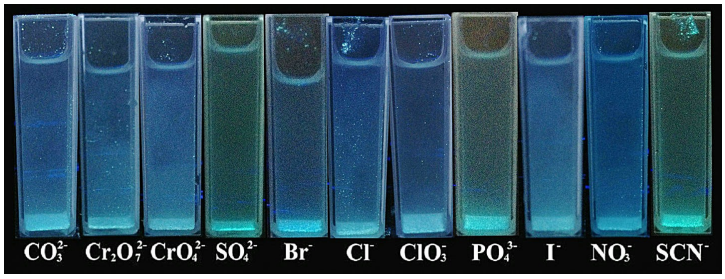

Figure S13. The visual fluorescence of complexes **1** after the addition of various anions.

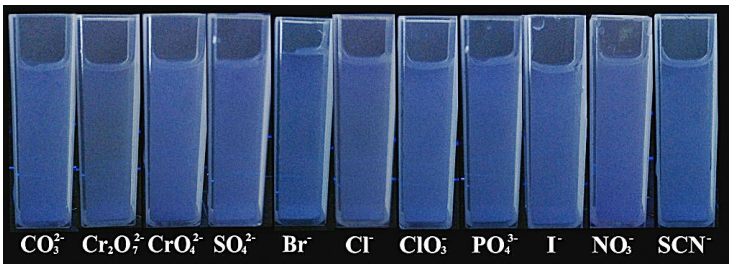

Figure S14. The visual fluorescence of complexes **2** after the addition of various anions.

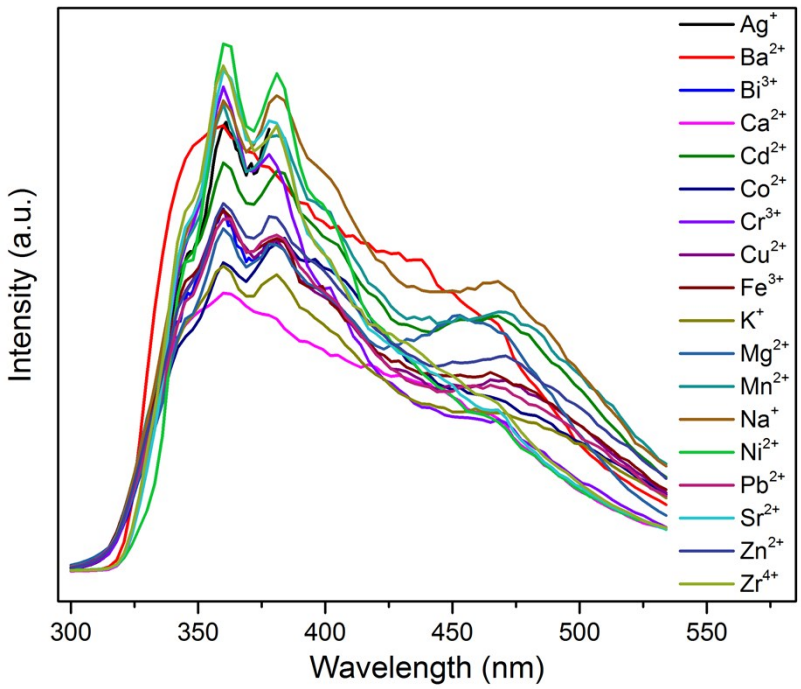

Figure S15. The fluorescence emission of complexes **1** suspension with various metal cations.

