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Five bis(imidazole)-based coordination polymers tuned by central metal ions and S-containing dicarboxylates: syntheses, structures and properties

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Table S1. Selected bond distances (Å) and angles (°) for complex **1**

Zn(1)-O(3)#1	1.932(2)	Zn(1)-O(1)	1.958(2)
Zn(1)-N(5)#2	1.994(3)	Zn(1)-N(1)	2.014(3)
O(3)#1-Zn(1)-O(1)	105.92(10)	O(3)#1-Zn(1)-N(5)#2	125.04(12)
O(1)-Zn(1)-N(5)#2	107.93(11)	O(3)#1-Zn(1)-N(1)	106.98(12)
O(1)-Zn(1)-N(1)	105.83(11)	N(5)#2-Zn(1)-N(1)	103.78(12)

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

Table S2. Selected bond distances (Å) and angles (°) for complex **2**

Co(1)-O(1)	2.028(6)	Co(1)-N(3)	2.100(9)
Co(1)-S(1)	2.592(3)	Co(2)-O(4)	2.097(6)
Co(2)-O(3W)	2.096(7)	Co(2)-O(2W)	2.115(8)
Co(3)-O(1W)	2.078(8)	Co(3)-O(6)	2.092(7)
Co(3)-O(4W)	2.115(7)	Co(4)-O(8)	2.067(7)
Co(4)-N(1)	2.089(10)	Co(4)-S(2)	2.600(3)
O(1)-Co(1)-O(1)#1	180.000(1)	O(1)-Co(1)-N(3)	90.5(3)
O(1)#1-Co(1)-N(3)	89.5(3)	O(1)-Co(1)-N(3)#1	89.5(3)
O(1)-Co(1)-S(1)#1	100.0(2)	N(3)-Co(1)-N(3)#1	179.999(1)
N(3)-Co(1)-S(1)#1	85.2(2)	O(4)-Co(2)-O(4)#2	179.999(1)

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O(1)-Co(1)-S(1)	80.0(2)	O(1)#1-Co(1)-S(1)	100.0(2)
N(3)-Co(1)-S(1)	94.5(3)	O(4)-Co(2)-O(2W)	91.5(3)
S(1)#1-Co(1)-S(1)	180.0	O(3W)-Co(2)-O(2W)	91.7(3)
O(3W)-Co(2)-O(2W)#2	88.3(3)	O(4)-Co(2)-O(2W)#2	88.5(3)
O(4)#2-Co(2)-O(2W)#2	91.5(3)	O(2W)-Co(2)-O(2W)#2	180.0
O(3W)-Co(2)-O(3W)#2	179.999(1)	O(6)#3-Co(3)-O(6)	179.999(2)
O(1W)-Co(3)-O(1W)#3	179.999(1)	O(1W)-Co(3)-O(6)	88.7(3)
O(1W)-Co(3)-O(4W)#3	88.5(3)	O(6)-Co(3)-O(4W)#3	88.3(3)
O(1W)-Co(3)-O(4W)	91.5(3)	O(1W)#3-Co(3)-O(4W)	88.5(3)
O(8)-Co(4)-N(1)#4	90.3(3)	O(6)-Co(3)-O(4W)	91.7(3)
O(4W)#3-Co(3)-O(4W)	179.998(1)	O(8)#4-Co(4)-O(8)	179.999(1)
O(8)#4-Co(4)-N(1)	90.3(3)	O(8)-Co(4)-N(1)	89.7(3)
N(1)#4-Co(4)-N(1)	179.999(1)	O(8)#4-Co(4)-S(2)	99.5(2)
O(8)-Co(4)-S(2)	80.5(2)	N(1)-Co(4)-S(2)#4	94.1(3)
N(1)-Co(4)-S(2)	85.9(3)	S(2)-Co(4)-S(2)#4	180.00(11)

