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

Design and construction of a series of metal–organic coordination polymers based on two isomeric semi-rigid bis-pyridyl-bis-amide ligands and three aromatic polycarboxylates †

Xiuli Wang,* Jian Luan, Hongyan Lin, Chuang Xu, Guocheng Liu, Juwen Zhang, and Aixiang Tian

Table S1 Selected bond distances (Å) and angles (°) for complexes **1–9**.

Complex **1**			
Cu(1)-O(7)#1	1.979(3)	Cu(2)-O(5)#3	1.951(3)
Cu(1)-O(7)	1.979(3)	Cu(2)-O(3)	1.995(3)
Cu(1)-N(5)#1	2.019(4)	Cu(2)-N(3)	2.044(4)
Cu(1)-N(5)	2.019(4)	Cu(2)-N(4)	2.048(4)
Cu(2)-O(1)#2	2.176(3)	O(5)#3-Cu(2)-O(3)	153.61(14)
O(7)#1-Cu(1)-O(7)	179.998(1)	O(5)#3-Cu(2)-N(3)	93.53(16)
O(7)#1-Cu(1)-N(5)#1	87.36(16)	O(3)-Cu(2)-N(3)	90.30(15)
O(7)-Cu(1)-N(5)#1	92.63(16)	O(5)#3-Cu(2)-N(4)	88.78(16)
O(7)#1-Cu(1)-N(5)	92.64(16)	O(3)-Cu(2)-N(4)	86.24(15)
O(7)-Cu(1)-N(5)	87.37(16)	N(3)-Cu(2)-N(4)	176.08(16)
N(5)#1-Cu(1)-N(5)	179.998(1)	O(5)#3-Cu(2)-O(1)#2	107.19(14)
N(3)-Cu(2)-O(1)#2	92.70(15)	O(3)-Cu(2)-O(1)#2	98.68(14)
N(4)-Cu(2)-O(1)#2	89.64(16)		
Symmetry code for **1**: #1 −*x*, −*y* + 1, -*z* + 1; #2 −*x*, −*y*, −*z*; #3 *x* + 1, *y*, *z*			
Complex **2**			
Cu(1)-O(1)	1.941(2)	Cu(2)-O(3)#2	1.953(3)
Cu(1)-O(5)	2.006(2)	Cu(2)-N(2)	2.006(4)
Cu(1)-N(1)	2.029(3)	Cu(2)-N(2)#2	2.006(4)
Cu(1)-N(5)#1	2.049(3)	Cu(1)-O(1W)	2.272(3)
Cu(2)-O(3)	1.953(3)	O(3)#2-Cu(2)-N(2)	92.34(14)
O(1)-Cu(1)-O(5)	177.36(10)	O(3)-Cu(2)-N(2)#2	92.34(14)
O(1)-Cu(1)-N(1)	93.46(12)	O(3)#2-Cu(2)-N(2)#2	156.35(13)
O(5)-Cu(1)-N(1)	84.63(11)	N(2)-Cu(2)-N(2)#2	94.4(2)
O(1)-Cu(1)-N(5)#1	92.06(11)	N(1)-Cu(1)-O(1W)	91.95(12)
O(5)-Cu(1)-N(5)#1	89.69(11)	N(5)#1-Cu(1)-O(1W)	93.08(12)
N(1)-Cu(1)-N(5)#1	172.60(12)	O(3)-Cu(2)-O(3)#2	90.46(18)
O(1)-Cu(1)-O(1W)	88.87(13)	O(3)-Cu(2)-N(2)	156.35(13)
O(5)-Cu(1)-O(1W)	93.01(12)		
Symmetry code for **2**: #1 *x* + 1, −*y*, *z* + 1/2; #2 − *x* + 1, *y*, −*z* + 1/2			
Complex **3**			
Cu(1)-O(3)	1.9434(15)	Cu(1)-O(1W)	2.2789(19)

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

Cu(1)-O(6)#1	1.9869(15)	Cu(1)-N(4)#2	2.0466(19)
Cu(1)-N(1)	2.0458(19)	N(1)-Cu(1)-N(4)#2	174.23(8)
O(3)-Cu(1)-O(6)#1	145.59(7)	O(3)-Cu(1)-O(1W)	113.35(7)
O(3)-Cu(1)-N(1)	91.33(7)	O(6)#1-Cu(1)-O(1W)	101.04(7)
O(6)#1-Cu(1)-N(1)	89.03(7)	N(1)-Cu(1)-O(1W)	87.00(8)
O(3)-Cu(1)-N(4)#2	91.83(7)	N(4)#2-Cu(1)-O(1W)	87.32(7)
O(6)#1-Cu(1)-N(4)#2	91.08(7)		

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

Complex **4**

Co(1)-O(1)	1.9807(13)	Co(1)-N(1)	2.1900(15)
Co(1)-O(4)#1	2.0439(13)	Co(1)-N(2)#2	2.1843(16)
Co(1)-O(1W)	2.0893(14)	O(1W)-Co(1)-N(2)#2	87.52(6)
O(1)-Co(1)-O(4)#1	140.98(6)	O(1)-Co(1)-N(1)	92.17(6)
O(1)-Co(1)-O(1W)	122.00(6)	O(4)#1-Co(1)-N(1)	90.41(6)
O(4)#1-Co(1)-O(1W)	97.00(5)	O(1W)-Co(1)-N(1)	87.88(6)
O(1)-Co(1)-N(2)#2	91.06(6)	N(2)#2-Co(1)-N(1)	175.31(6)
O(4)#1-Co(1)-N(2)#2	89.21(6)		

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

Complex **5**

Ni(1)-O(1)	1.9772(11)	Ni(1)-O(2)#1	2.2418(12)
Ni(1)-O(3)#1	2.0532(11)	Ni(1)-N(1)	2.1335(14)
Ni(1)-O(1W)	2.0788(13)	Ni(1)-N(2)	2.1242(14)
O(1)-Ni(1)-O(3)#1	154.00(5)	O(3)#1-Ni(1)-O(2)#1	61.43(4)
O(1)-Ni(1)-O(1W)	109.83(5)	O(1W)-Ni(1)-O(2)#1	157.59(5)
O(3)#1-Ni(1)-O(1W)	96.16(5)	N(2)-Ni(1)-O(2)#1	92.01(5)
O(1)-Ni(1)-N(2)	91.30(5)	N(1)-Ni(1)-O(2)#1	92.14(5)
O(3)#1-Ni(1)-N(2)	89.15(5)	O(1W)-Ni(1)-N(1)	87.73(5)
O(1W)-Ni(1)-N(2)	87.30(6)	N(2)-Ni(1)-N(1)	174.90(5)
O(1)-Ni(1)-N(1)	91.46(5)	O(1)-Ni(1)-O(2)#1	92.58(4)
O(3)#1-Ni(1)-N(1)	90.24(5)		

Symmetry code for **5**: #1 $x + 1, y, z$

Complex **6**

Zn(1)-O(1)	1.9515(14)	Zn(1)-N(1)	2.2343(18)
Zn(1)-O(2)#1	1.9836(14)	Zn(1)-N(2)#2	2.2308(18)
Zn(1)-O(1W)	2.0457(15)	O(1W)-Zn(1)-N(2)#2	86.59(7)
O(1)-Zn(1)-O(2)#1	129.89(6)	O(1)-Zn(1)-N(1)	92.67(7)
O(1)-Zn(1)-O(1W)	124.84(6)	O(2)#1-Zn(1)-N(1)	90.10(6)
O(2)#1-Zn(1)-O(1W)	105.25(6)	O(1W)-Zn(1)-N(1)	88.28(7)
O(1)-Zn(1)-N(2)#2	91.17(7)	N(2)#2-Zn(1)-N(1)	174.75(7)
O(2)#1-Zn(1)-N(2)#2	90.17(6)		