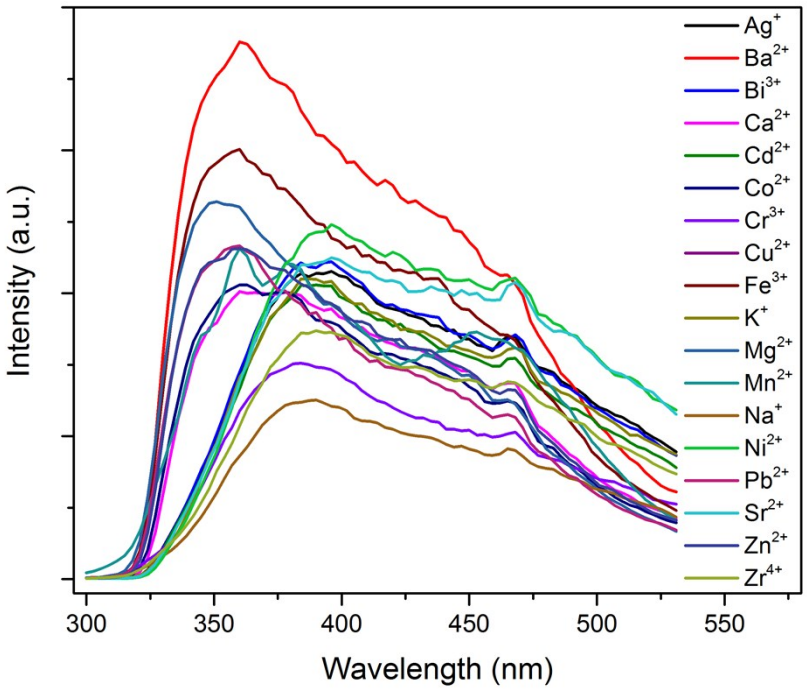

Figure S16. The fluorescence emission of complexes **2** suspension with various metal cations.

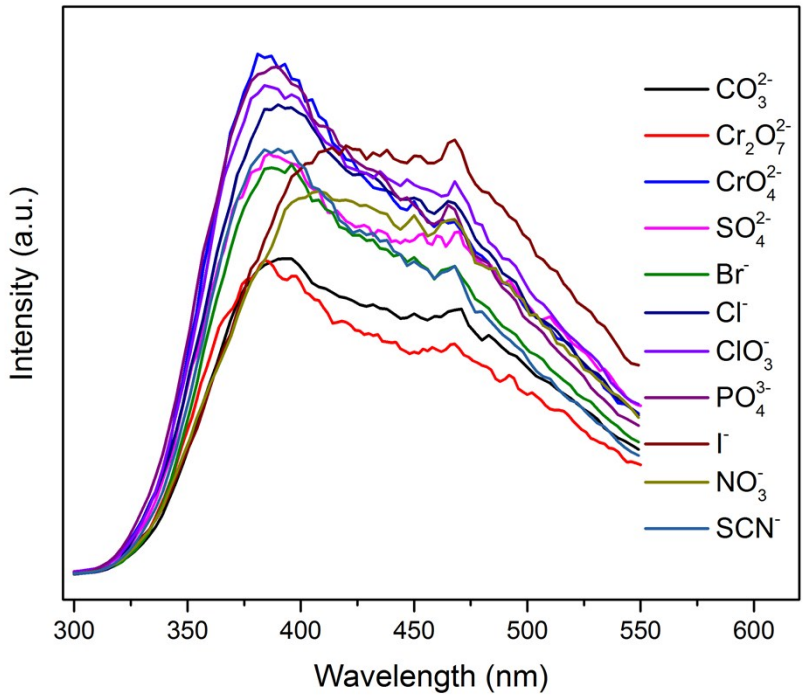

Figure S17. The fluorescence emission of complexes **1** suspension with various anions.

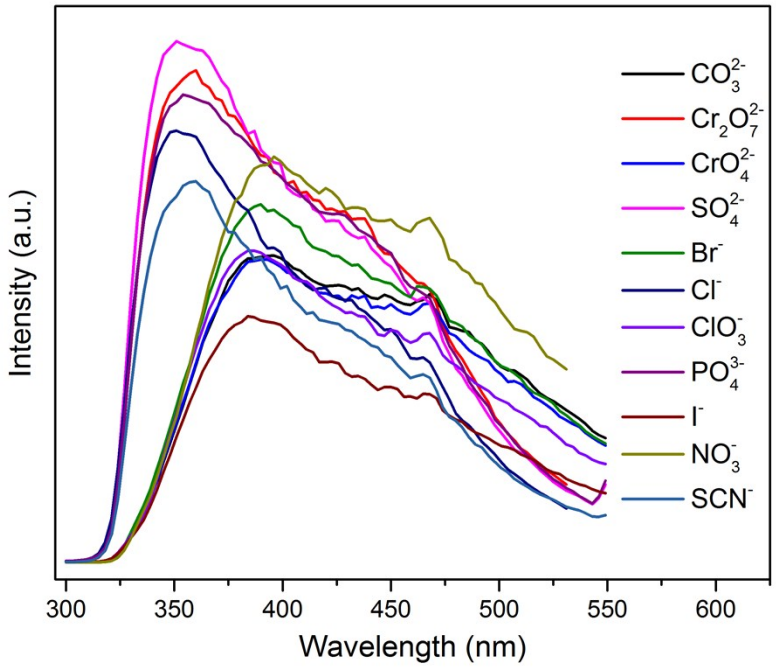

Figure S18. The fluorescence emission of complexes **2** suspension with various anions.