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

Table S3. Selected bond distances (Å) and angles (°) for complex **3**

Ni(1)-O(2W)	2.017(11)	Ni(1)-O(2W)#1	2.017(11)
Ni(1)-O(1W)#1	2.040(13)	Ni(1)-O(1W)	2.041(13)
Ni(1)-O(3)	2.070(13)	Ni(1)-O(3)#1	2.070(13)
S(1)-Ni(2)	2.536(5)	O(1)-Ni(2)	2.041(13)
N(1)-Ni(2)	2.058(15)	Ni(2)-O(1)#2	2.041(13)
Ni(2)-N(1)#2	2.058(15)	Ni(2)-S(1)#2	2.536(5)
O(2W)-Ni(1)-O(2W)#1	180.000(1)	O(2W)-Ni(1)-O(1W)#1	88.2(4)
O(2W)#1-Ni(1)-O(1W)#1	91.8(4)	O(2W)-Ni(1)-O(1W)	91.8(4)
O(2W)#1-Ni(1)-O(1W)	88.2(4)	O(1W)#1-Ni(1)-O(1W)	180.0
O(2W)-Ni(1)-O(3)	87.2(5)	O(2W)#1-Ni(1)-O(3)	92.8(5)
O(1W)#1-Ni(1)-O(3)	88.9(5)	O(1W)-Ni(1)-O(3)	91.1(5)
O(2W)-Ni(1)-O(3)#1	92.8(5)	O(2W)#1-Ni(1)-O(3)#1	87.2(5)
O(1W)#1-Ni(1)-O(3)#1	91.1(5)	O(1W)-Ni(1)-O(3)#1	88.9(5)
O(3)-Ni(1)-O(3)#1	179.999(1)	O(1)#2-Ni(2)-O(1)	179.999(1)
O(1)#2-Ni(2)-N(1)#2	89.4(5)	O(1)-Ni(2)-N(1)#2	90.6(5)
O(1)#2-Ni(2)-N(1)	90.6(5)	O(1)-Ni(2)-N(1	89.4(5)
N(1)#2-Ni(2)-N(1)	180.000(1)	O(1)#2-Ni(2)-S(1)	98.4(4)
O(1)-Ni(2)-S(1)	81.6(4)	N(1)#2-Ni(2)-S(1)	94.5(4)
N(1)-Ni(2)-S(1)	85.5(4)	O(1)#2-Ni(2)-S(1)#2	81.6(4)

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O(1)-Ni(2)-S(1)#2	98.4(4)	N(1)#2-Ni(2)-S(1)#2	85.5(4)
N(1)-Ni(2)-S(1)#2	94.5(4)	S(1)-Ni(2)-S(1)#2	180.0
Symmetry code: #1 $-x-1, -y+1, -z$; #2 $-x, -y, -z$; #3 $-x, -y-1, -z+1$			

Table S4. Selected bond distances (Å) and angles (°) for complex **4**

Cd(1)-O(1W)	2.278(2)	Cd(1)-O(1)	2.283(2)
Cd(2)-O(3)	2.286(2)	Cd(1)-O(2W)	2.289(2)
S(1)-Cd(2)	2.7853(8)	N(1)-Cd(2)	2.282(2)
O(1W)-Cd(1)-O(1W)#1	180.0	O(1W)-Cd(1)-O(1)	90.12(10)
O(1W)#1-Cd(1)-O(1)	89.88(10)	O(1)#1-Cd(1)-O(2W)	87.63(8)
O(1W)#1-Cd(1)-O(1)#1	90.12(10)	O(1)-Cd(1)-O(1)#1	180.0
O(1W)-Cd(1)-O(2W)#1	91.84(8)	O(1W)#1-Cd(1)-O(2W)#1	88.16(8)
O(1)-Cd(1)-O(2W)#1	87.63(8)	O(1)#1-Cd(1)-O(2W)#1	91.84(8)
O(1W)-Cd(1)-O(2W)	88.16(8)	O(1W)#1-Cd(1)-O(2W)	91.84(8)
O(1)-Cd(1)-O(2W	92.37(8)	N(1)-Cd(2)-O(3)#2	89.93(8)
O(2W)#1-Cd(1)-O(2W)	179.999(1)	N(1)#2-Cd(2)-N(1)	180.00(10)
N(1)#2-Cd(2)-O(3)	89.93(8)	N(1)-Cd(2)-O(3)	90.07(9)
O(3)-Cd(2)-O(3)#2	180.0	N(1)#2-Cd(2)-S(1)	94.85(7)
N(1)-Cd(2)-S(1)	85.15(7)	O(3)-Cd(2)-S(1)	73.36(5)
O(3)#2-Cd(2)-S(1)	106.64(5)	N(1)#2-Cd(2)-S(1)#2	85.15(7)
N(1)-Cd(2)-S(1)#2	94.86(7)	O(3)-Cd(2)-S(1)#2	106.64(5)
O(3)#2-Cd(2)-S(1)#2	73.36(5)	S(1)-Cd(2)-S(1)#2	179.999(1)
Symmetry code: #1 $-x, -y+2, -z$; #2 $-x, -y+1, -z$; #3 $-x-1, -y, -z-1$			