Symmetry code for **6**: #1 $x + 1, y, z$; #2 $-x + 1/2, y + 1/2, -z + 1/2$

Complex **7**

Cd(1)-O(1)	2.306(3)	Cd(1)-O(4)#2	2.431(3)
Cd(1)-O(2)#1	2.352(3)	Cd(1)-O(3)#2	2.365(3)

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

Cd(1)-N(1)	2.360(3)	Cd(1)-N(2)#3	2.395(3)
O(1)-Cd(1)-O(2)#1	100.05(10)	O(2)#1-Cd(1)-O(4)#2	99.37(10)
O(1)-Cd(1)-N(1)	135.75(10)	N(1)-Cd(1)-O(4)#2	85.70(10)
O(2)#1-Cd(1)-N(1)	90.81(10)	O(3)#2-Cd(1)-O(4)#2	54.19(9)
O(1)-Cd(1)-O(3)#2	83.38(10)	N(2)#3-Cd(1)-O(4)#2	86.02(11)
O(2)#1-Cd(1)-O(3)#2	91.12(10)	N(1)-Cd(1)-N(2)#3	84.21(11)
N(1)-Cd(1)-O(3)#2	139.59(10)	O(3)#2-Cd(1)-N(2)#3	96.40(10)
O(1)-Cd(1)-N(2)#3	79.76(11)	O(1)-Cd(1)-O(4)#2	133.31(10)
O(2)#1-Cd(1)-N(2)#3	172.39(10)		

Symmetry code for **7**: #1 −*x* + 1, −*y*, −*z* + 2; #2 *x*, *y* + 1, *z*; #3 −*x*, −*y*, −*z* + 1

Complex **8**

Cd(1)-O(1)	2.2750(16)	Cd(1)-O(4)#2	2.3785(16)
Cd(1)-N(1)	2.3365(18)	Cd(1)-N(2)#3	2.434(2)
Cd(1)-O(2)#1	2.3598(17)	Cd(1)-O(3)#1	2.4346(17)
O(1)-Cd(1)-N(1)	129.53(6)	O(1)-Cd(1)-O(3)#1	136.54(6)
O(1)-Cd(1)-O(2)#1	87.15(6)	N(1)-Cd(1)-O(3)#1	89.58(6)
N(1)-Cd(1)-O(2)#1	143.10(6)	O(2)#1-Cd(1)-O(3)#1	54.67(6)
O(1)-Cd(1)-O(4)#2	100.25(6)	O(4)#2-Cd(1)-O(3)#1	99.65(6)
N(1)-Cd(1)-O(4)#2	87.31(6)	N(2)#3-Cd(1)-O(3)#1	80.25(6)
O(2)#1-Cd(1)-O(4)#2	89.94(6)	O(2)#1-Cd(1)-N(2)#3	94.55(7)
O(1)-Cd(1)-N(2)#3	83.43(7)	O(4)#2-Cd(1)-N(2)#3	174.35(6)
N(1)-Cd(1)-N(2)#3	87.04(7)		

Symmetry code for **8**: #1 *x* + 1, *y*, *z*; #2 −*x*, −*y*, −*z*; #3 *x* − 1, *y* + 1, *z*

Complex **9**

Cu(1)-O(8)#1	1.9637(19)	Cu(2)-O(5)	2.0380(19)
Cu(1)-O(7)#2	1.9707(18)	Cu(2)-O(9)#5	2.314(2)
Cu(1)-O(2)#3	1.975(2)	Cu(2)-O(6)	2.006(2)
Cu(1)-O(1)	1.978(2)	N(1)-Cu(2)	1.986(2)
Cu(1)-N(4)#4	2.181(2)	Cu(2)-O(3)	1.936(2)
N(4)#4-Cu(1)-Cu(1)#3	172.47(7)	O(3)-Cu(2)-N(1)	96.34(10)
O(8)#1-Cu(1)-O(7)#2	167.02(8)	O(3)-Cu(2)-O(6)	160.21(9)
O(8)#1-Cu(1)-O(2)#3	89.47(9)	N(1)-Cu(2)-O(6)	96.86(9)
O(7)#2-Cu(1)-O(2)#3	87.18(9)	O(3)-Cu(2)-O(5)	100.75(8)
O(8)#1-Cu(1)-O(1)	89.10(9)	N(1)-Cu(2)-O(5)	161.85(9)
O(7)#2-Cu(1)-O(1)	91.40(9)	O(6)-Cu(2)-O(5)	65.06(8)
O(2)#3-Cu(1)-O(1)	167.30(8)	O(3)-Cu(2)-O(9)#5	99.95(8)
O(8)#1-Cu(1)-N(4)#4	97.15(8)	N(1)-Cu(2)-O(9)#5	90.28(9)
O(7)#2-Cu(1)-N(4)#4	95.76(8)	O(6)-Cu(2)-O(9)#5	94.67(9)
O(2)#3-Cu(1)-N(4)#4	99.23(9)	O(5)-Cu(2)-O(9)#5	92.73(8)
O(1)-Cu(1)-N(4)#4	93.47(9)	O(2)#3-Cu(1)-Cu(1)#3	88.28(6)
O(8)#1-Cu(1)-Cu(1)#3	83.30(6)	O(1)-Cu(1)-Cu(1)#3	79.02(6)
O(7)#2-Cu(1)-Cu(1)#3	84.06(6)		

Symmetry code for **9**: #1 *x* + 1, *y* + 1, *z*; #2 −*x*, −*y* − 1, −*z*; #3 −*x* + 1, −*y*, −*z*; #4 *x* + 1, *y* + 1, *z* + 1; #5 −*x* - 1, −*y* − 1, −*z* − 1

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

Table S2. Selected hydrogen-bonding geometry (Å, °) for complex **1**, **3**, **7**, **8**

Complex	D–H···A	D–H	H···A	D···A	D–H···A
1	N(1)–H(1A)···O(6)	0.86	2.10	2.9457	166
3	N(3)–H(3A)···O(4)	0.86	2.17	2.8961	142
7	N(4)–H(4B)···O(3)	0.86	2.15	2.9378	151
8	N(3)–H(3B)···O(6)	0.86	2.22	2.9803	148

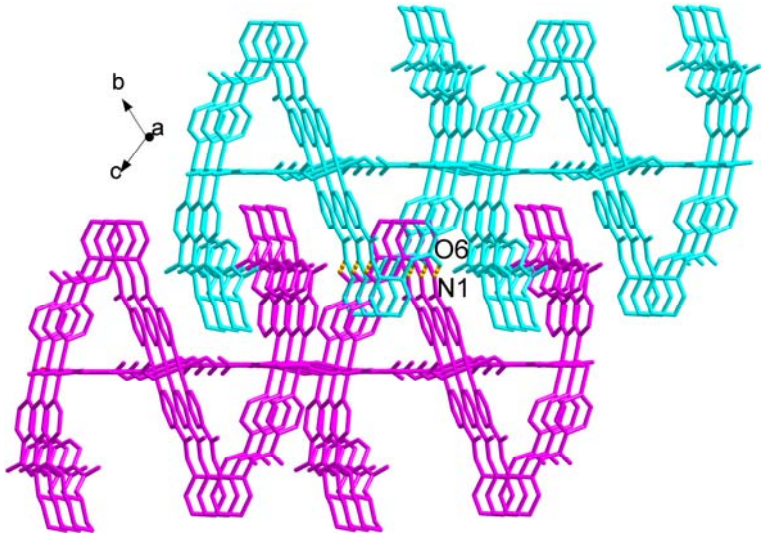


Fig. S1 View of 3D supramolecular architecture of **1**.