(5) ADSORPTION OF DYES

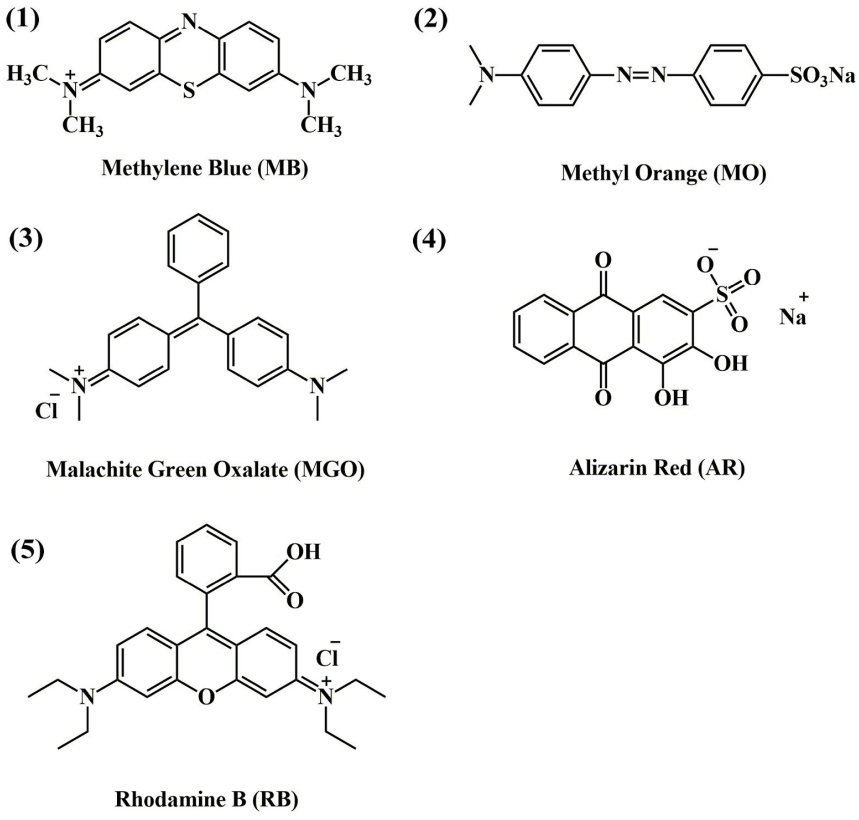

Figure S19. The structures of five kinds of dyes.

Figure S20. The naked-eye photos of dyes in 2 hours after the additions of complexes **1**.

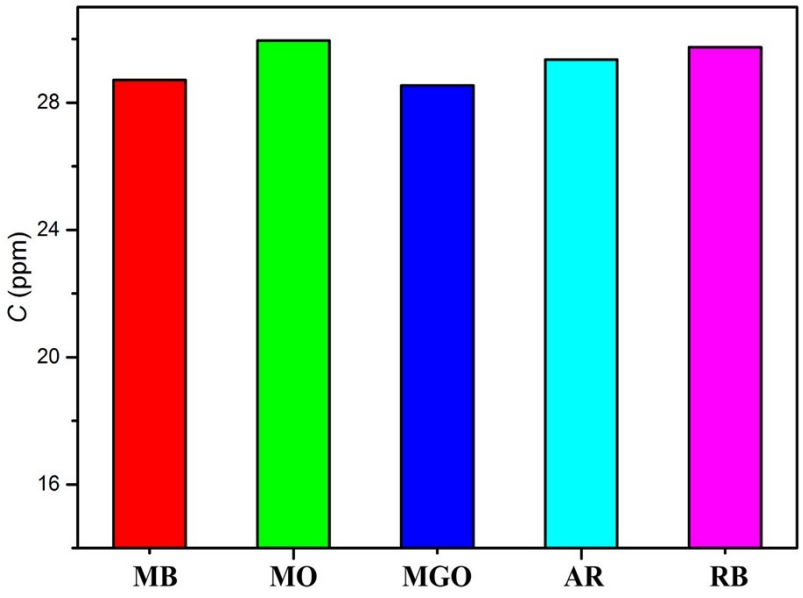

Figure S21. The concentrations of dyes in 2 hours after the additions of complexes **1**.

