Supplementary Material (ESI) for CrystEngComm
This journal is © The Royal Society of Chemistry

Bis(pyridyl)-bis(amide)-modulated a series of metal-1,2-phenylenediacetate coordination polymers: Construction and selective dye adsorption

Xiuli Wang,* Jing Zhao, Mao Le, Hongyan Lin, Guocheng Liu and Xiang Wang

Table S1 Selected bond distances (Å) and angles (°) for complexes **1–5**.

Complex **1**			
Cu(1)-O(1)	1.9311(15)	Cu(1)-N(1)	2.0425(18)
Cu(1)-O(3)#1	1.9962(15)	Cu(1)-O(2)#3	2.3355(16)
Cu(1)-N(2)#2	2.0314(18)	N(2)#2-Cu(1)-N(1)	177.54(7)
O(1)-Cu(1)-O(3)#1	161.73(7)	O(1)-Cu(1)-O(2)#3	111.94(7)
O(1)-Cu(1)-N(2)#2	92.28(7)	O(3)#1-Cu(1)-O(2)#3	86.29(6)
O(3)#1-Cu(1)-N(2)#2	87.51(7)	N(2)#2-Cu(1)-O(2)#3	93.80(7)
O(1)-Cu(1)-N(1)	89.82(7)	N(1)-Cu(1)-O(2)#3	86.59(7)
O(3)#1-Cu(1)-N(1)	90.09(7)		
Symmetry code for **1**: #1 $x-1, y, z$; #2 $x, y+1, z-1$; #3 $-x, -y+1, -z+1$			
Complex **2**			
Cu(1)-O(1)	1.917(3)	Cu(1)-N(2)#2	2.065(3)
Cu(1)-O(4)#1	1.940(3)	Cu(1)-O(1W)	2.298(3)
Cu(1)-N(1)	2.048(3)	N(1)-Cu(1)-N(2)#2	175.71(14)
O(1)-Cu(1)-O(4)#1	160.48(12)	O(1)-Cu(1)-O(1W)	103.24(11)
O(1)-Cu(1)-N(1)	88.79(12)	O(4)#1-Cu(1)-O(1W)	96.20(11)
O(4)#1-Cu(1)-N(1)	90.57(12)	N(1)-Cu(1)-O(1W)	86.99(12)
O(1)-Cu(1)-N(2)#2	90.24(13)	N(2)#2-Cu(1)-O(1W)	89.17(12)
O(4)#1-Cu(1)-N(2)#2	91.75(12)		
Symmetry code for **2**: #1 $x-1, y, z$; #2 $-x-1, y-1/2, -z+3/2$			
Complex **3**			
Ni(1)-O(4)#1	2.026(2)	Ni(2)-O(5)	2.026(2)
Ni(1)-O(1)	2.056(2)	Ni(2)-O(3)	2.059(2)
Ni(1)-O(6)#1	2.063(2)	Ni(2)-O(8)#1	2.070(2)
Ni(1)-O(1W)	2.080(2)	Ni(2)-N(3)	2.115(3)
Ni(1)-N(1)	2.121(3)	Ni(2)-O(1W)#3	2.119(2)
Ni(1)-N(4)#2	2.179(3)	Ni(2)-N(2)	2.138(3)
O(4)#1-Ni(1)-O(1)	172.98(10)	O(5)-Ni(2)-O(3)	99.27(10)
O(4)#1-Ni(1)-O(6)#1	99.09(10)	O(5)-Ni(2)-O(8)#1	174.75(10)
O(1)-Ni(1)-O(6)#1	86.22(10)	O(3)-Ni(2)-O(8)#1	85.44(10)
O(4)#1-Ni(1)-O(1W)	90.78(9)	O(5)-Ni(2)-N(3)	90.28(10)
O(1)-Ni(1)-O(1W)	93.65(9)	O(3)-Ni(2)-N(3)	82.35(10)
O(6)#1-Ni(1)-O(1W)	91.96(9)	O(8)#1-Ni(2)-N(3)	88.07(11)
O(4)#1-Ni(1)-N(1)	87.28(10)	O(5)-Ni(2)-O(1W)#3	90.60(9)
O(1)-Ni(1)-N(1)	88.87(11)	O(3)-Ni(2)-O(1W)#3	91.70(9)

