

Table S1† Selected Bond lengths [Å] and angles [deg] for complex 1-6

Complex 1			
Co1—O1	2.200 (6)	O6—Co1—C12	136.9 (3)
Co1—O2	2.089 (7)	O6—Co1—N1 ⁱ	90.0 (3)
Co1—N1 ⁱ	2.101(9)	O6—Co1—O2	91.2 (3)
Co1—N5	2.135 (8)	O7—Co1—O1	59.8 (2)
Co1—O6	2.079 (6)	O7—Co1—C12	29.6 (3)
Co1—O7	2.174 (6)	N1 ⁱ —Co1—O1	91.8 (3)
O1—Co1—C12	30.7 (3)	N1 ⁱ —Co1—N5	176.3 (3)
N5—Co1—O1	84.6 (3)	N1 ⁱ —Co1—O7	91.5 (3)
N5—Co1—O7	86.1 (3)	N1 ⁱ —Co1—C12	95.8 (3)
N5—Co1—C12	80.7 (3)	O2—Co1—O1	161.6 (2)
O6—Co1—O1	106.6 (3)	O2—Co1—N5	90.2 (3)
O6—Co1—N5	91.7 (3)	O2—Co1—O7	102.3 (2)
O6—Co1—O7	166.4 (3)	O2—Co1—C12	130.9 (3)
Complex 2			
Co1—O1	1.988 (6)	O1—Co1—N4 ⁱ	106.5 (3)
Co1—O4	2.022 (6)	O4—Co1—N4 ⁱ	95.6 (2)
Co1—N2	2.033 (6)	N2—Co1—N4 ⁱ	101.3 (3)
Co1—N4 ⁱ	2.046 (6)	O1—Co1—O3	93.5 (2)
Co1—O3	2.379 (6)	O4—Co1—O3	58.5 (2)
O1—Co1—O4	140.8 (3)	N2—Co1—O3	90.6 (3)
O1—Co1—N2	101.9 (3)	N4 ⁱ —Co1—O3	153.8 (2)
O4—Co1—N2	105.0 (3)		
Complex 3			
Co1—O1 ⁱ	1.9828 (11)	O1 ⁱ —Co1—N2	121.73 (5)
Co1—O1	1.9828 (11)	O1—Co1—N2	112.89 (6)
Co1—N2	2.0411 (14)	O1 ⁱ —Co1—N2 ⁱ	112.89 (6)
Co1—N2 ⁱ	2.0411 (14)	O1—Co1—N2 ⁱ	121.73 (5)
O1 ⁱ —Co1—O1	93.84 (7)	N2—Co1—N2 ⁱ	95.89 (8)
Complex 4			
Co1—O9	2.034 (3)	O9—Co1—O3	81.56 (10)
Co1—O2	2.085 (3)	O2—Co1—O3	84.35 (11)
Co1—N4 ⁱ	2.110 (4)	N4 ⁱ —Co1—O3	91.84 (12)
Co1—O4 ⁱⁱ	2.119 (3)	O4 ⁱⁱ —Co1—O3	102.96 (11)
Co1—N5	2.133 (4)	N5—Co1—O3	169.85 (13)
Co1—O3	2.184 (3)	O1—Co2—O9 ⁱⁱ	176.70 (12)
Co2—O1	2.051 (3)	O1—Co2—O9	93.16 (11)
Co2—O9 ⁱⁱ	2.063 (3)	O9 ⁱⁱ —Co2—O9	84.12 (11)
Co2—O9	2.085 (3)	O1—Co2—O5	90.71 (14)
Co2—O5	2.111 (3)	O9 ⁱⁱ —Co2—O5	91.34 (13)
Co2—N2	2.119 (4)	O9—Co2—O5	93.79 (13)
Co2—O3	2.180 (3)	O1—Co2—N2	90.19 (13)

O9—Co1—O2	91.30 (11)	O9 ⁱⁱ —Co2—N2	92.44 (13)
O9—Co1—N4 ⁱ	173.38 (12)	O9—Co2—N2	175.76 (13)
O2—Co1—N4 ⁱ	87.48 (13)	O5—Co2—N2	88.76 (15)
O9—Co1—O4 ⁱⁱ	95.73 (11)	O1—Co2—O3	87.91 (12)
O2—Co1—O4 ⁱⁱ	170.51 (12)	O9 ⁱⁱ —Co2—O3	89.78 (11)
N4 ⁱ —Co1—O4 ⁱⁱ	86.26 (12)	O9—Co2—O3	80.53 (10)
O9—Co1—N5	93.52 (13)	O5—Co2—O3	174.07 (13)
O2—Co1—N5	86.90 (13)	N2—Co2—O3	97.01 (13)
N4 ⁱ —Co1—N5	92.91 (15)	O9—Co1—O3	81.56 (10)
O4 ⁱⁱ —Co1—N5	86.30 (13)		