Table S5. Selected bond distances (Å) and angles (°) for complex **5**

Cd(1)-N(3)	2.262(2)	Cd(1)-N(2)	2.280(3)
Cd(1)-N(1)	2.342(3)	Cd(1)-O(2)#1	2.478(3)
Cd(1)-O(4)#1	2.489(2)	Cd(1)-O(1)	2.512(2)
Cd(1)-O(3)	2.584(3)	N(3)-Cd(1)-N(2)	173.04(9)
N(3)-Cd(1)-N(1)	90.30(9)	N(2)-Cd(1)-N(1)	90.90(9)
N(3)-Cd(1)-O(2)#1	95.62(8)	N(2)-Cd(1)-O(2)#1	88.34(9)
N(1)-Cd(1)-O(2)#1	135.26(9)	N(3)-Cd(1)-O(4)#1	86.87(8)
N(2)-Cd(1)-O(4)#1	100.07(9)	N(1)-Cd(1)-O(4)#1	83.98(9)
O(2)#1-Cd(1)-O(4)#1	52.30(8)	N(3)-Cd(1)-O(1)	86.44(8)
N(2)-Cd(1)-O(1)	87.94(8)	N(1)-Cd(1)-O(1)	136.00(9)

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O(2)#1-Cd(1)-O(1)	88.69(8)	O(4)#1-Cd(1)-O(1)	139.42(8)
N(3)-Cd(1)-O(3)	89.80(9)	N(2)-Cd(1)-O(3)	83.47(9)
N(1)-Cd(1)-O(3)	85.09(9)	O(2)#1-Cd(1)-O(3)	139.04(9)
O(4)#1-Cd(1)-O(3)	168.56(8)	O(1)-Cd(1)-O(3)	51.07(8)

Symmetry code: #1 –*x*, –*y*, –*z*; #2 –*x* + 1, –*y*, –*z* + 1; #3 –*x*, –*y* + 1, –*z* + 1; #4 –*x* + 1, –*y*, –*z*

Table S6. Hydrogen-bonding geometries (Å, °) of complexes **1**, **2** and **4**

D–H···A	D–H	H···A	D···A	D–H···A
		1		
C11–H11A···O2	0.97	2.58	3.283(52)	129
		2		
O2W–H2WA···O2	0.85	2.01	2.749(93)	148
		4		
O1W–H1WA···O4	0.85	2.14	2.713(29)	125

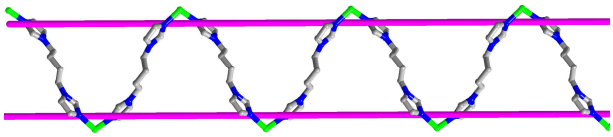

Fig. S1. The 1D [Zn-biim-4]$_n$ meso-helical chain in complex **1**.

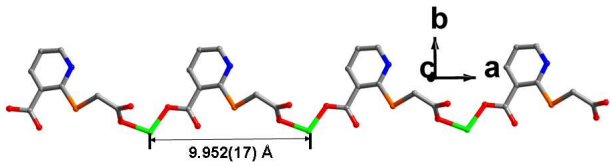

Fig. S2. View of the 1D linear chain constructed by Zn^{II} ions and 2-CMSN anions in complex **1**.

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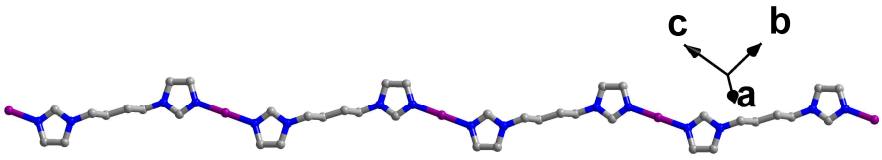

Fig. S3. View of the 1D linear chain constructed by Co^{II} ions and biim-4 ligands in complex **2**.

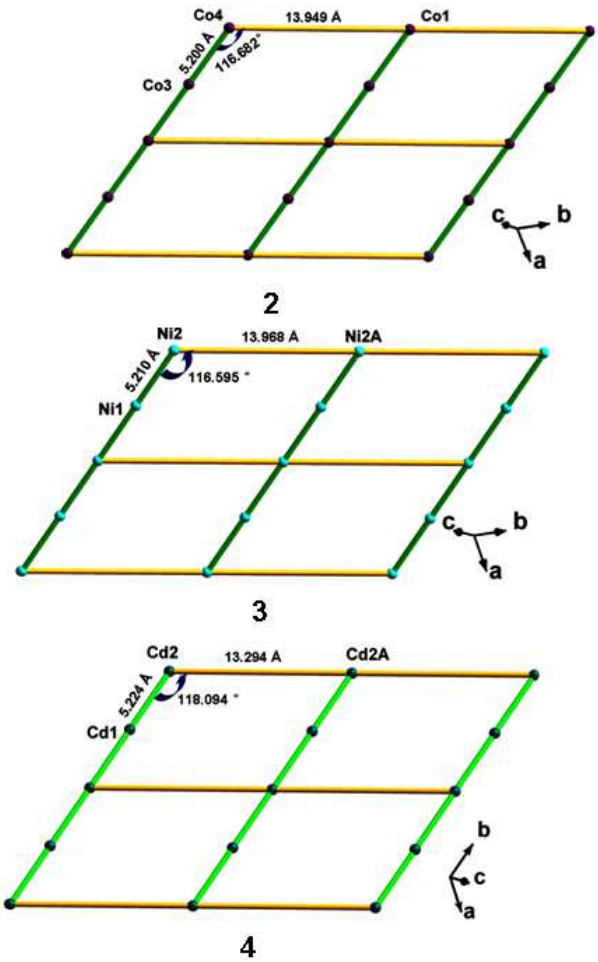

Fig. S4. The simplified representation of the 2D structure in complexes **2**–**4**.