O(6)#1-Ni(1)-N(1)	82.48(10)	O(8)#1-Ni(2)-O(1W)#3	91.56(9)
O(1W)-Ni(1)-N(1)	173.74(10)	N(3)-Ni(2)-O(1W)#3	174.05(10)
O(4)#1-Ni(1)-N(4)#2	85.96(11)	O(5)-Ni(2)-N(2)	86.82(11)
O(1)-Ni(1)-N(4)#2	88.84(11)	O(3)-Ni(2)-N(2)	173.27(10)
O(6)#1-Ni(1)-N(4)#2	174.82(11)	O(8)#1-Ni(2)-N(2)	88.36(10)
O(1W)-Ni(1)-N(4)#2	86.77(10)	N(3)-Ni(2)-N(2)	94.85(11)
N(1)-Ni(1)-N(4)#2	99.02(11)	O(1W)#3-Ni(2)-N(2)	91.08(10)

Symmetry code for **3**: #1 $x + 1/2, -y + 1/2, -z$; #2 $-x, y, -z - 1/2$; #3 $x - 1/2, -y + 1/2, -z$

Complex **4**

Cu(1)-O(2)#1	1.944(5)	Cu(2)-O(1)	1.957(5)
Cu(1)-O(6)	1.960(4)	Cu(2)-O(6)#4	1.947(4)
Cu(1)-O(6)#2	1.993(5)	Cu(2)-O(6)	1.947(4)
Cu(1)-N(1)	2.067(6)	Cu(2)-O(1)#4	1.957(5)
Cu(1)-O(3)#3	2.235(5)	O(6)#2-Cu(1)-O(3)#3	87.36(19)
O(2)#1-Cu(1)-O(6)	163.8(2)	N(1)-Cu(1)-O(3)#3	93.7(2)
O(2)#1-Cu(1)-O(6)#2	91.2(2)	O(6)#4-Cu(2)-O(6)	180
O(6)-Cu(1)-O(6)#2	81.3(2)	O(6)#4-Cu(2)-O(1)#4	86.81(19)
O(2)#1-Cu(1)-N(1)	88.0(2)	O(6)-Cu(2)-O(1)#4	93.19(19)
O(6)-Cu(1)-N(1)	99.2(2)	O(6)#4-Cu(2)-O(1)	93.19(19)
O(6)#2-Cu(1)-N(1)	178.8(2)	O(6)-Cu(2)-O(1)	86.81(19)
O(2)#1-Cu(1)-O(3)#3	102.1(2)	O(1)#4-Cu(2)-O(1)	180.000(2)
O(6)-Cu(1)-O(3)#3	91.91(18)		

Symmetry code for **4**: #1 $x - 1, y, z$; #2 $-x, -y + 1, -z + 1$; #3 $x - 1, y - 1, z$; #4 $-x + 1, -y + 1, -z + 1$

Complex **5**

Co(1)-O(1)	2.0513(14)	Co(1)-O(3)#2	2.1309(14)
Co(1)-O(2)#1	2.0575(13)	Co(1)-N(1)	2.1616(16)
Co(1)-O(1W)	2.0763(16)	Co(1)-O(4)#2	2.2082(13)
O(1)-Co(1)-O(2)#1	94.44(6)	O(1W)-Co(1)-N(1)	174.86(7)
O(1)-Co(1)-O(1W)	97.86(7)	O(3)#2-Co(1)-N(1)	85.11(6)
O(2)#1-Co(1)-O(1W)	90.40(6)	O(1)-Co(1)-O(4)#2	106.50(5)
O(1)-Co(1)-O(3)#2	164.08(6)	O(2)#1-Co(1)-O(4)#2	158.93(6)
O(2)#1-Co(1)-O(3)#2	99.12(6)	O(1W)-Co(1)-O(4)#2	84.48(6)
O(1W)-Co(1)-O(3)#2	90.39(7)	O(3)#2-Co(1)-O(4)#2	60.59(5)
O(1)-Co(1)-N(1)	87.11(6)	N(1)-Co(1)-O(4)#2	95.41(6)
O(2)#1-Co(1)-N(1)	87.88(6)		

