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The modulation effect of carboxylic acid ligands on the electron transfer photochromism of naphthalene diimide-derived coordination polymers

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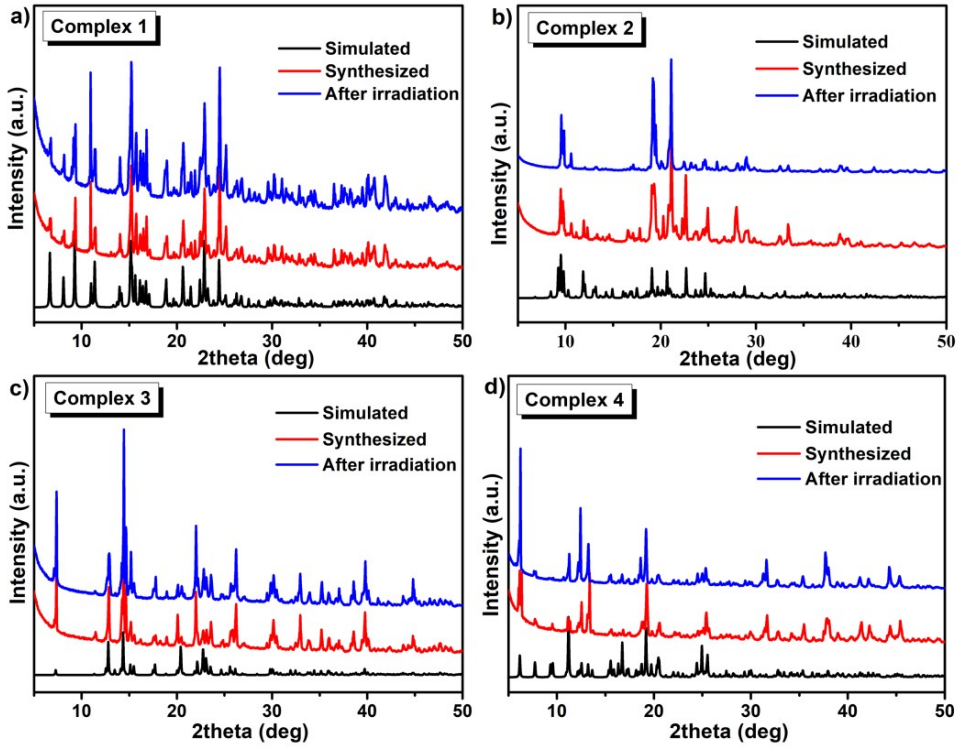

Fig. S1 PXRD patterns of **1-4** simulated from the X-ray single-crystal structures, as-synthesized samples and after irradiation samples.