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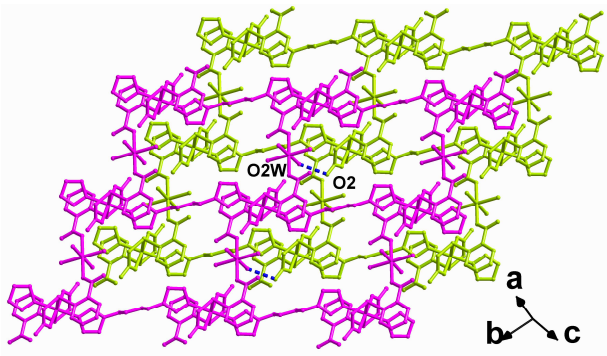
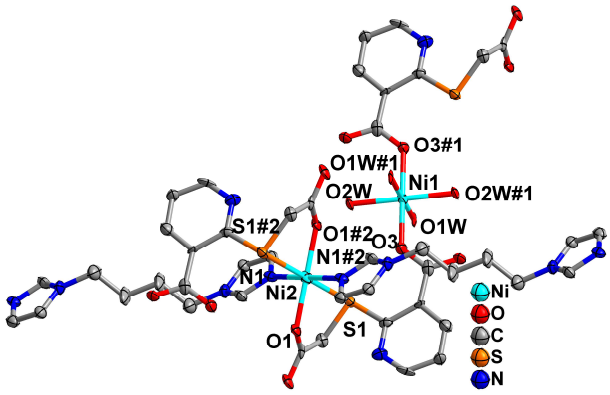
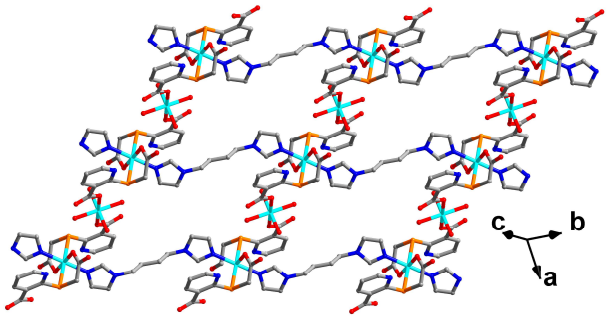


Fig. S5. The 3D supramolecular architecture connected by hydrogen bonding interactions in **2**.



(a)



(b)

Fig. S6. (a) The coordination environment of Ni^{II} centers in complex **3** with 30% thermal ellipsoids; **(b)** The 2D layer in complex **3**.

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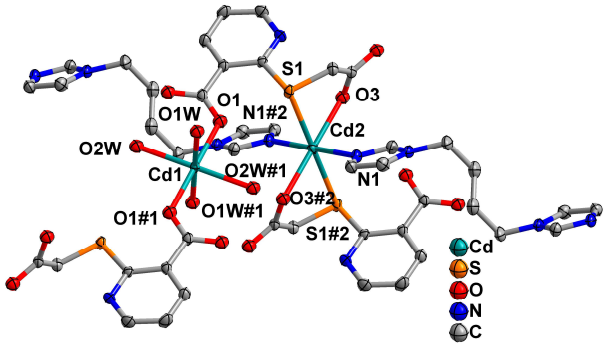
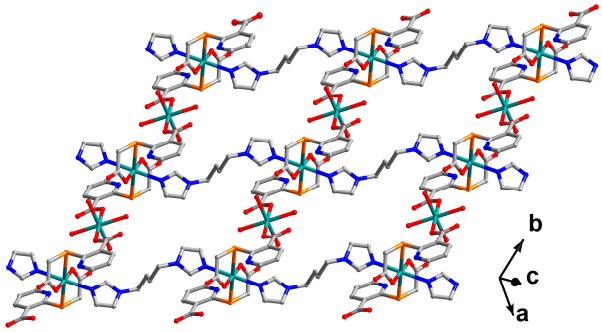


(a)