Symmetry code for **5**: #1 $-x, y - 1/2, -z + 1/2$; #2 $-x, -y, -z + 1$

Table S2. Selected hydrogen-bonding geometry (Å, º) for complex **1**–**3**

Complex	D–H···A	D–H	H···A	D···A	D–H···A
1	N(3)–H(3B)···O(2W) [i]	0.86	2.04	2.8488	157
	O(2W)–H(2WB)···O(4)	0.85	2.02	2.6870	135
2	N(3)–H(3A)···O(3) [iii]	0.86	2.27	3.1133	167
3	N(5)–H(5B)···O(12) [iv]	0.86	2.03	2.8592	163

Symmetry code: [i] 1 – *x*, –*y*, 1 – *z*; [ii] 1–*x*, –1/2+ *y*, 1/2 – *z*; [iii] 2 – *x*,1 – *y*,1 – *z*; [iv] 3/2 – *x*, –1/2 + *y*, *z*

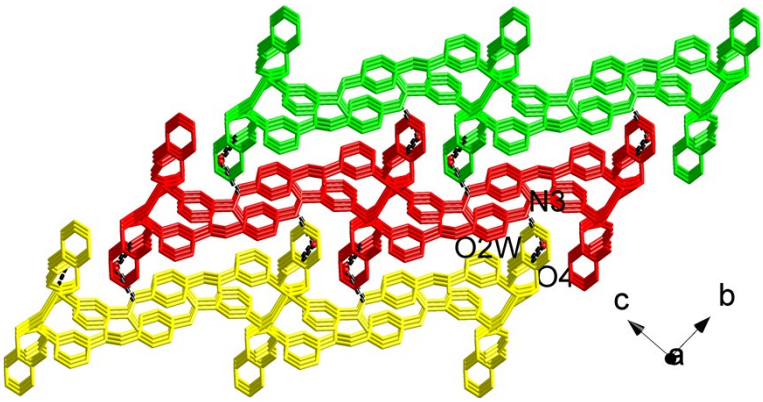


Fig. S1 View of 3D supramolecular architecture of **1**.

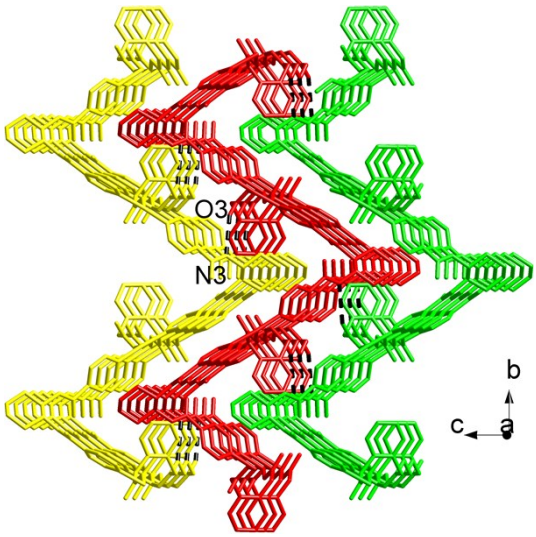


Fig. S2 View of 3D supramolecular architecture of **2**.

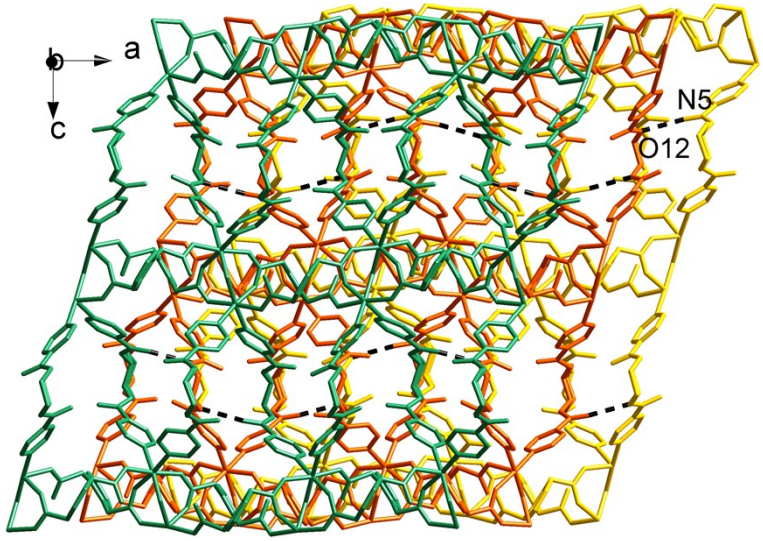


Fig. S3 View of 3D supramolecular architecture of **3**.