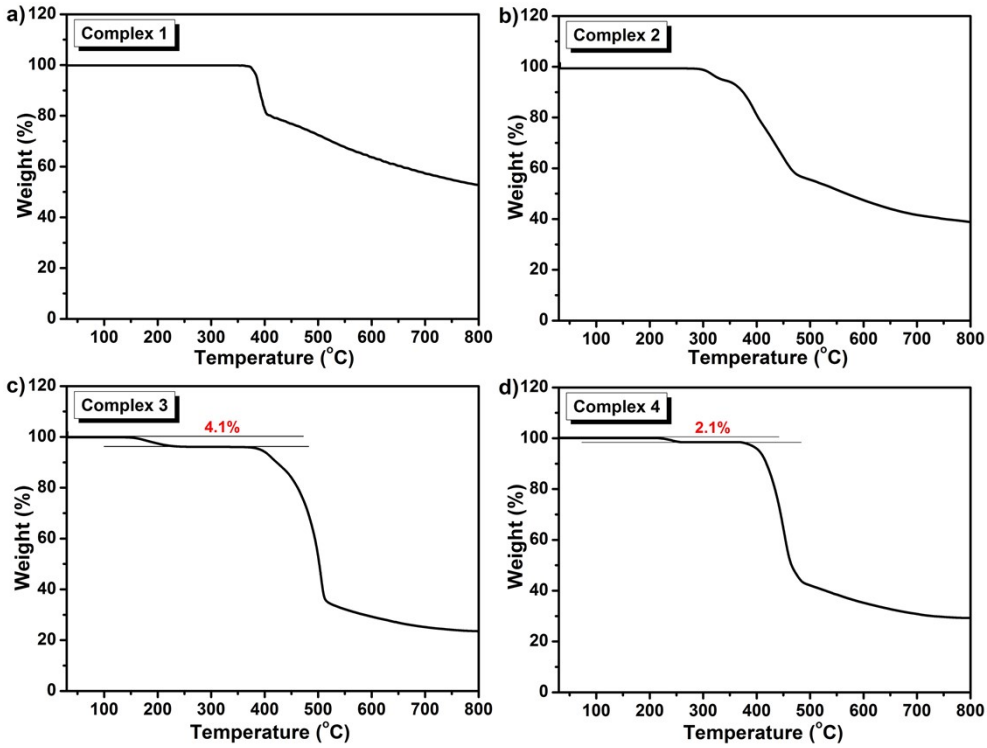

Fig. S2 TGA curves of **1-4**.

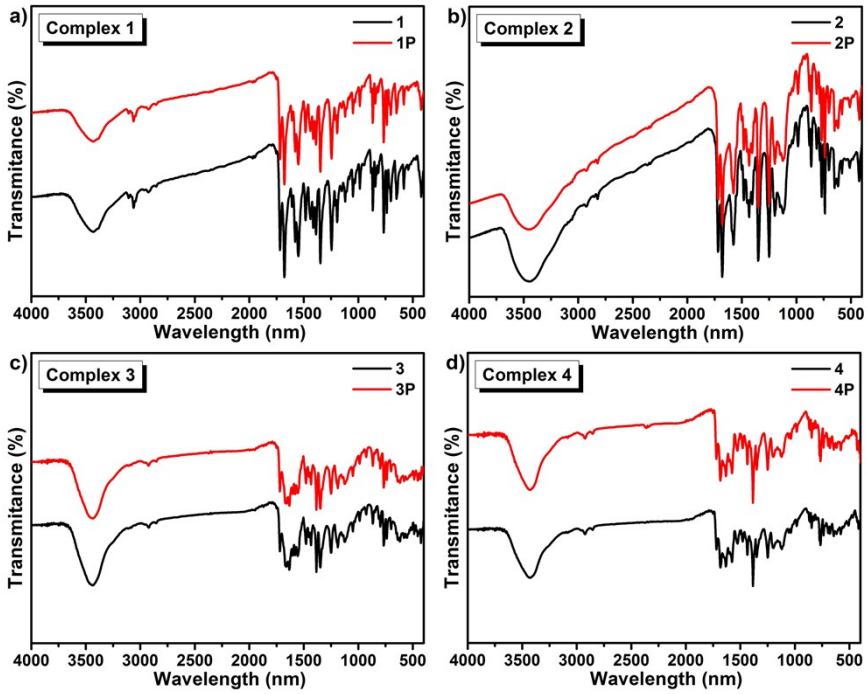

Fig. S3 FT-IR spectra of **1-4**.

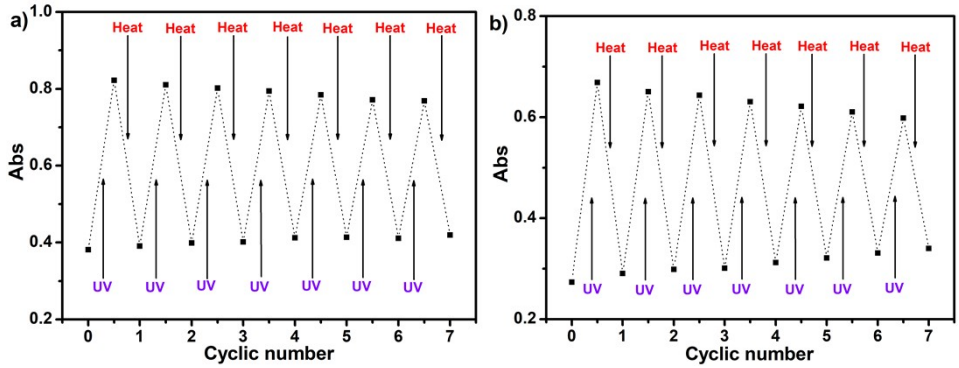

Fig. S4 The switching cycles of coloration-decoloration processes of **1** (a) and **2** (b) upon alternating UV light illumination and thermal treatment.