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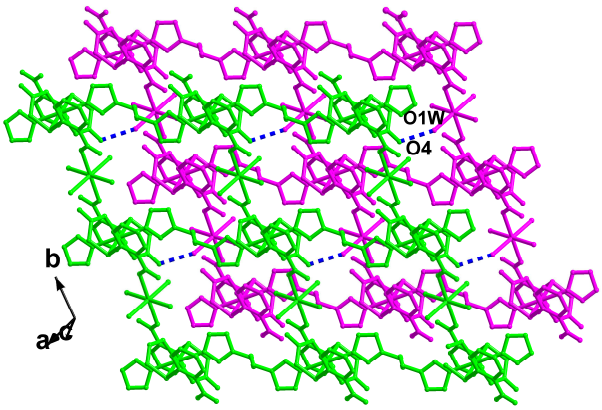

(c)

Fig. S7. (a) The coordination environment of Cd^{II} center in complex **4** with 30% thermal ellipsoids; **(b)** The 2D layer in complex **4**; **(c)** The 3D supramolecular architecture connected by hydrogen bonding interactions.

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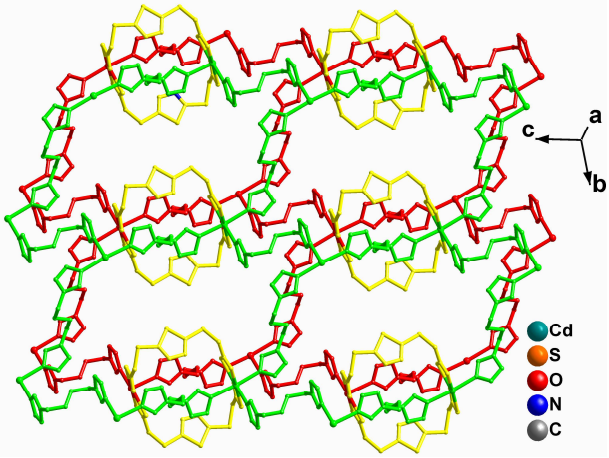
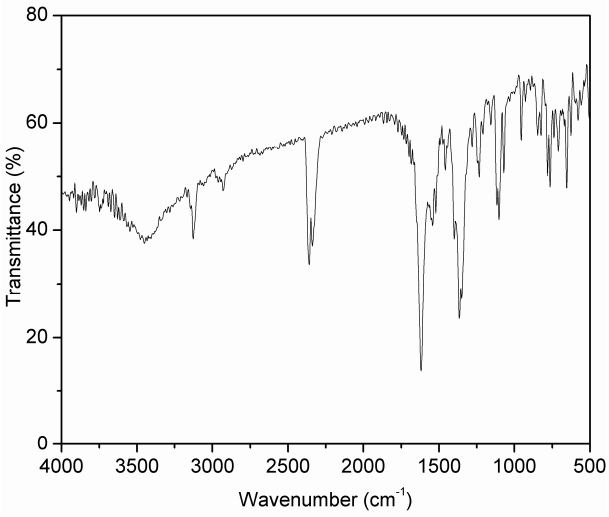
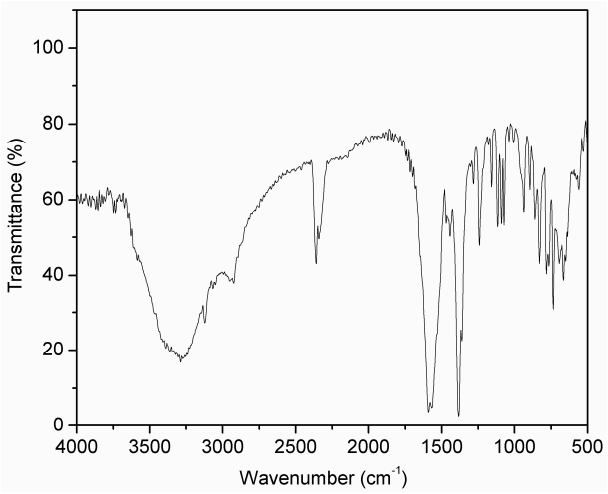


Fig. S8. The 3D framework of complex **5**.



(a)



(b)

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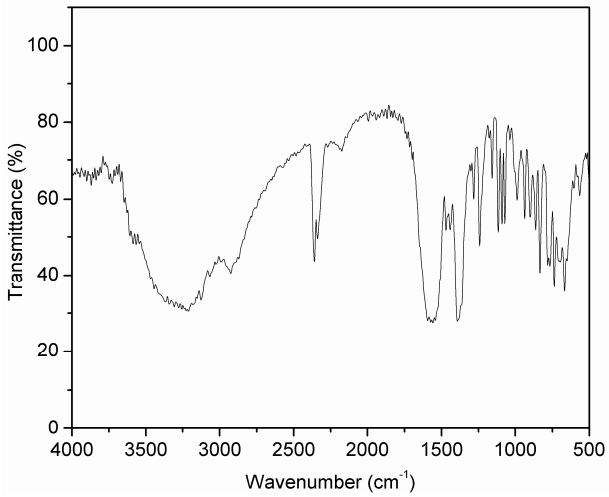