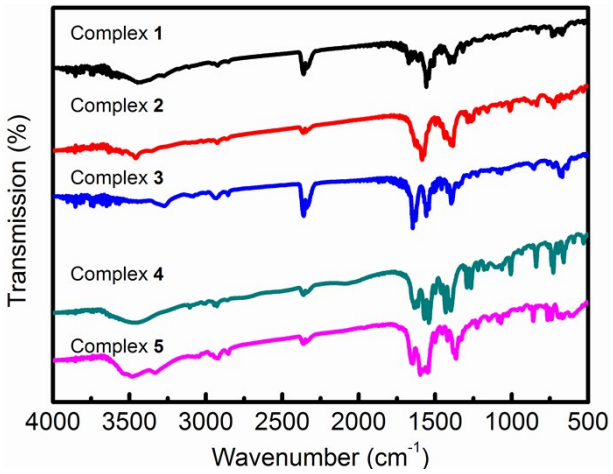
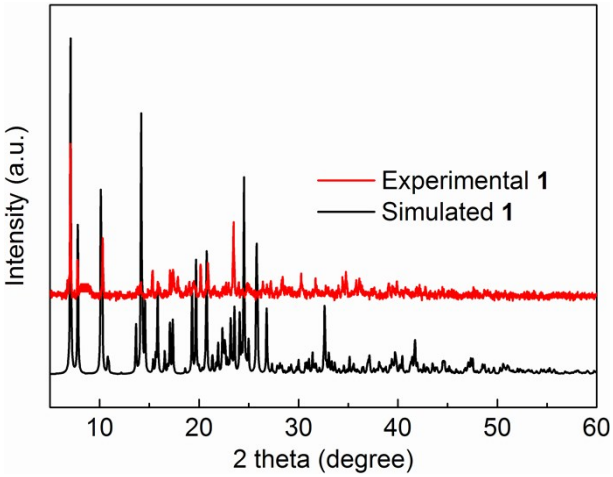
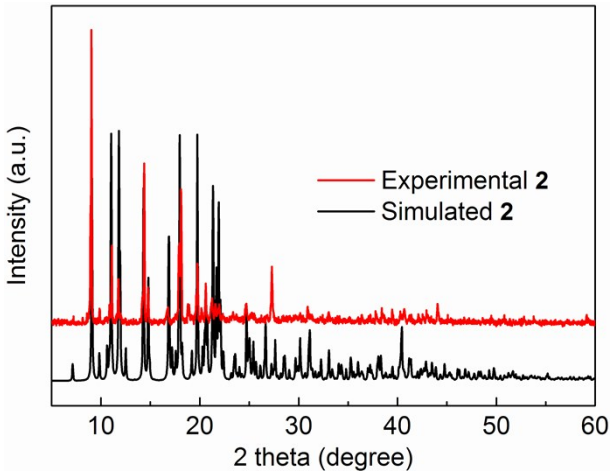
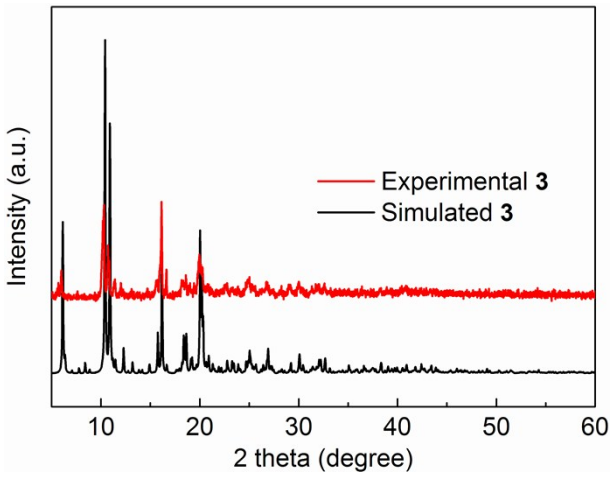


Fig. S4 The IR spectra of complexes **1–5**.