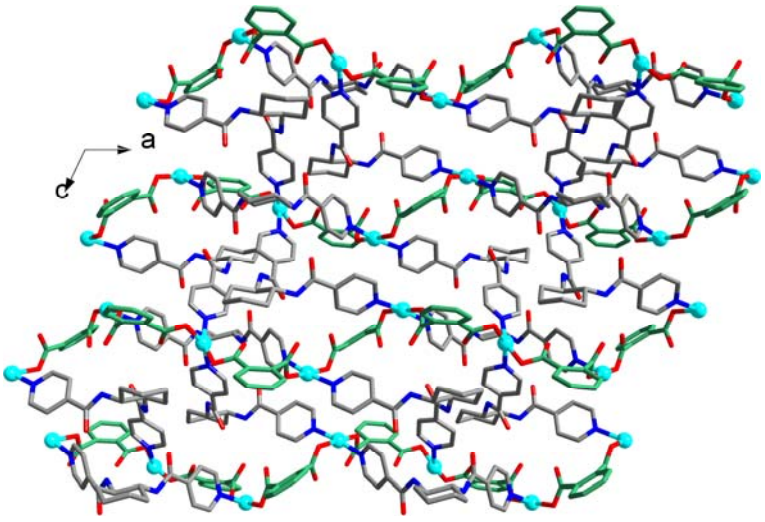


Fig. S2 View of the 2D layer in **2**.

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

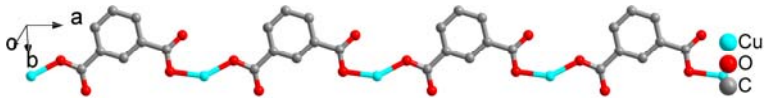


Fig. S3 View of 1D $[Cu\text{-}1,3\text{-}BDC]_n$ chain in **3**.

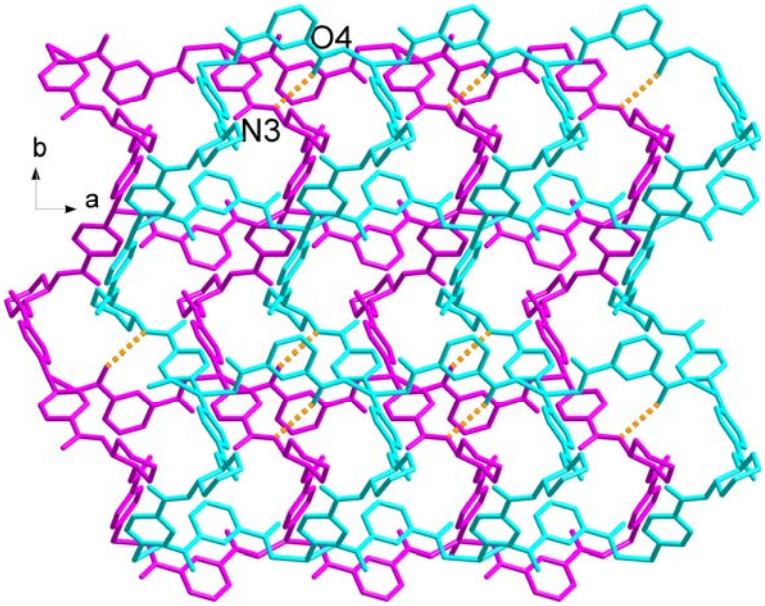


Fig. S4 View of 3D supramolecular architecture of **3**.

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

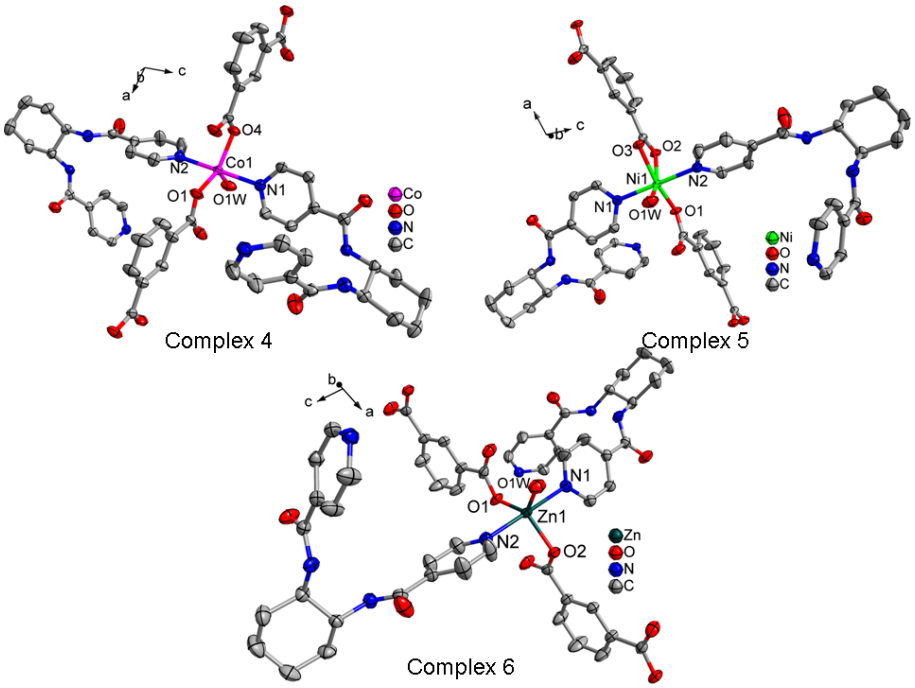


Fig. S5 The coordination geometries of the metal ions in **4**–**6**.

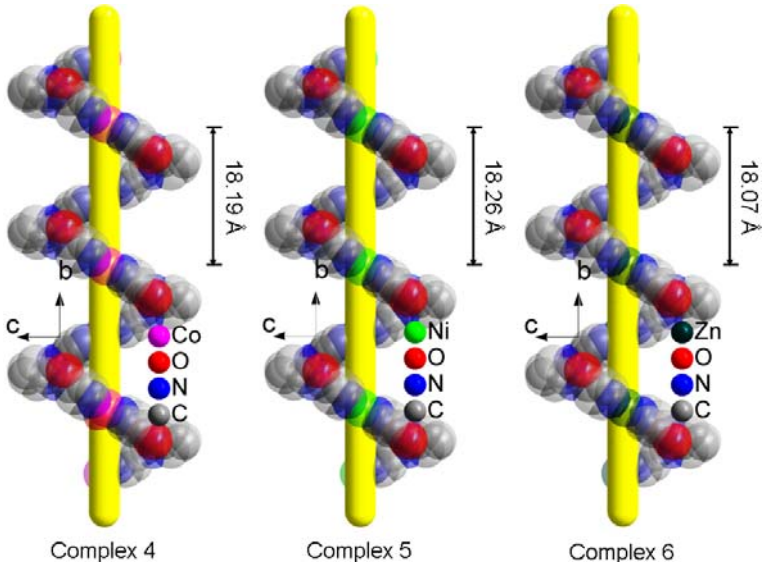


Fig. S6 View of the right-handed helix chains in **4**–**6**.