Complex 5

Ni1—N4 ⁱ	2.037 (3)	N2—Ni1—O4 ⁱⁱ	88.15 (9)
Ni1—O1	2.0469 (19)	N4 ⁱ —Ni1—O6	91.24 (10)
Ni1—N2	2.051 (3)	O1—Ni1—O6	87.83 (8)
Ni1—O4 ⁱⁱ	2.0756 (19)	N2—Ni1—O6	89.68 (10)
Ni1—O6	2.125 (2)	O4 ⁱⁱ —Ni1—O6	90.32 (8)
Ni1—O7	2.137 (2)	N4 ⁱ —Ni1—O7	87.27 (10)
N4 ⁱ —Ni1—O1	87.72 (10)	O1—Ni1—O7	94.53 (9)
N4 ⁱ —Ni1—N2	178.63 (11)	N2—Ni1—O7	91.85 (10)
O1—Ni1—N2	91.30 (10)	O4 ⁱⁱ —Ni1—O7	87.34 (8)
N4 ⁱ —Ni1—O4 ⁱⁱ	92.86 (9)	O6—Ni1—O7	177.16 (9)
O1—Ni1—O4 ⁱⁱ	178.07 (9)		

Complex 6

Ni1—N2 ⁱ	2.100 (5)	O1—Ni1—N2 ⁱ	87.11 (18)
Ni1—N2	2.100 (5)	O1—Ni1—N6	92.34 (19)
Ni1—N6	2.103 (5)	O1 ⁱ —Ni1—N6	87.66 (19)
Ni1—N6 ⁱ	2.103 (5)	O1—Ni1—N6 ⁱ	87.66 (19)
Ni1—O1 ⁱ	2.068 (4)	O1 ⁱ —Ni1—N6 ⁱ	92.34 (19)
Ni1—O1	2.068 (4)	O1 ⁱ —Ni1—O1	180.000 (1)
Ni2—N4 ⁱⁱ	2.061 (5)	N4 ⁱⁱⁱ —Ni2—N4 ⁱⁱ	180.0
Ni2—N4 ⁱⁱⁱ	2.061 (5)	N4 ⁱⁱⁱ —Ni2—O3	86.8 (2)
Ni2—O3	2.101 (4)	N4 ⁱⁱ —Ni2—O3	93.2 (2)
Ni2—O3 ^{iv}	2.101 (4)	N4 ⁱⁱⁱ —Ni2—O3 ^{iv}	93.2 (2)
Ni2—O5	2.091 (4)	N4 ⁱⁱ —Ni2—O3 ^{iv}	86.8 (2)
Ni2—O5 ^{iv}	2.091 (4)	N4 ⁱⁱ —Ni2—O5 ^{iv}	89.63 (19)
N2—Ni1—N2 ⁱ	180.000 (1)	N4 ⁱⁱⁱ —Ni2—O5 ^{iv}	90.37 (19)
N2—Ni1—N6	95.99 (19)	N4 ⁱⁱⁱ —Ni2—O5	89.63 (19)
N2 ⁱ —Ni1—N6	84.01 (19)	N4 ⁱⁱ —Ni2—O5	90.37 (19)
N2—Ni1—N6 ⁱ	84.01 (19)	O3—Ni2—O3 ^{iv}	180.000 (1)
N2 ⁱ —Ni1—N6 ⁱ	95.99 (19)	O5—Ni2—O3 ^{iv}	87.12 (17)
N6—Ni1—N6 ⁱ	180.0 (3)	O5 ^{iv} —Ni2—O3 ^{iv}	92.88 (17)
O1—Ni1—N2	92.89 (18)	O5 ^{iv} —Ni2—O3	87.12 (17)
O1 ⁱ —Ni1—N2	87.11 (18)	O5—Ni2—O3	92.88 (17)
O1 ⁱ —Ni1—N2 ⁱ	92.89 (18)	O5 ^{iv} —Ni2—O5	180.000 (1)

Table S2† Photocatalytic degradation first-order kinetic for MB of complex 6

Complex	k (min ⁻¹)	R
1	0.02511	0.99856
2	0.04224	0.99114
3	0.03323	0.95968
4	0.03395	0.99173
5	0.01358	0.99147
6	0.01571	0.9909