Intensity (a.u.)
Experimental 1
Simulated 1
10
20
30
40
50
60
2 theta (degree)


Intensity (a.u.)
Experimental 2
Simulated 2
10
20
30
40
50
60
2 theta (degree)


Intensity (a.u.)
Experimental 3
Simulated 3
10
20
30
40
50
60
2 theta (degree)

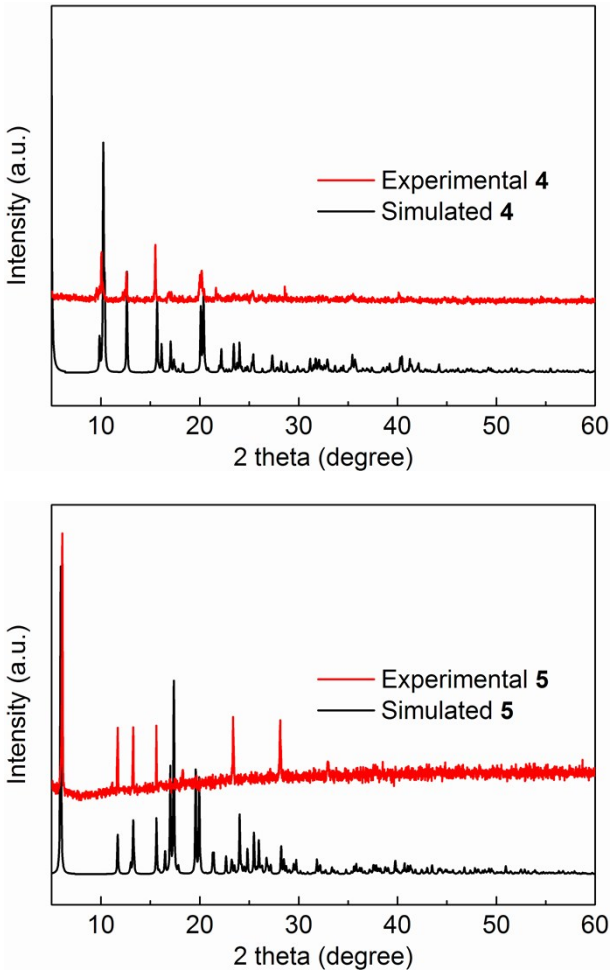


Fig. S5 The simulated (black line) and experimental (red line) powder X-ray diffraction patterns for complexes **1**–**5**.

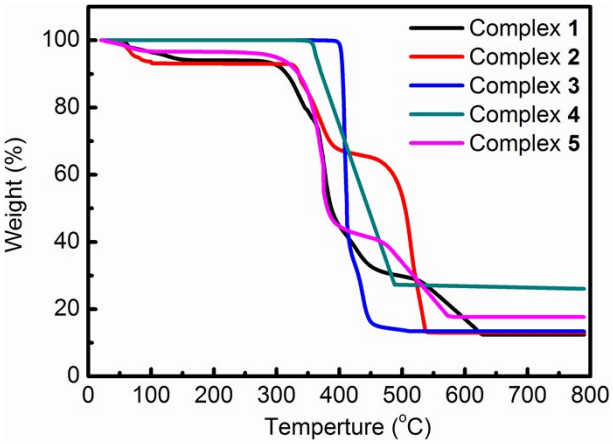


Fig. S6 The TG curves of complexes **1**–**5**.