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

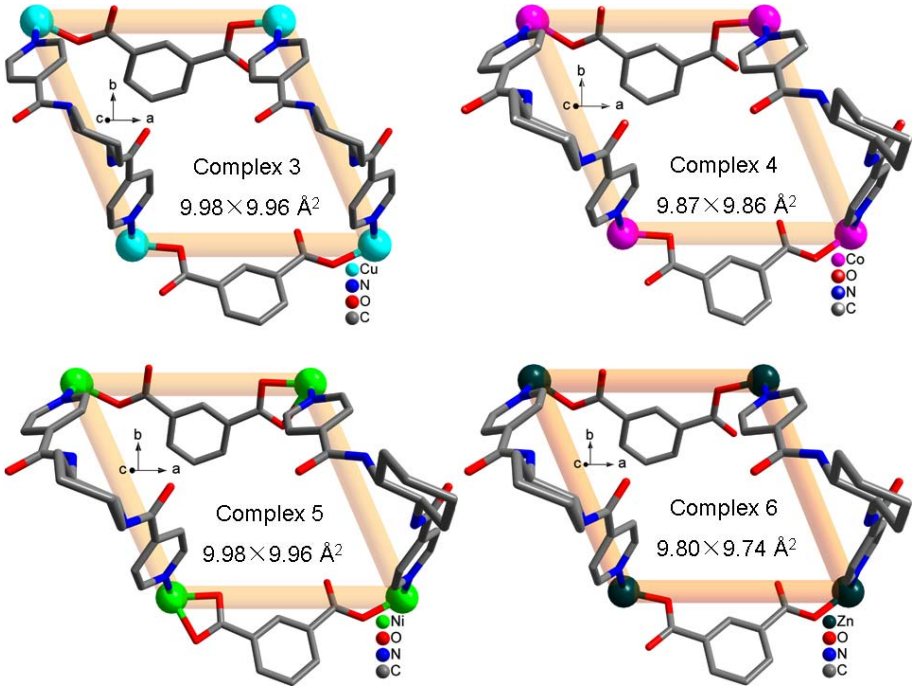


Fig. S7 The $[M_4(4\text{-bpah})_2(1,3\text{-BDC})_2]$ rings with similar sizes in complexes **3**–**6** (M = Cu(II)/Co(II)/Ni(II)/Zn(II)).

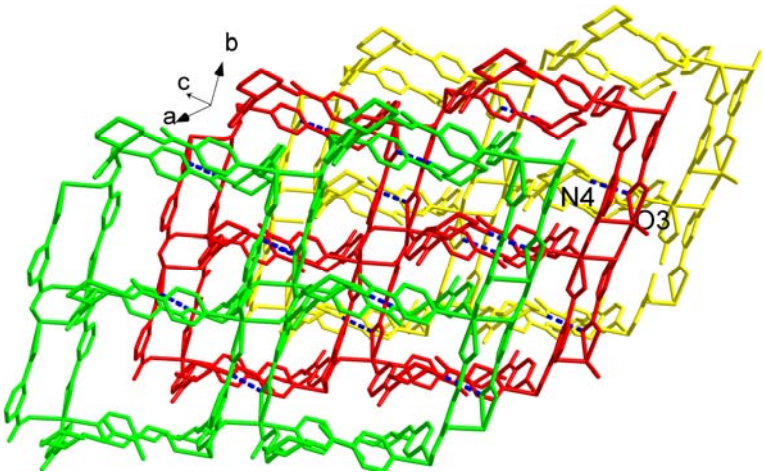


Fig. S8 View of 3D supramolecular architecture of **7**

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

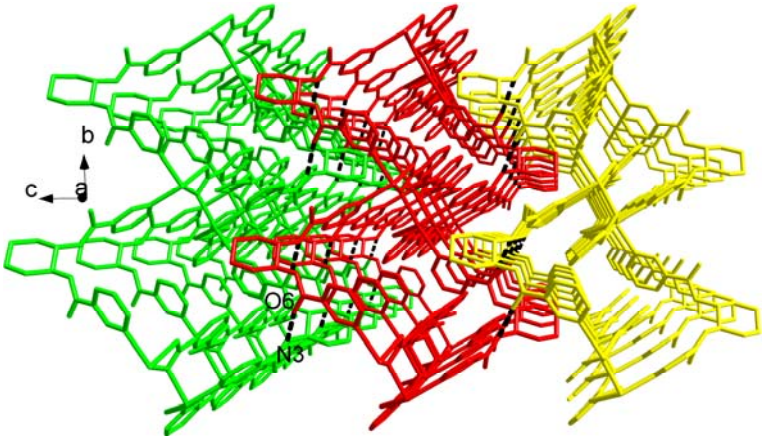
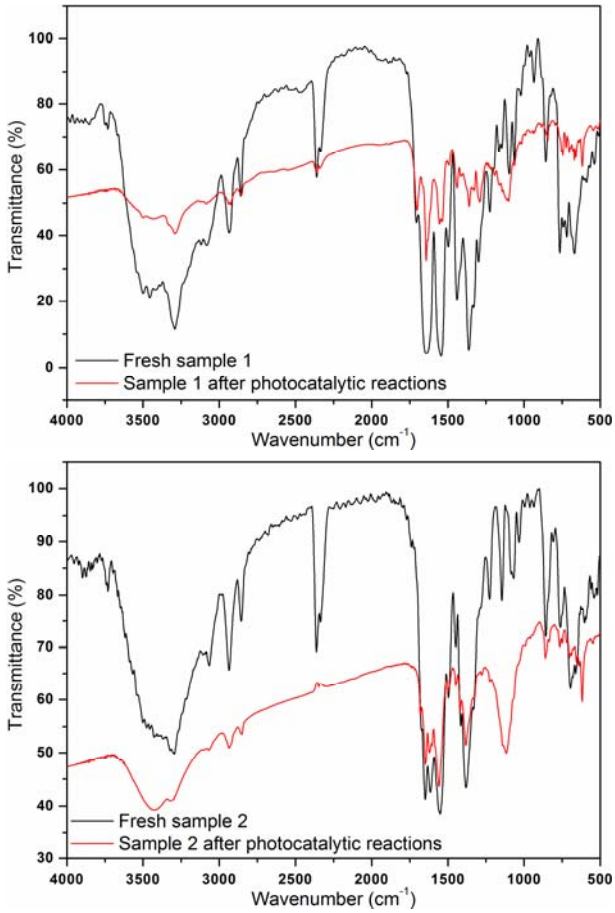
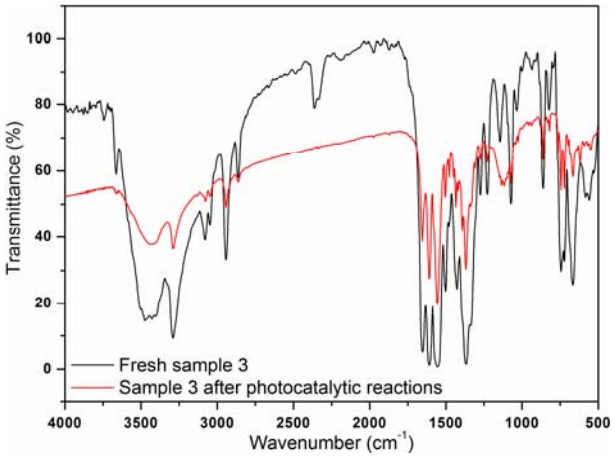
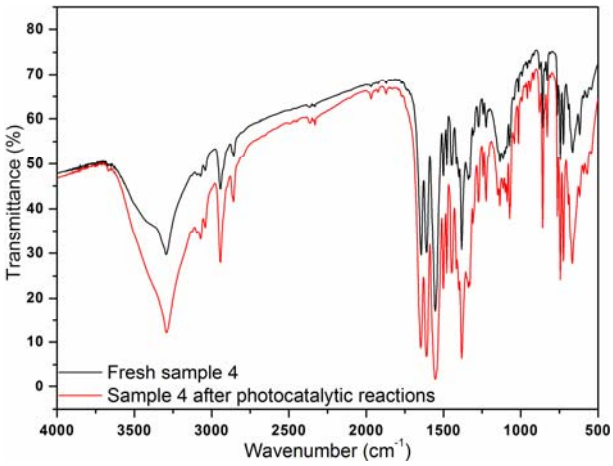


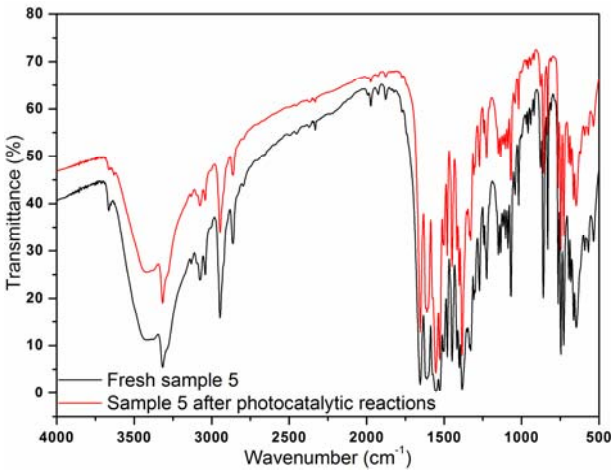
Fig. S9 View of 3D supramolecular architecture of **8**.