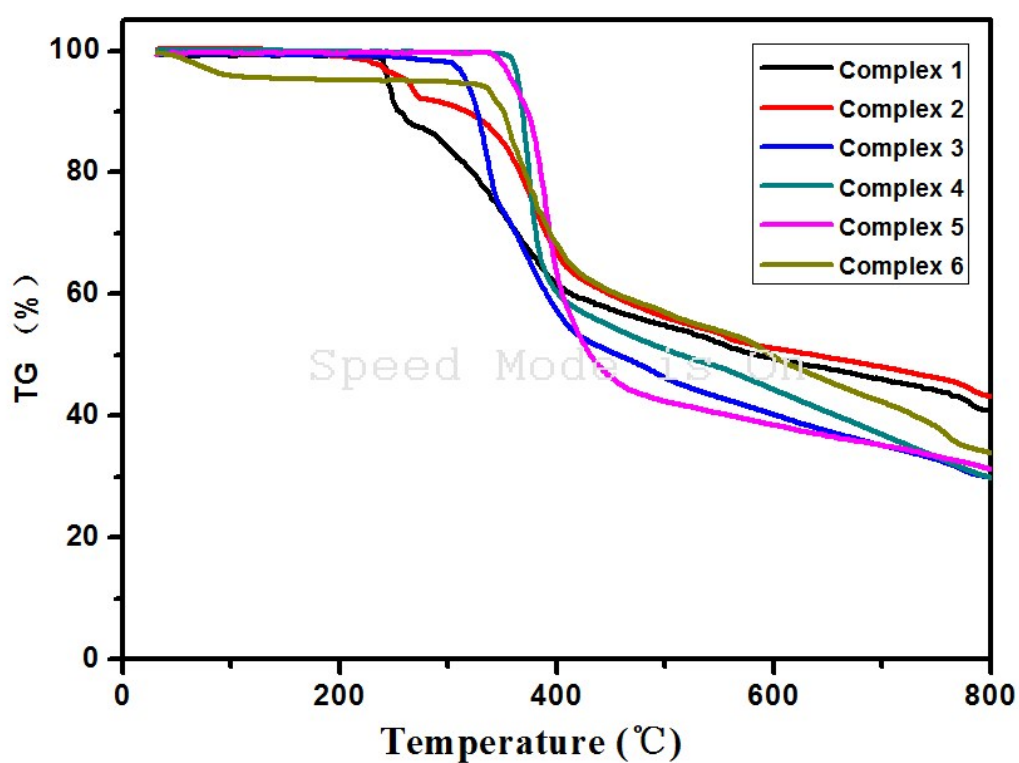


Fig. S1† TG curves of complex 1-6.