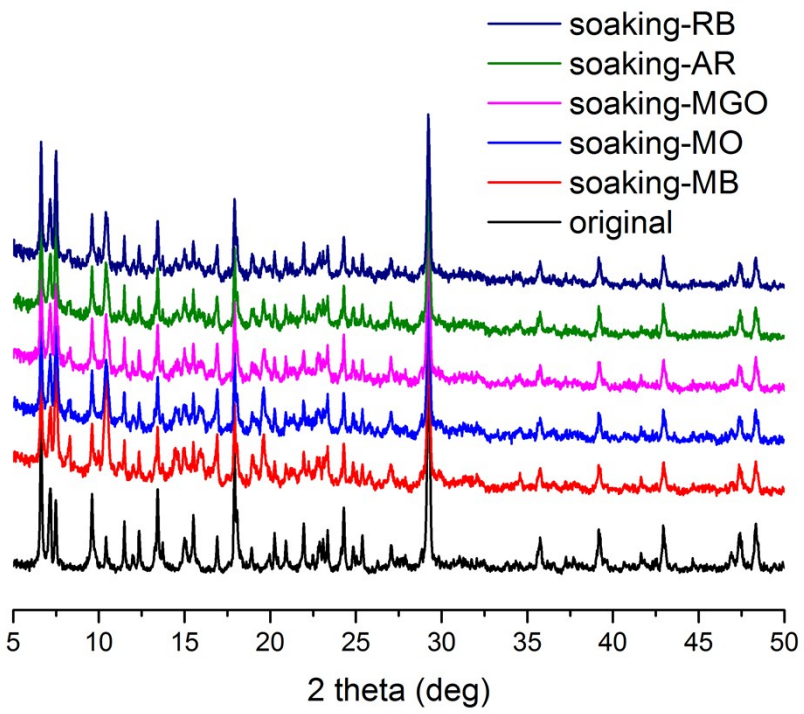

Figure S22. The PXRD results of complexes **1** after soaking in five dyes.

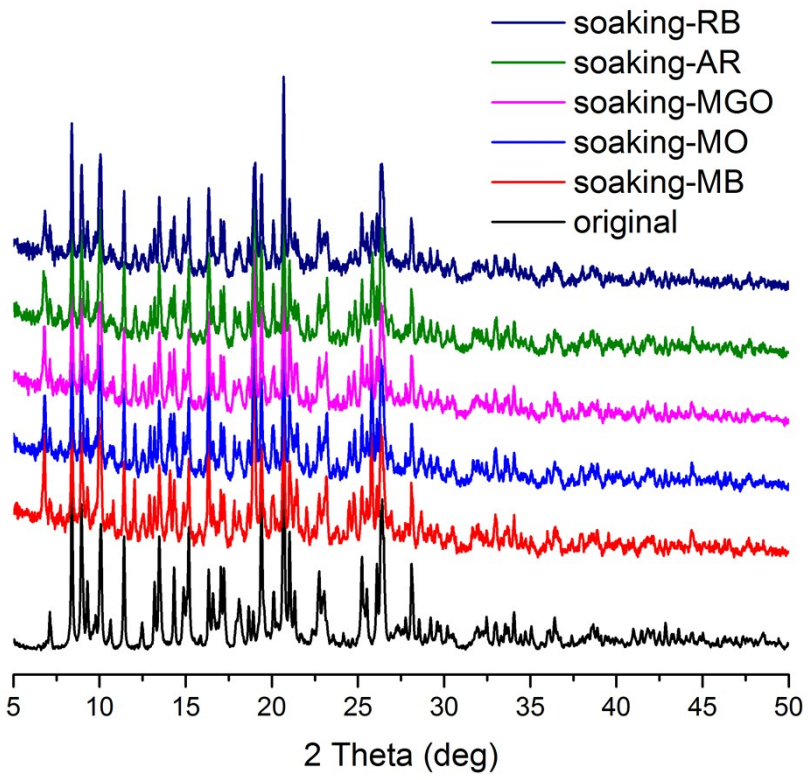

Figure S23. The PXRD results of complexes **2** after soaking in five dyes.