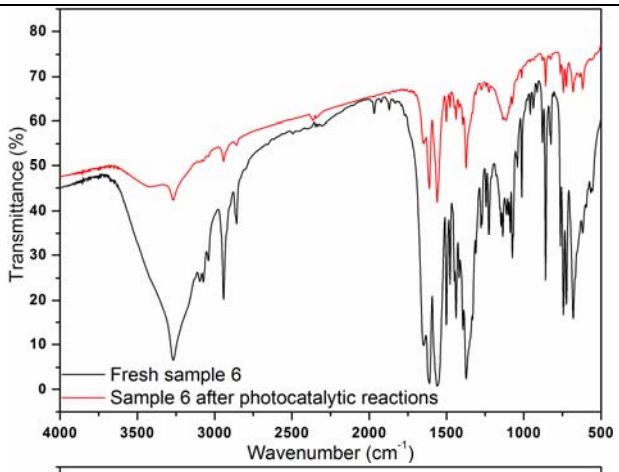
Supplementary Material (ESI) for CrystEngComm
This journal is © The Royal Society of Chemistry

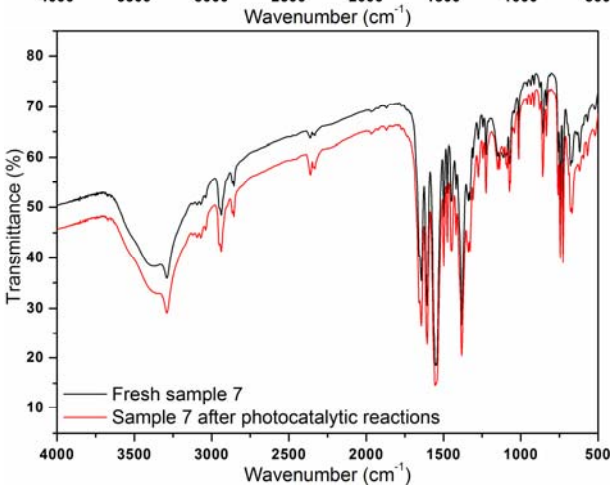


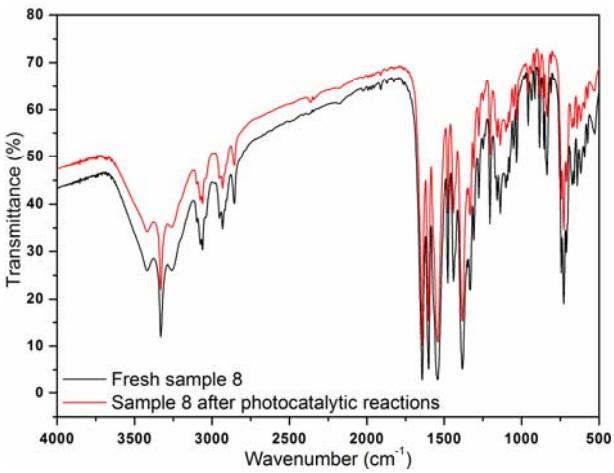




Supplementary Material (ESI) for CrystEngComm
This journal is © The Royal Society of Chemistry







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

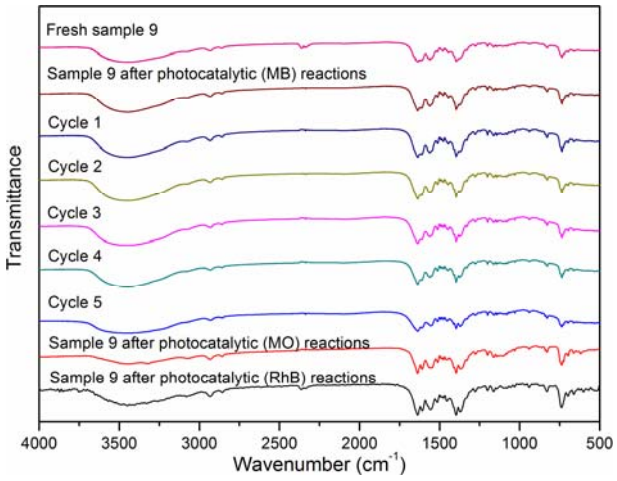
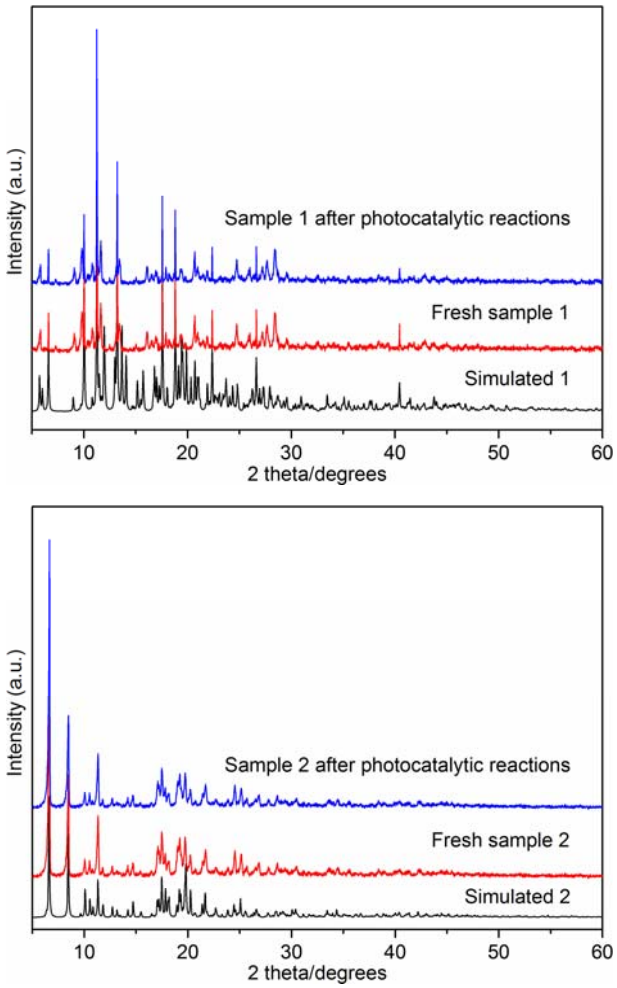
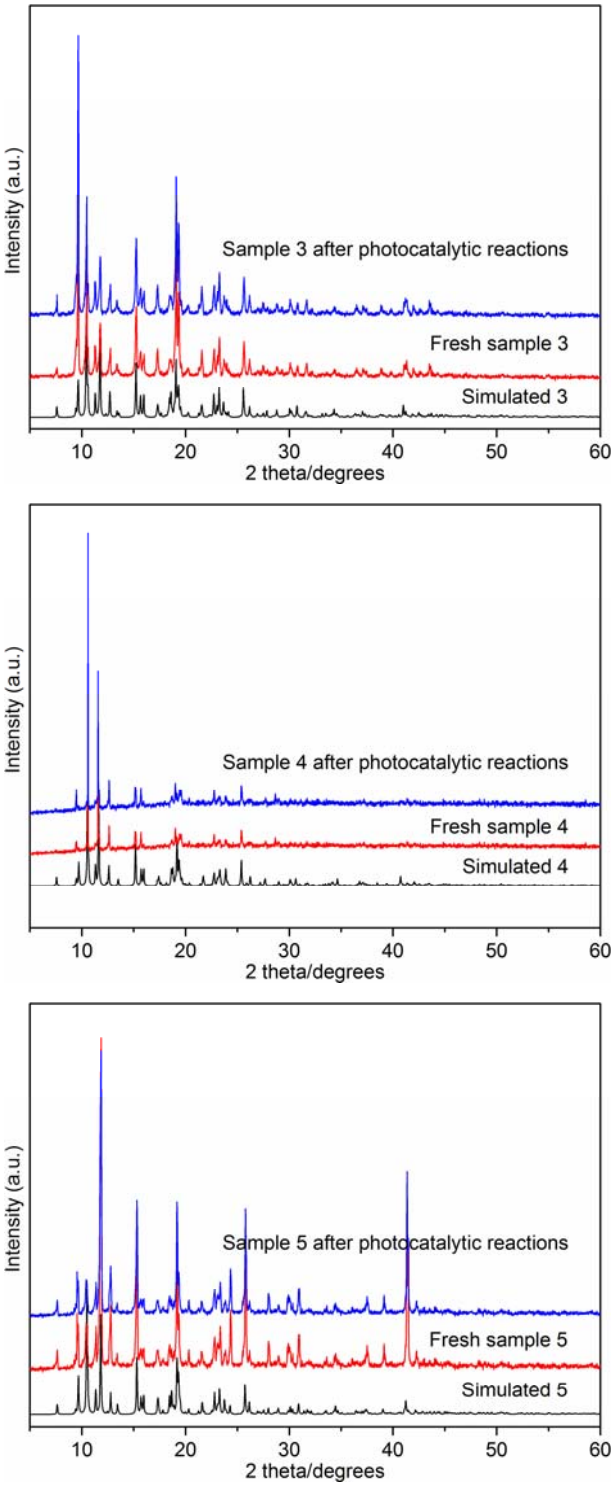