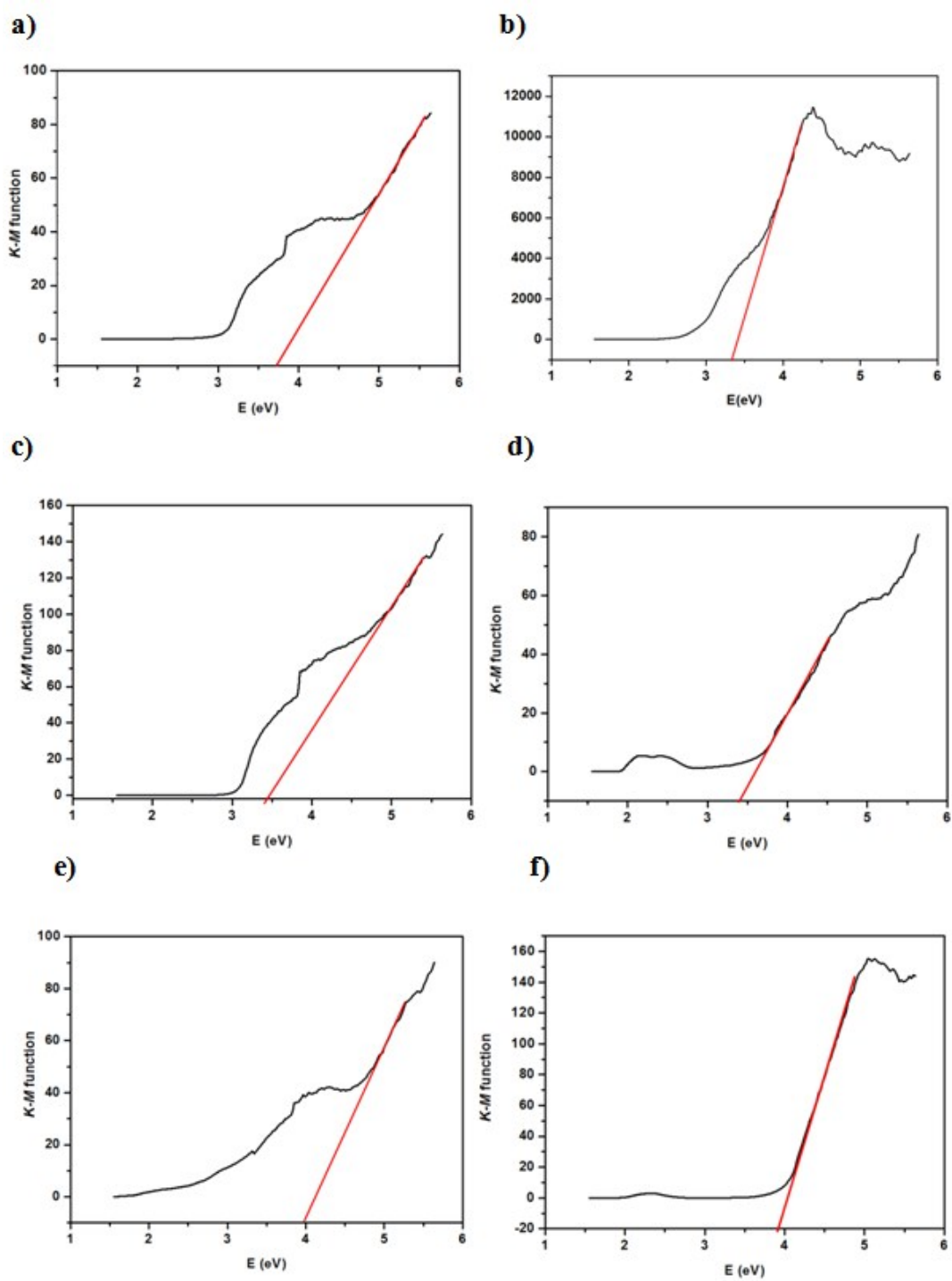


Fig. S2† Kubelka–Munk-transformed diffuse reflectance spectra of complex 1-6 (a-f)