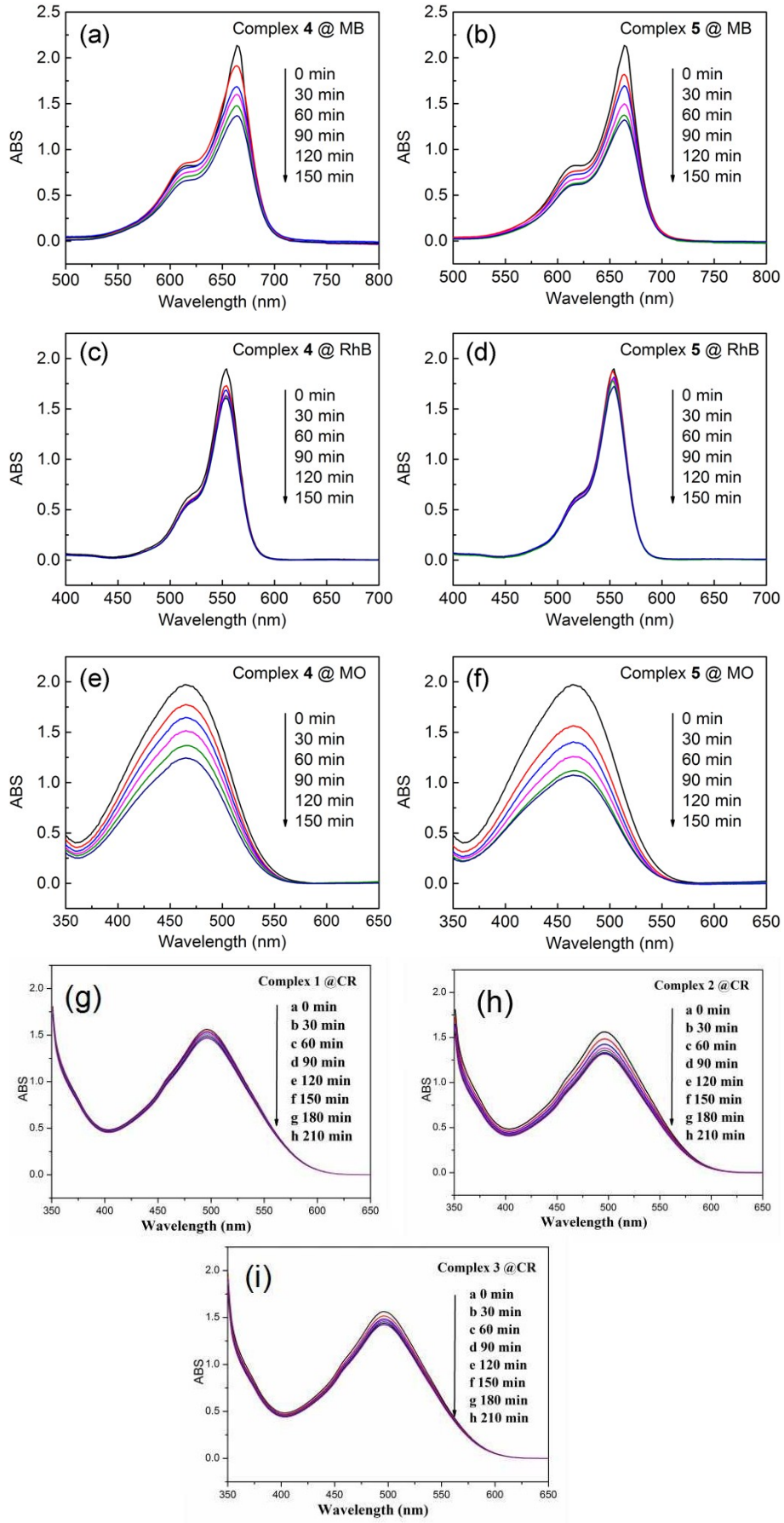

(a)
Complex 4 @ MB
0 min
30 min
60 min
90 min
120 min
150 min
ABS
Wavelength (nm)
(b)
Complex 5 @ MB
0 min
30 min
60 min
90 min
120 min
150 min
ABS
Wavelength (nm)
(c)
Complex 4 @ RhB
0 min
30 min
60 min
90 min
120 min
150 min
ABS
Wavelength (nm)
(d)
Complex 5 @ RhB
0 min
30 min
60 min
90 min
120 min
150 min
ABS
Wavelength (nm)
(e)
Complex 4 @ MO
0 min
30 min
60 min
90 min
120 min
150 min
ABS
Wavelength (nm)
(f)
Complex 5 @ MO
0 min
30 min
60 min
90 min
120 min
150 min
ABS
Wavelength (nm)
(g)
Complex 1 @CR
a 0 min
b 30 min
c 60 min
d 90 min
e 120 min
f 150 min
g 180 min
h 210 min
ABS
Wavelength (nm)
(h)
Complex 2 @CR
a 0 min
b 30 min
c 60 min
d 90 min
e 120 min
f 150 min
g 180 min
h 210 min
ABS
Wavelength (nm)
(i)
Complex 3 @CR
a 0 min
b 30 min
c 60 min
d 90 min
e 120 min
f 150 min
g 180 min
h 210 min
ABS
Wavelength (nm)

Fig. S7 UV-vis absorption spectra of the MB (a), RhB (c) and MO (e) solutions after 150 min with complex **4** in dark; UV-vis spectra of the MB (b), RhB (d) and MO (f) solutions after 150 min with complex **5** in dark; UV-vis spectra of the CR solutions after 210 min with complex **1** (g), **2** (h) and **3** (i) in dark.