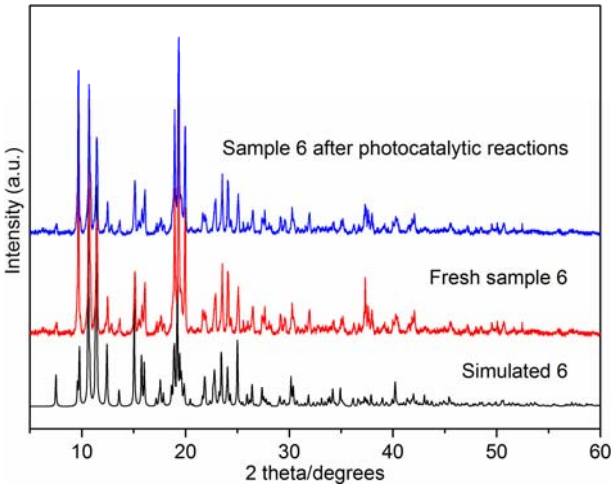
Fig. S10 The IR spectra of complexes **1–9** and after photocatalytic reactions.

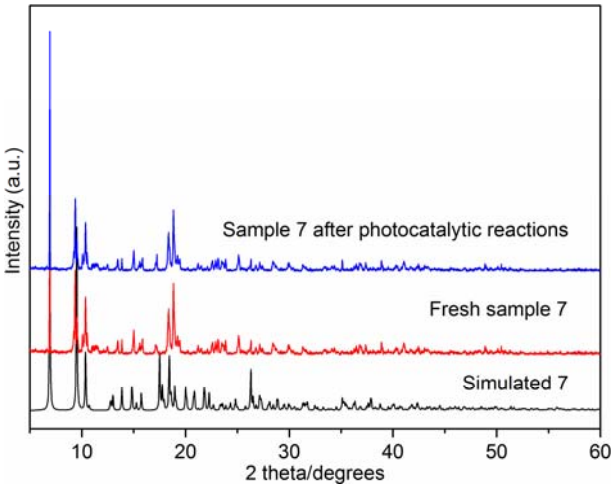


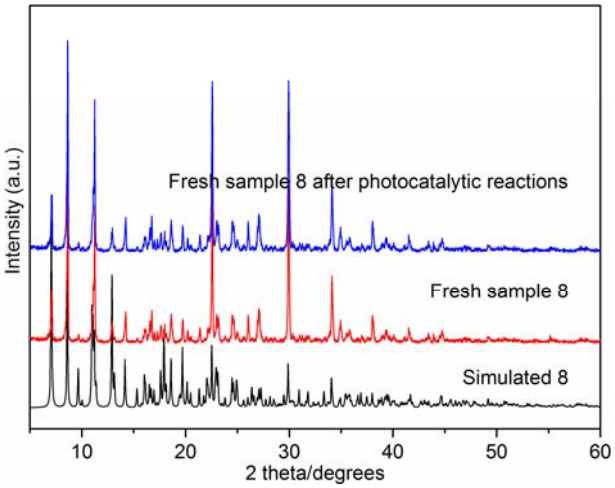
Supplementary Material (ESI) for CrystEngComm
This journal is © The Royal Society of Chemistry



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







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

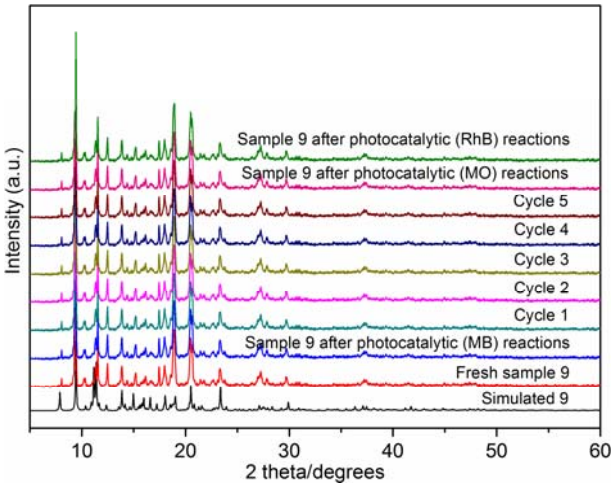


Figure S11 The powder X-ray diffraction patterns of simulated, fresh samples, and samples after photocatalytic experiments for complexes 1−9.