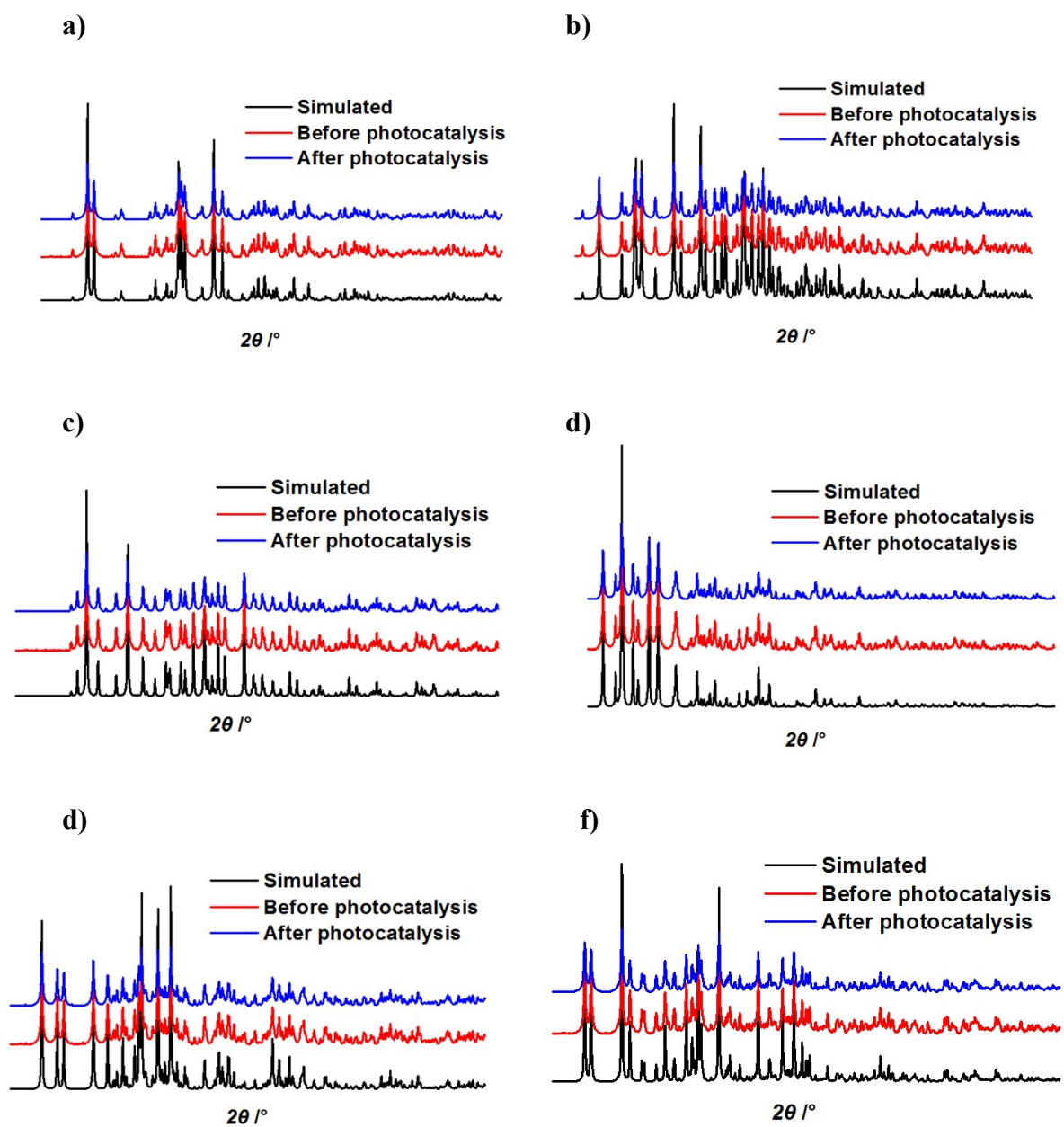


Fig. S3† The experimental crystals' PXRD patterns of complex 1- 6 (a-f) compared with the simulated pattern



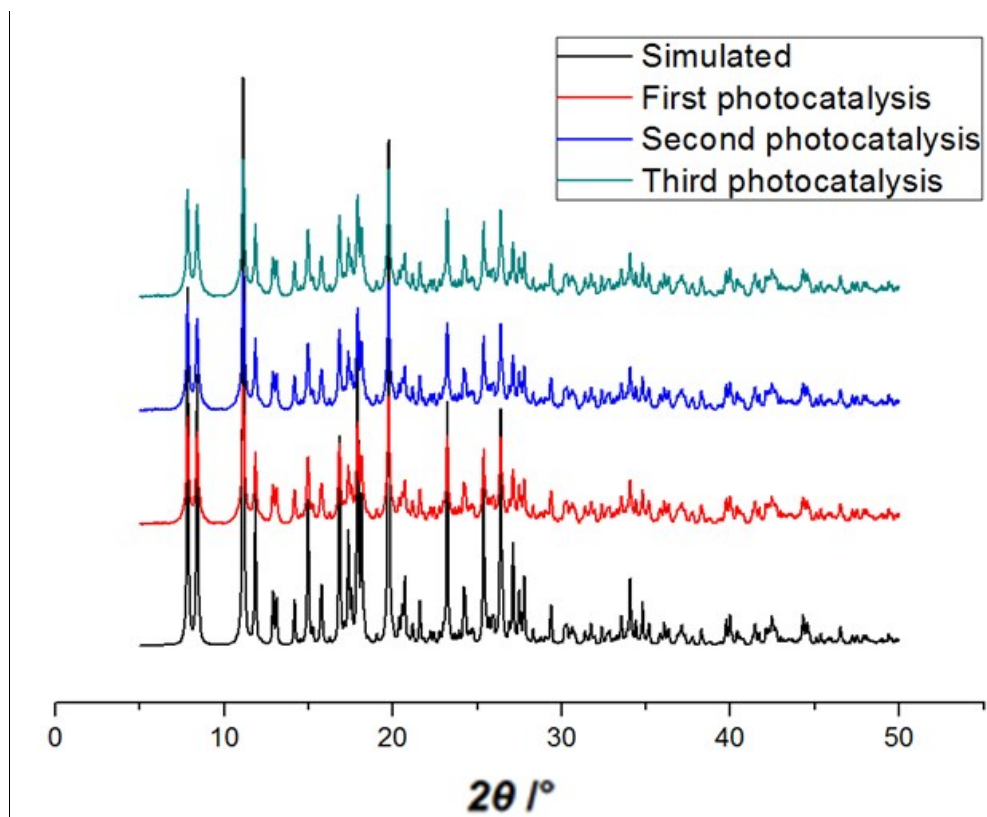


Fig. S4† The three experimental crystals' PXRD patterns of complex 6 compared with the simulated pattern