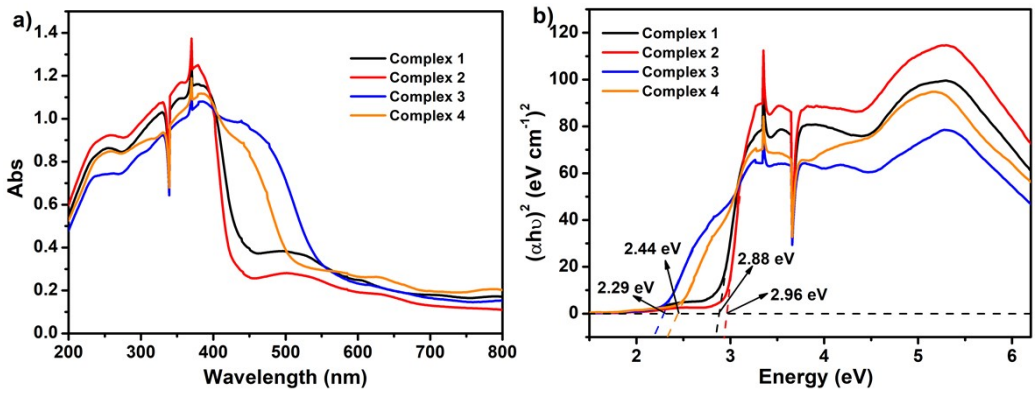

Fig. S5 (a) UV-vis spectra of complexes **1-4** and (b) Kubelka-Munk transformed reflectivity *vs* energy of complexes **1-4**.