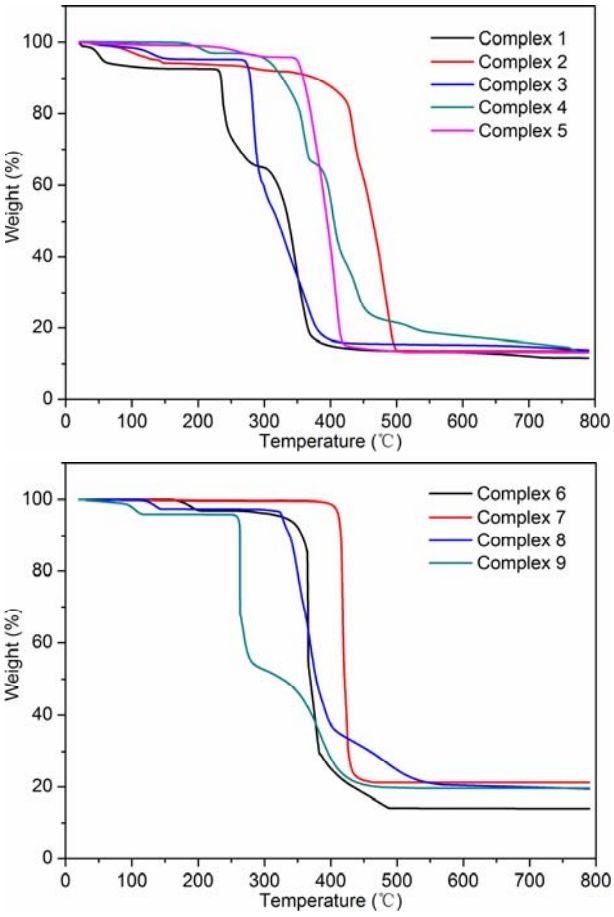
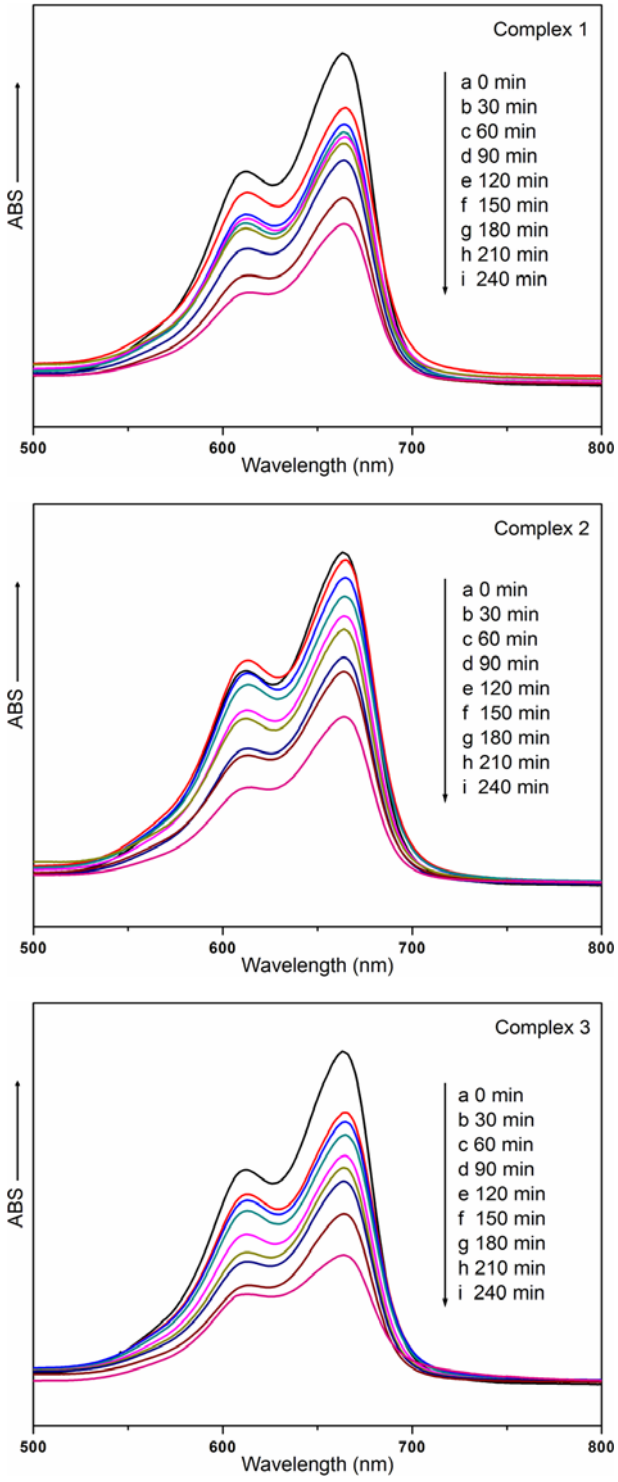
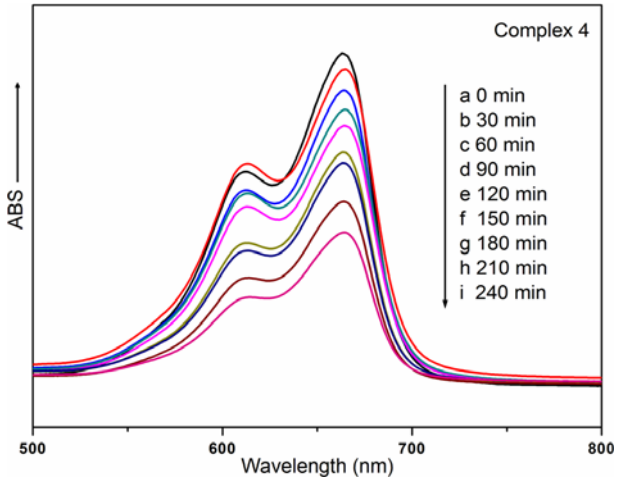


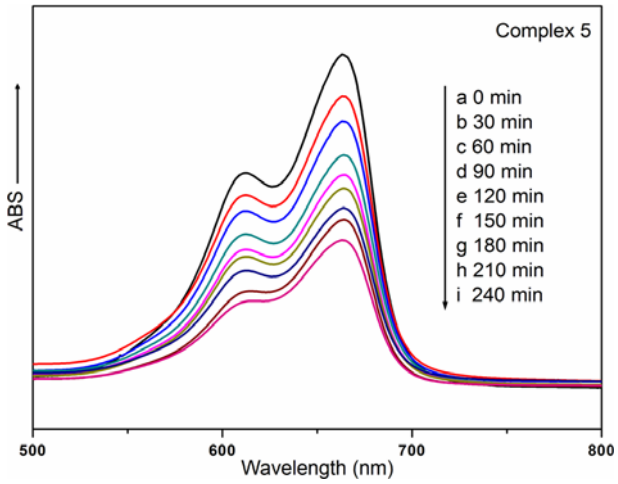
Fig. S12 The TG curves of complexes **1–9**.

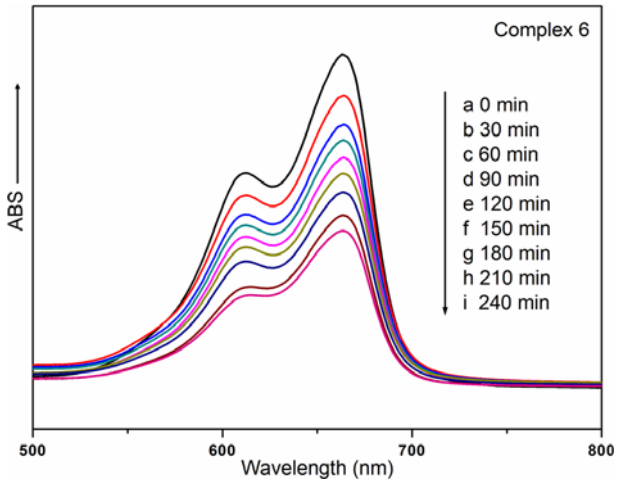
Supplementary Material (ESI) for CrystEngComm
This journal is © The Royal Society of Chemistry