(6) CRYSTALLOGRAPHIC DATAS TABLES

Table S1. Crystallographic data and details of diffraction experiments for complexes **1-2**.

Complex 1			
Formula	$C_{66}H_{60}Cd_3N_4O_{23}$	V (Å^3)	5227(5)
M_r	1614.36	Z	3
Crystal system	Trigonal	ρ (g cm^{-3})	1.537
Space group	$P3_221$	μ (mm^{-1})	0.985
a (Å)	15.398(8)	T (K)	293(2)
b (Å)	15.398(8)	Goof	1.027
c (Å)	25.456(14)	R [$I > 2\sigma(I)$]	R1 = 0.0703
α (°)	90		wR2 = 0.1780
β (°)	90	R (all data)	R1 = 0.1043
γ (°)	120		wR2 = 0.2044
Complex 2			
Formula	$C_{48}H_{34}CdNO_{17}$	V (Å^3)	2092.0(4)
M_r	1009.16	Z	2
Crystal system	Triclinic	ρ (g cm^{-3})	1.602
Space group	P-1	μ (mm^{-1})	0.605
a (Å)	10.0495(13)	T (K)	296(2)
b (Å)	11.2187(14)	Goof	1.068
c (Å)	19.950(2)	R [$I > 2\sigma(I)$]	R1 = 0.0415
α (°)	79.844(2)		wR2 = 0.1176
β (°)	82.668(2)	R (all data)	R1 = 0.0500
γ (°)	71.385(2)		wR2 = 0.1347

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

Table S2. Selected Bond Lengths (Å) and Angles (deg) for **1-2**.

Complex **1**			
Cd(1)-O(5)#2	2.239(5)	Cd(1)-N(1B)	2.315(8)
Cd(1)-O(7)#3	2.315 (8)	Cd(1)-N(1A)	2.341(7)
Cd(1)-O(1)	2.345(6)	Cd(1)-O(2)	2.385(6)
Cd(1)-O(8)#3	2.544(7)	Cd(1)-O(4)#2	2.582(7)
Cd(2)-N(2)#4	2.223(8)	Cd(2)-O(1W)	2.160(7)
Cd(2)-O(3W)	2.350(14)	Cd(2)-O(2W)	2.264(17)
Cd(2)-N(2)	2.346(7)	Cd(2)-O(1W)#4	2.348(7)
Cd(2)-O(2W)#4	2.283(16)	Cd(2)-O(3W)#4	2.387(14)
O(5)#2-Cd(1)-N(1B)	105.0(4)	O(5)#2-Cd(1)-O(7)#3	114.3(2)
N(1B)-Cd(1)-O(7)#3	88.2(4)	O(5)#2-Cd(1)-N(1A)	100.9(3)
O(5)#2-Cd(1)-O(1)	138.3(3)	O(7)#3-Cd(1)-N(1A)	82.2(3)