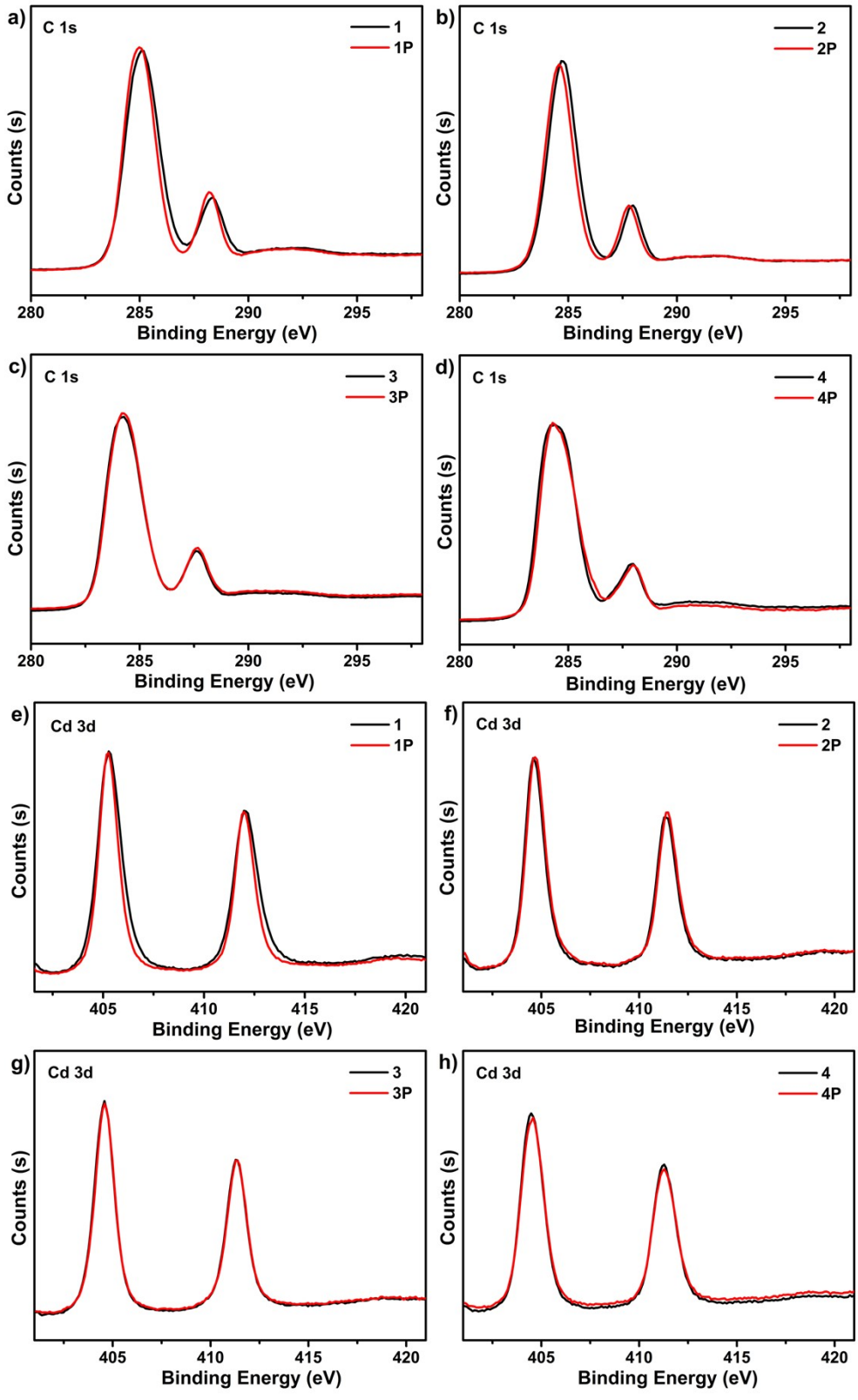

Fig. S6 C 1s (a-d) and Cd 3d (e-h) XPS core-level spectra of **1-4** and **1P-4P**.

2. Tables

Table S1. Crystallographic data and refinement of complexes **1-4**.

Complex	**1**	**2**	**3**	**4**
CCDC number	2095774	2095775	2095776	2095777
Formula	$C_{32}H_{16}CdN_4O_8$	$C_{56}H_{28}CdN_9O_{15}$	$C_{18}H_{11}Cd_{0.5}N_2O_5$	$C_{38}H_{22}CdN_4O_9$
M (g mol^{-1})	696.89	1179.27	391.49	790.99
Crystal system	Triclinic	Triclinic	Triclinic	Orthorhombic
Space group	*P-1*	*P-1*	*P-1*	*Pbca*
a (Å)	9.0370(8)	10.1715(7)	7.8636(2)	18.933(6)
b (Å)	11.9459(11)	13.7543(10)	8.6510(3)	11.390(4)
c (Å)	14.2200(13)	18.1085(13)	12.3167(3)	28.638(9)
α (deg)	72.514(2)	87.319(2)	92.507(2)	90
β (deg)	73.088(2)	84.683(2)	97.146(2)	90
γ (deg)	69.414(2)	70.671(2)	114.756(3)	90
V (Å^3)	1340.9(2)	2380.0(3)	750.69(4)	6175(4)
Z	2	2	2	8
D_c (g cm^{-3})	1.726	1.646	1.732	1.702
μ (mm^{-1})	0.879	0.547	6.458	0.777
Reflns collected/unique	19308/6577	43793/11777	5918/2606	36229/7144
R_{int}	0.0177	0.0274	0.0351	0.0317
GOF	1.063	1.055	1.059	1.020
R_1[a], wR_2[b] [I > 2σ(I)]	0.0226/0.0609	0.0346/0.0727	0.0341/0.0862	0.0324/0.0728
R_1, wR_2 (all data)	0.0242/0.0618	0.0476/0.0778	0.0343/0.0865	0.0528/0.0820

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

Table S2. Selected bond lengths (Å) and angles (°) for complexes **1-4**.