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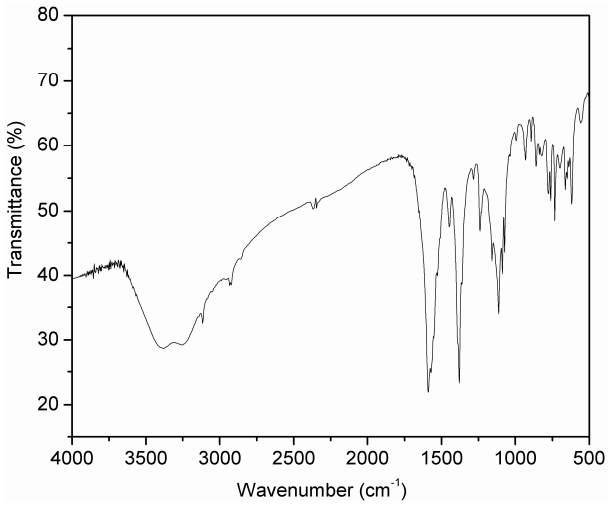

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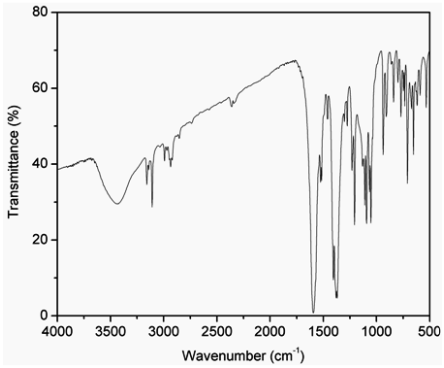

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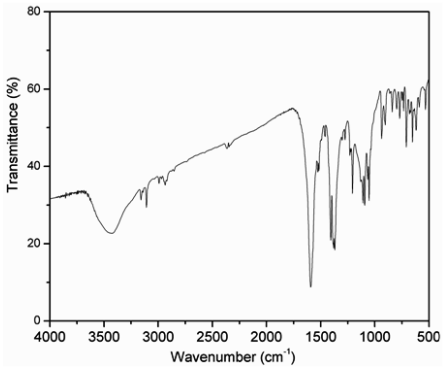

(f)

Fig. S9. (a)–(e) The IR spectra of complexes **1**–**5**; **(f)** The IR spectrum of complex **5** after the photocatalysis experiments.

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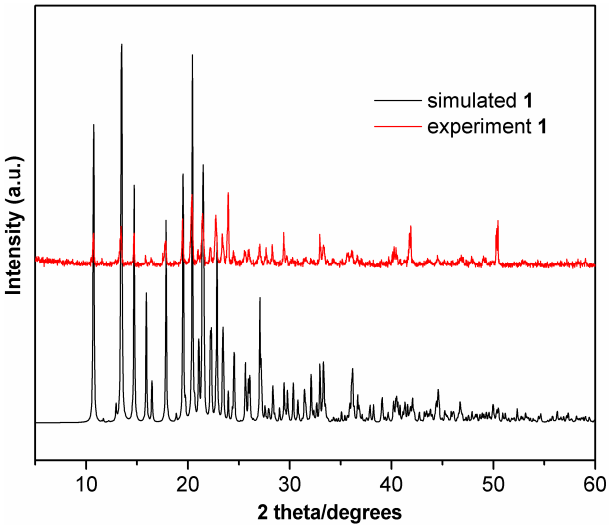

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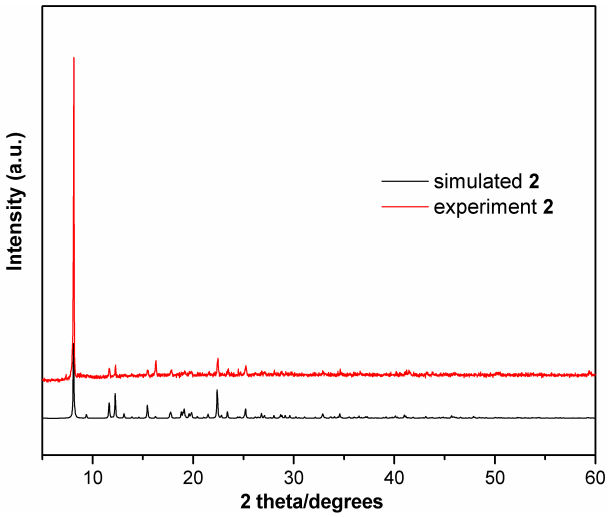