O(7)#3-Cd(1)-O(1)	107.4(3)	N(1B)-Cd(1)-O(1)	77.4(3)
O(5)#2-Cd(1)-O(2)	110.0(2)	N(1A)-Cd(1)-O(1)	86.1(3)
O(7)#3-Cd(1)-O(2)	106.0(2)	N(1B)-Cd(1)-O(2)	131.6(3)
O(1)-Cd(1)-O(2)	54.2(2)	N(1A)-Cd(1)-O(2)	140.3(3)
N(1B)-Cd(1)-O(8)#3	138.1(3)	O(5)#2-Cd(1)-O(8)#3	83.6(2)
N(1A)-Cd(1)-O(8)#3	130.0(3)	O(7)#3-Cd(1)-O(8)#3	52.2(2)
O(2)-Cd(1)-O(8)#3	79.0(2)	O(1)-Cd(1)-O(8)#3	122.9(2)
N(1B)-Cd(1)-O(4)#2	85.4(4)	O(5)#2-Cd(1)-O(4)#2	52.8(2)
N(1A)-Cd(1)-O(4)#2	89.2(3)	O(7)#3-Cd(1)-O(4)#2	163.0(2)
O(2)-Cd(1)-O(4)#2	90.0(2)	O(1)-Cd(1)-O(4)#2	86.6(2)
O(1W)#4-Cd(2)-O(1W)	167.9(5)	O(8)#3-Cd(1)-O(4)#2	128.1 (2)
O(1W)-Cd(2)-N(2)	88.8(3)	O(1W)#4-Cd(2)-N(2)	88.0(3)
O(1W)-Cd(2)-N(2)#4	96.1(3)	O(1W)#4-Cd(2)-N(2)#4	87.3(3)
O(1W)#4-Cd(2)-O(2W)	86.4(8)	N(2)-Cd(2)-N(2)#4	175.06(16)
N(2)-Cd(2)-O(2W)	91.0(9)	O(1W)-Cd(2)-O(2W)	82.0(8)
O(1W)#4-Cd(2)-O(3W)#4	81.0(4)	N(2)#4-Cd(2)-O(2W)	90.1(9)
N(2)-Cd(2)-O(3W)#4	89.3(6)	O(1W)-Cd(2)-O(3W)#4	110.6(4)
O(2W)-Cd(2)-O(3W)#4	167.4(8)	N(2)#4-Cd(2)-O(3W)#4	88.5(6)
O(1W)-Cd(2)-O(3W)	85.8(5)	O(1W)#4-Cd(2)-O(3W)	105.6(4)
N(2)#4-Cd(2)-O(3W)	93.3(6)	N(2)-Cd(2)-O(3W)	86.6(6)
O(3W)#4-Cd(2)-O(3W)	24.9(7)	O(2W)-Cd(2)-O(3W)	167.7(8)
O(1W)-Cd(2)-O(2W)#4	90.5(8)	N(2)#4-Cd(2)-O(2W)#4	93.8(9)
O(2W)#4-Cd(2)-N(2)	86.6(9)	O(1W)-Cd(2)-O(1W)#4	167.9(5)

Symmetry transformations used to generate equivalent atoms: #1 x-y+1,-y+1,-z+1/3; #2 x-y,-y+1,-z+1/3; #3 -x+y+1,-x+1,z+1/3; #4 x-y+1,-y+2,-z-2/3; #5 -y+1,x-y,z-1/3.

Table S3. Selected Bond Lengths (Å) and Angles (deg) for **2**.

Complex **2**			
Cd(1)-O(10)	2.265(3)	Cd(1)-O(4)#1	2.361(3)
Cd(1)-O(1)	2.346(3)	Cd(1)-O(1W)#2	2.411(3)
Cd(1)-O(1W)	2.383(3)	Cd(1)-N(1)	2.313(4)
Cd(1)-O(9)	2.560(3)		
O(10)-Cd(1)-N(1)	98.77(12)	O(10)-Cd(1)-O(1)	167.91(10)
N(1)-Cd(1)-O(1)	91.59(12)	O(10)-Cd(1)-O(4)#1	94.66(10)
N(1)-Cd(1)-O(4)#1	85.07(11)	O(1)-Cd(1)-O(4)#1	79.96(10)
O(10)-Cd(1)-O(1W)	84.64(11)	N(1)-Cd(1)-O(1W)	163.69(12)
O(1)-Cd(1)-O(1W)	83.70(11)	O(4)#1-Cd(1)-O(1W)	78.74(11)
O(10)-Cd(1)-O(1W)#2	103.65(11)	N(1)-Cd(1)-O(1W)#2	117.81(11)
O(1)-Cd(1)-O(1W)#2	76.61(11)	O(4)#1-Cd(1)-O(1W)#2	147.32(11)
O(1W)-Cd(1)-O(1W)#2	76.34(12)	O(10)-Cd(1)-O(9)	53.57(10)
N(1)-Cd(1)-O(9)	78.92(11)	O(1)-Cd(1)-O(9)	135.54(9)
O(4)#1-Cd(1)-O(9)	140.75(10)	O(1W)-Cd(1)-O(9)	115.18(11)
O(1W)#2-Cd(1)-O(9)	70.30(10)		

Symmetry transformations used to generate equivalent atoms: #1 x+1,y-1,z ; #2 -x,-y+1,-z+1; #3 x-1,y+1,z; #4 -x+1,-y+2,-z+1.

REFERENCES

[1] Sheldrick G M. *SHELXL-97*, *Program for Crystal Structure Determination*, University of Göttingen, Germany, 1997.

[2] Sheldrick G M. *SHELXL-97*, P*rogram for Crystal Structure Refinement*, University of Göttingen, Germany, 1997.