Complex 1			
Cd(1)-O(4)#1	2.2825(14)	Cd(1)-N(1)	2.2982(13)
Cd(1)-O(1)	2.1934(13)	Cd(1)-O(3)#1	2.4618(15)
Cd(1)-N(3)	2.2770(14)	Cd(1)-C(8)#1	2.6917(17)
O(4)-Cd(1)#1	2.2825(14)	O(3)-Cd(1)#1	2.4618(15)
C(8)-Cd(1)#1	2.6917(17)		
O(4)#1-Cd(1)-N(1)	86.93(5)	O(4)#1-Cd(1)-O(3)#1	55.05(5)
O(4)#1-Cd(1)-C(8)#1	27.71(5)	N(1)-Cd(1)-O(3)#1	141.83(5)
N(1)-Cd(1)-C(8)#1	114.63(5)	O(1)-Cd(1)-O(4)#1	111.78(6)
O(1)-Cd(1)-N(1)	100.16(5)	O(1)-Cd(1)-O(3)#1	97.51(5)
O(1)-Cd(1)-N(3)	118.79(6)	O(1)-Cd(1)-C(8)#1	104.28(5)
O(3)#1-Cd(1)-C(8)#1	27.50(5)	N(3)-Cd(1)-O(4)#1	114.38(5)
N(3)-Cd(1)-N(1)	119.96(5)	N(3)-Cd(1)-O(3)#1	78.82(5)
N(3)-Cd(1)-C(8)#1	98.67(5)		
Symmetry codes: #1: -x+1, -y+1, -z; #2: -x, -y, -z+1; #3 -x+2, -y+1, -z+1			
Complex 2			
Cd(1)-O(10)	2.3787(16)	Cd(1)-O(14)	2.5170(16)
Cd(1)-O(9)	2.4142(15)	Cd(1)-N(5)	2.3039(17)
Cd(1)-N(1)	2.3622(17)	Cd(1)-N(7)	2.3357(17)
Cd(1)-O(13)	2.5474(18)	Cd(1)-C(49)	2.7301(19)
O(10)-Cd(1)-O(14)	165.72(5)	O(10)-Cd(1)-O(9)	54.17(5)
O(10)-Cd(1)-O(13)	143.30(5)	O(10)-Cd(1)-C(49)	27.14(6)
O(14)-Cd(1)-O(13)	50.34(5)	O(14)-Cd(1)-C(49)	167.04(6)
O(9)-Cd(1)-O(14)	140.11(5)	O(9)-Cd(1)-O(13)	90.70(5)
O(9)-Cd(1)-C(49)	27.17(6)	N(5)-Cd(1)-O(10)	101.69(6)
N(5)-Cd(1)-O(14)	80.62(6)	N(5)-Cd(1)-O(9)	90.76(6)
N(5)-Cd(1)-N(1)	97.58(6)	N(5)-Cd(1)-N(7)	163.08(6)
N(5)-Cd(1)-O(13)	87.52(6)	N(5)-Cd(1)-C(49)	98.96(6)
N(1)-Cd(1)-O(10)	82.47(5)	N(1)-Cd(1)-O(14)	83.25(5)
N(1)-Cd(1)-O(9)	136.63(6)	N(1)-Cd(1)-O(13)	131.95(6)
N(1)-Cd(1)-C(49)	109.58(6)	N(7)-Cd(1)-O(10)	92.76(6)
N(7)-Cd(1)-O(14)	87.54(5)	N(7)-Cd(1)-O(9)	90.65(6)
N(7)-Cd(1)-N(1)	92.94(6)	N(7)-Cd(1)-O(13)	75.60(6)
N(7)-Cd(1)-C(49)	89.88(6)	O(13)-Cd(1)-C(49)	116.75(6)
Symmetry codes: #1 -x-1, -y+2, -z+1; #2 -x+1, -y, -z+2			
Complex 3			
Cd(1)-O(3)#1	2.264(2)	Cd(1)-O(3)	2.264(2)
Cd(1)-O(5)#1	2.346(2)	Cd(1)-O(5)	2.346(2)