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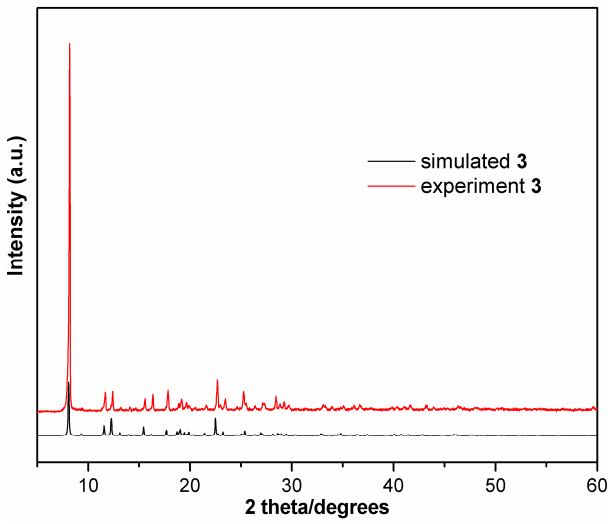

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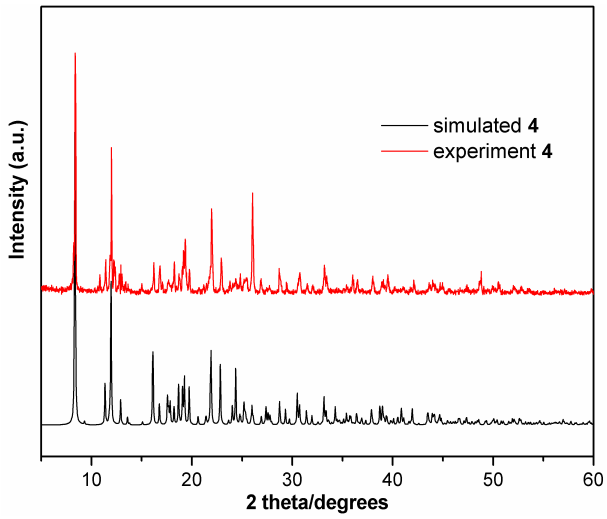
(c)



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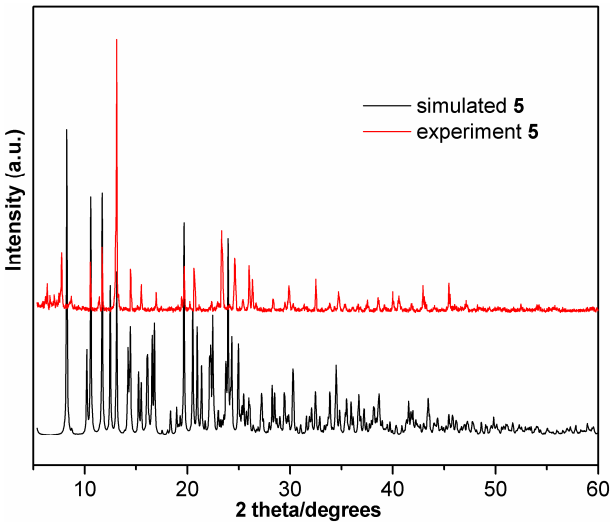

(e)

Fig. S10. The PXRD curves of complexes **1**–**5**.

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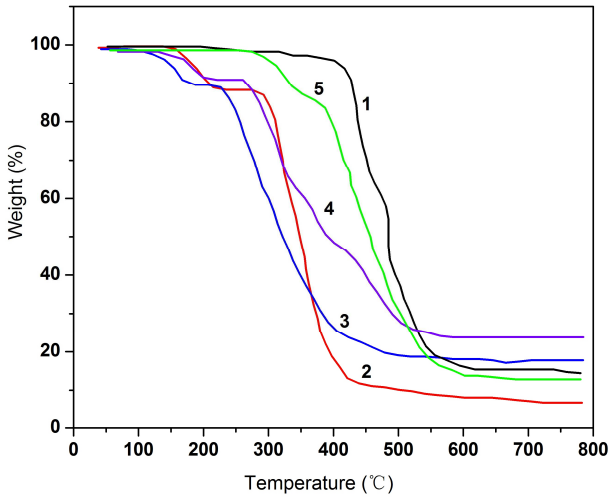


Fig. S11. The TG curves of complexes **1**–**5**.