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







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

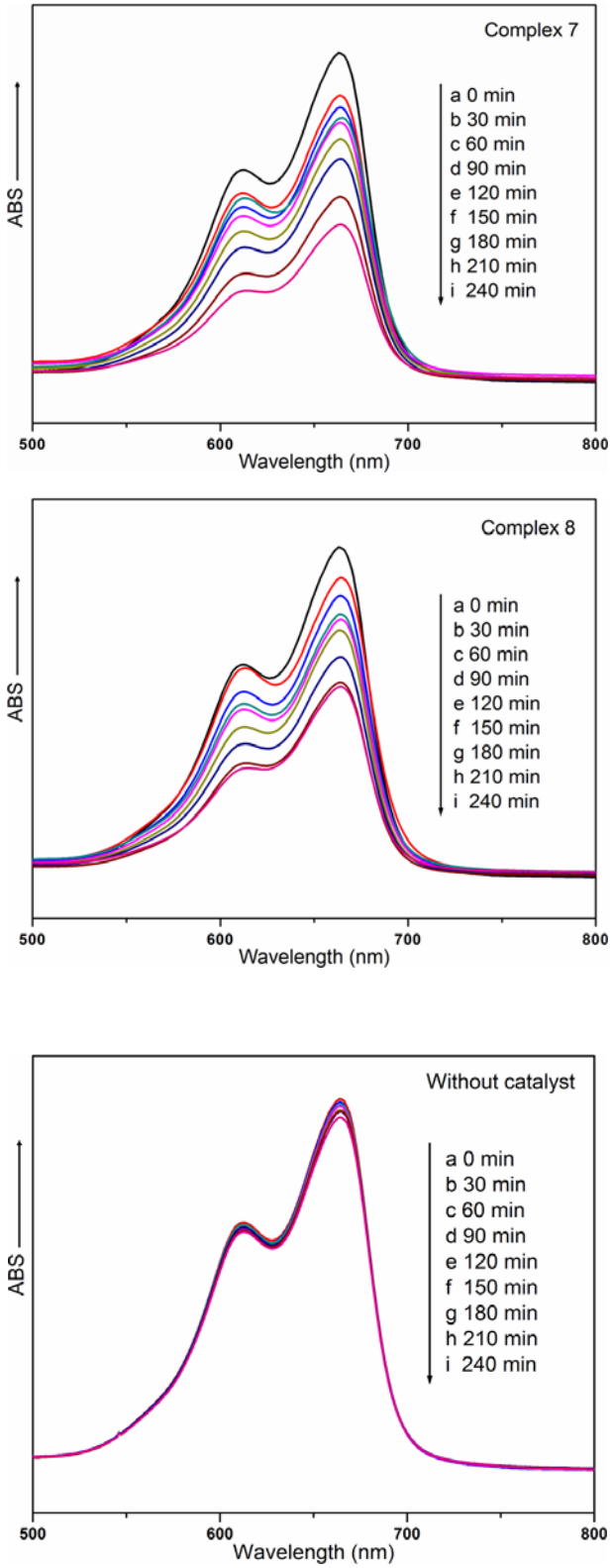


Fig. S13 Absorption spectra of the MB solution during the decomposition reaction under UV irradiation with the presence of complexes **1**–**8**, and without catalyst.

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

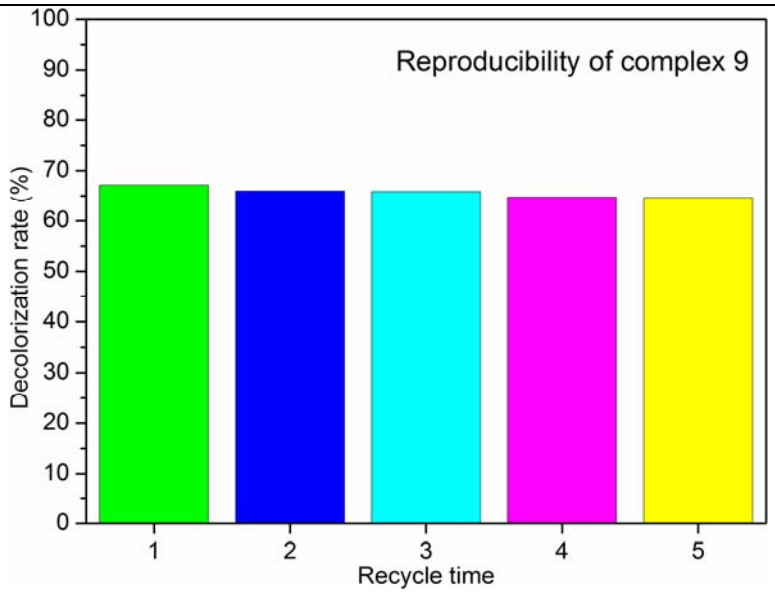


Fig. S14 Cycling runs of **9** in the degradation of MB solution.

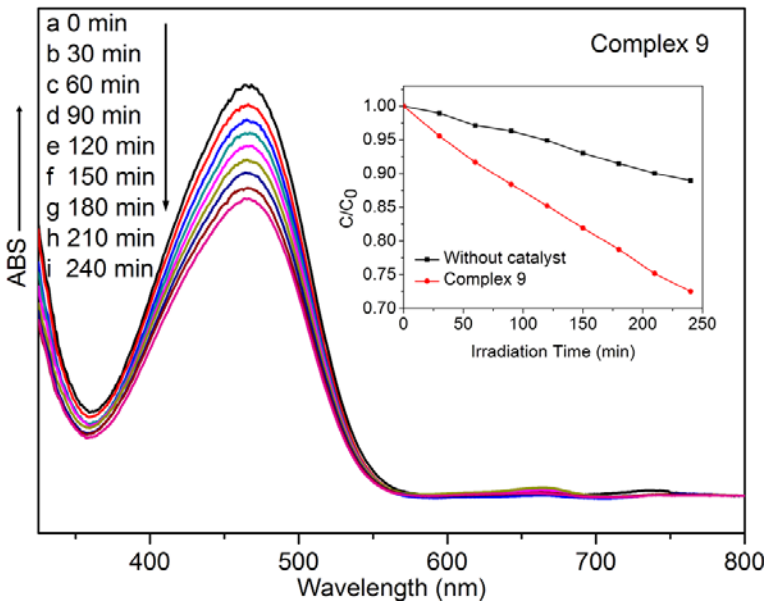


Fig. S15 Absorption spectra of the MO solution during the decomposition reaction under UV irradiation with the presence of complex **9**. The inset shows photocatalytic decomposition rates of MO solution under UV irradiation with the use of complex **9** and no crystal in the same conditions.

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

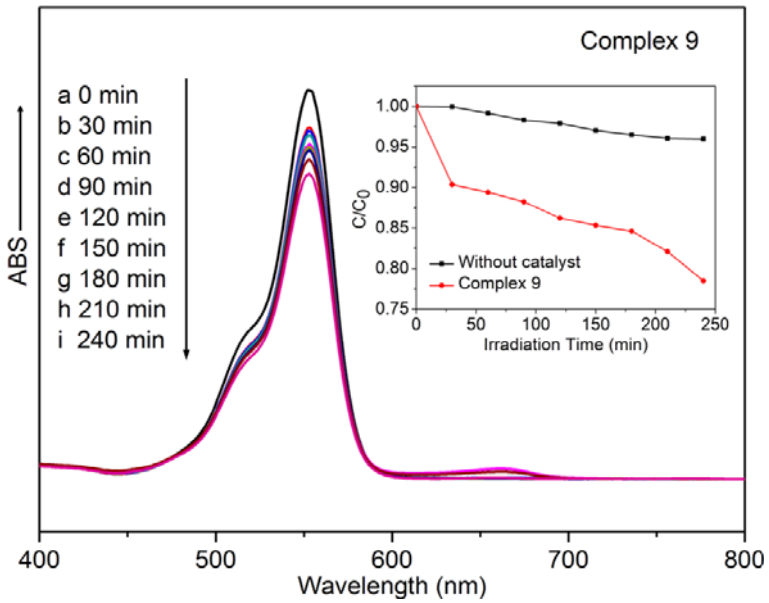


Fig. S16 Absorption spectra of the RhB solution during the decomposition reaction under UV irradiation with the presence of complex **9**. The inset shows photocatalytic decomposition rates of RhB solution under UV irradiation with the use of complex **9** and no crystal in the same conditions.