Cd(1)-N(1)	2.348(3)	Cd(1)-N(1)#1	2.348(3)
O(3)#1-Cd(1)-O(3)	180.00(12)	O(3)-Cd(1)-O(5)	91.10(9)
O(3)-Cd(1)-O(5)#1	88.90(9)	O(3)#1-Cd(1)-O(5)	88.90(9)
O(3)#1-Cd(1)-O(5)#1	91.10(9)	O(3)-Cd(1)-N(1)#1	88.50(9)
O(3)-Cd(1)-N(1)	91.50(9)	O(3)#1-Cd(1)-N(1)	88.50(9)
O(3)#1-Cd(1)-N(1)#1	91.50(9)	O(5)-Cd(1)-O(5)#1	180.00(13)
O(5)-Cd(1)-N(1)#1	87.89(9)	O(5)#1-Cd(1)-N(1)	87.89(9)
O(5)-Cd(1)-N(1)	92.11(9)	O(5)#1-Cd(1)-N(1)#1	92.11(9)
N(1)#1-Cd(1)-N(1)	180.0		
Symmetry codes: #1 -x, -y, -z+1; #2 -x+2, -y+1, -z+2; #3 -x-1, -y, -z			
Complex 4			
Cd(1)-O(8)#1	2.4075(19)	Cd(1)-O(9)	2.310(2)
Cd(1)-O(7)#1	2.508(2)	Cd(1)-O(5)	2.400(2)
Cd(1)-O(6)	2.499(2)	Cd(1)-N(1)	2.339(2)
Cd(1)-N(4)#2	2.340(2)	O(8)-Cd(1)#2	2.4075(19)
O(7)-Cd(1)#2	2.508(2)	N(4)-Cd(1)#1	2.340(2)
O(8)#1-Cd(1)-O(7)#1	53.01(6)	O(8)#1-Cd(1)-O(6)	141.19(7)
O(9)-Cd(1)-O(8)#1	134.54(7)	O(9)-Cd(1)-O(7)#1	81.57(6)
O(9)-Cd(1)-O(5)	137.14(7)	O(9)-Cd(1)-O(6)	84.11(7)
O(9)-Cd(1)-N(1)	95.20(7)	O(5)-Cd(1)-O(7)#1	141.02(6)
O(9)-Cd(1)-N(4)#2	87.59(8)	O(5)-Cd(1)-O(6)	53.13(7)
O(5)-Cd(1)-O(8)#1	88.07(7)	O(6)-Cd(1)-O(7)#1	165.59(7)
N(1)-Cd(1)-O(7)#1	91.51(7)	N(1)-Cd(1)-O(8)#1	88.57(7)
N(1)-Cd(1)-O(5)	89.36(7)	N(1)-Cd(1)-N(4)#2	177.21(7)
N(1)-Cd(1)-O(6)	91.44(7)	N(4)#2-Cd(1)-O(8)#1	89.47(7)
N(4)#2-Cd(1)-O(7)#1	88.89(7)	N(4)#2-Cd(1)-O(6)	88.85(7)
N(4)#2-Cd(1)-O(5)	88.59(7)		
Symmetry codes: #1: -x+3/2, -y+1, z-1/2; #2: -x+3/2, -y+1, z+1/2			

Table S3. Hydrogen bonds of for complexes **1-4** (Å and °).

Complex 1				
D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
C(9)-H(9)···O(4)	0.93	2.48	3.081(2)	123
C(9)-H(9)···O(5)	0.93	2.51	3.195(2)	130
C(10)-H(10)···O(3)	0.93	2.57	3.306(3)	136
C(11)-H(11)···O(1)	0.93	2.45	3.376(3)	171
C(13)-H(13)···O(2)	0.93	2.36	3.102(3)	136
C(25)-H(25)···O(2)	0.93	2.54	3.255(2)	134
C(25)-H(25)···O(6)	0.93	2.55	3.236(2)	131
Complex 2				
D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
C(1)-H(1)···O(10)	0.93	2.28	2.978(3)	132
C(3)-H(3)···O(9)	0.93	2.45	3.336(3)	159
C(5)-H(5)···O(12)	0.93	2.60	3.355(3)	139
C(5)-H(5)···O(14)	0.93	2.41	3.105(3)	132
C(12)-H(12)···O(5)	0.93	2.55	3.134(3)	121
C(16)-H(16)···O(3)	0.93	2.38	3.078(3)	131
C(27)-H(27)···O(10)	0.93	2.56	3.254(3)	132
C(29)-H(29)···O(14)	0.93	2.50	3.048(3)	118
C(39)-H(39)···O(15)	0.93	2.55	3.440(3)	160
C(52)-H(52)···O(4)	0.93	2.57	3.416(3)	152
Complex 3				
D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(5)-H(5A)···O(4)	0.85	1.92	2.679(4)	148
O(5)-H(5B)···O(2)	0.85	2.09	2.906(4)	161
C(5)-H(5)···O(3)	0.93	2.55	3.186(4)	126
C(17)-H(17)···O(4)	0.93	2.59	3.478(5)	161
Complex 4				
D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(9)-H(9A)···O(8)	0.85	1.94	2.747(3)	156
O(9)-H(9B)···O(5)	0.85	2.08	2.831(3)	146
C(3)-H(3)···O(3)	0.93	2.59	3.215(3)	125
C(11)-H(11)···O(1)	0.93	2.35	3.262(3)	167
C(22)-H(22)···O(4)	0.93	2.57	3.095(3)	116
C(23)-H(23)···O(4)	0.93	2.51	3.083(3)	120

Table S4. Photochromic kinetic parameters at room temperature of **1-2**.

Complex	A_0	A_1	k_1 (s^{-1})	k_2 (s^{-1})	R
1	0.81491	-0.20712	0.00226	0.03522	0.99201
2	0.67026	-0.19431	0.0239	0.00108	0.9888