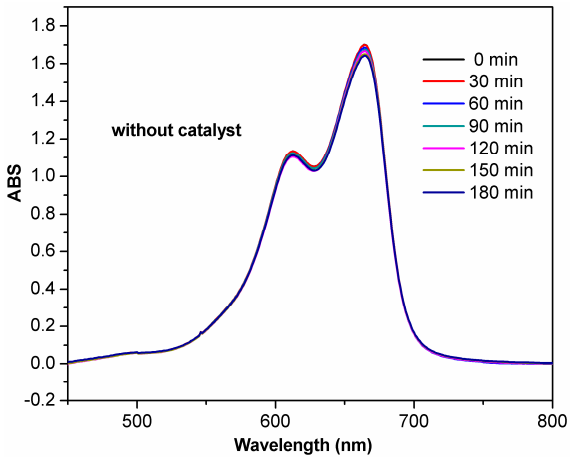
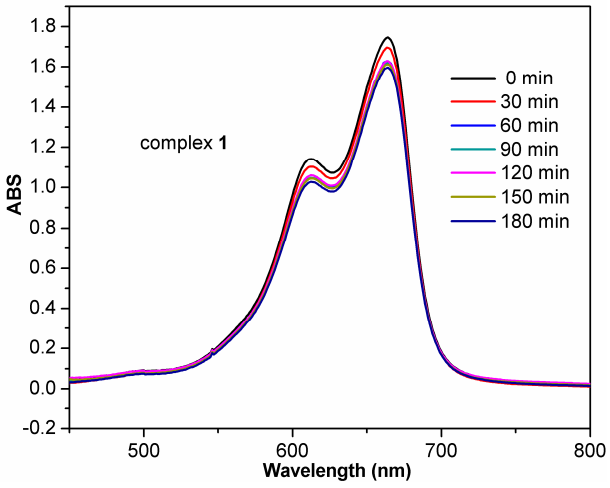


Fig. S12. Absorption spectra of the MB solution during the decomposition reaction under UV light irradiation without catalyst.



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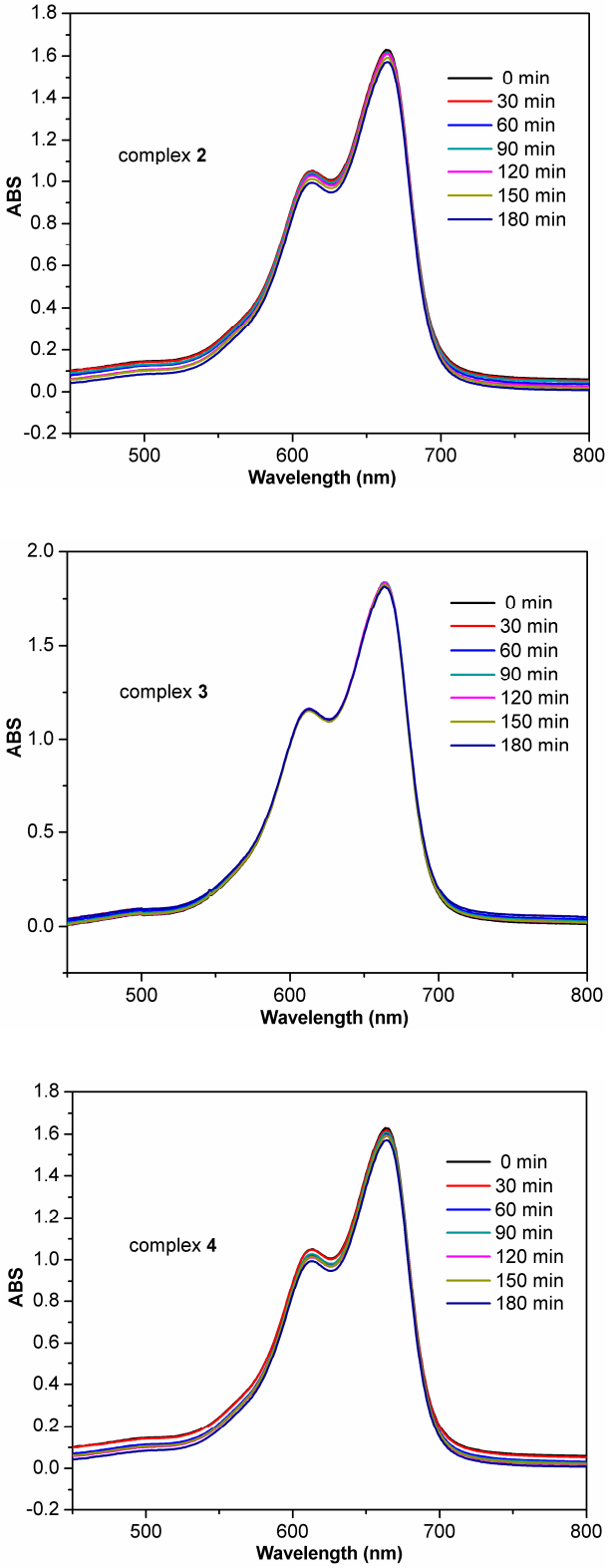

Fig. S13. Absorption spectra of the MB solution during the decomposition reaction under UV light irradiation with the use of complexes **1**–**4**.