Supporting Information

Synthesis, crystal structures, and luminescent properties of Zn(II) and Cd(II) coordination compounds assembled from flexible bis(quinolyl) ligands with symmetrical spacers: the influence of coordinated anions

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Table S1. Selected bond lengths (Å) for compound **1**

bond	length	bond	length
Zn(1)–N(1)	2.186(3)	Zn(1)–N(2)	2.060(3)
Zn(1)–N(7)	2.144(3)	Zn(1)–N(8)	2.068(3)
Zn(1)–O(1)	2.196(3)	Zn(1)–O(2)	2.192(2)
Zn(2)–N(3)	2.157(3)	Zn(2)–N(5)	2.112(3)
Zn(2)–N(6)	2.244(3)	Zn(2)–N(13)	1.971(4)
Zn(2)–Cl(1)	2.2669(11)	Zn(3)–N(9)	2.131(3)
Zn(3)–N(11)	2.125(3)	Zn(3)–N(12)	2.220(3)
Zn(3)–N(14)	1.969(3)	Zn(3)–N(15)	1.964(3)

Table S2. Selected bond angles (°) for compound **1**

bond angle	degree	bond angle	degree
N(1)–Zn(1)–N(2)	76.87(11)	N(1)–Zn(1)–N(7)	100.26(11)
N(1)–Zn(1)–N(8)	115.03(11)	N(2)–Zn(1)–N(7)	120.10(11)
N(2)–Zn(1)–N(8)	158.34(12)	N(7)–Zn(1)–N(8)	77.09(10)
O(1)–Zn(1)–N(1)	150.04(10)	O(1)–Zn(1)–N(2)	74.15(10)
O(1)–Zn(1)–N(7)	87.86(10)	O(1)–Zn(1)–N(8)	94.85(10)
O(2)–Zn(1)–N(1)	88.32(10)	O(2)–Zn(1)–N(2)	89.08(10)
O(2)–Zn(1)–N(7)	150.69(10)	N(3)–Zn(2)–N(5)	73.07(12)
N(3)–Zn(2)–N(6)	146.85(12)	N(3)–Zn(2)–N(13)	95.32(14)
N(5)–Zn(2)–N(6)	73.78(12)	N(5)–Zn(2)–N(13)	124.45(15)
N(6)–Zn(2)–N(13)	103.44(14)	N(3)–Zn(2)–Cl(1)	101.48(9)
N(5)–Zn(2)–Cl(1)	123.85(10)	N(6)–Zn(2)–Cl(1)	96.69(9)
N(13)–Zn(2)–Cl(1)	111.66(12)	N(9)–Zn(3)–N(11)	73.83(11)
N(9)–Zn(3)–N(12)	147.53(11)	N(9)–Zn(3)–N(14)	100.97(11)
N(9)–Zn(3)–N(15)	97.37(12)	N(11)–Zn(3)–N(12)	73.73(11)
N(11)–Zn(3)–N(14)	121.66(12)	N(11)–Zn(3)–N(15)	121.14(12)
N(12)–Zn(3)–N(14)	97.08(11)	N(12)–Zn(3)–N(15)	98.06(12)
N(14)–Zn(3)–N(15)	117.17(13)		

Table S3. Hydrogen bond parameters (Å, °) of compound **1**

D-H···A	D(D—H)	d(H···A)	d(D···A)	∠(DHA)	Symmetry transformation for A
O(5)—H(5)···O(4)	0.9672	1.989(9)	2.761(9)	135.2(3)	
O(5)—H(5F)···Cl(1)	1.045(6)	2.283(4)	3.252(4)	153.6(5)	1 — x, 2 — y, — z
N(4)—H(4)···O(5)	0.8800	1.860(5)	2.731(5)	169.82(16)	
N(10)—H(10)···O(3)	0.8800	1.892(4)	2.746(4)	163.19(16)	

Table S4. Selected bond lengths (Å) for compound **2**

bond	length	bond	length
Zn(1)–Cl(1)	2.3103(5)	Zn(1)–O(2)	1.9358(15)
Zn(1)–N(1)	2.2434(17)	Zn(1)–N(2)	2.1278(18)
Zn(1)–N(4)	2.1430(17)	Zn(2)–Cl(2)	2.2570(18)
Zn(2)–I(2)	2.548(4)	Zn(2)–O(1)	2.2973(15)
Zn(2)–O(2A)	1.9350(14)	Zn(2)–N(5)	2.0762(16)
Zn(2)–N(6)	2.2067(18)		

Symmetry transformations used to generate equivalent atoms: A: 2 — x, 2 — y, — z.

Table S5. Selected bond angles (°) for compound **2**

bond angle	degree	bond angle	degree
N(1)–Zn(1)–Cl(1)	96.07(5)	N(2)–Zn(1)–Cl(1)	122.83(5)
N(4)–Zn(1)–Cl(1)	100.23(5)	N(1)–Zn(1)–N(4)	146.36(7)
N(2)–Zn(1)–N(1)	73.42(7)	N(2)–Zn(1)–N(4)	73.01(7)
N(1)–Zn(1)–O(2)	104.70(6)	N(2)–Zn(1)–O(2)	120.95(6)
N(4)–Zn(1)–O(2)	94.23(6)	O(2)–Zn(1)–Cl(1)	116.10(5)
Cl(2)–Zn(2)–N(5)	118.24(6)	Cl(2)–Zn(2)–N(6)	103.79(6)
Cl(2)–Zn(2)–O(1)	94.11(6)	Cl(2)–Zn(2)–O(2A)	115.39(6)
I(2)–Zn(2)–N(5)	125.85(11)	I(2)–Zn(2)–N(6)	109.42(11)
I(2)–Zn(2)–O(1)	92.09(11)	I(2)–Zn(2)–O(2A)	107.08(11)
N(5)–Zn(2)–N(6)	75.88(6)	N(5)–Zn(2)–O(1)	72.08(6)

Table S5. (continued)

bond angle	degree	bond angle	degree
N(5)–Zn(2)–O(2A)	125.86(6)	N(6)–Zn(2)–O(1)	147.80(6)
N(6)–Zn(2)–O(2A)	98.45(6)	O(1)–Zn(2)–O(2A)	97.65(6)

Symmetry transformations used to generate equivalent atoms: A: 2 — x, 2 — y, — z.

Table S6. Hydrogen bond parameters (Å, °) of compound **2**

D-H···A	D(D—H)	d(H···A)	d(D···A)	∠(DHA)	Symmetry transformation for A
N(3)—H(3)···O(3)	0.88	1.91	2.761(2)	162.0	
O(3)—H(3C)···Cl(1)	0.87	2.79	3.429(3)	132	2 — x, 1 —y, — z
O(5)—H(5)···Cl(1)	0.87	2.31	3.175(2)	176	
O(6)—H(6D)···Cl(2)	0.87	2.45	3.259(3)	155	—1 + x, y, 1 + z
O(6)—H(6D)···I(2)	0.87	2.25	3.060(6)	155	—1 + x, y, 1 + z
O(3)—H(3E)···O(5)	0.87	1.87	2.742(5)	176	x, y, — 1 + z
O(4)—H(4)···O(1)	0.87	2.00	2.87(3)	172.0	
O(4)—H(4E)···O(5)	0.87	1.95	2.75(3)	150.4	x, y, — 1 + z
O(5)—H(5)···O(6)	0.87	1.90	2.739(3)	160.6	
O(6)—H(6A)···O(4)	0.87	1.79	2.50(3)	137.0	2 — x, 2 — y, — z

Table S7. Selected bond lengths (Å) for compound **3**

bond	length	bond	length
Cd(1)–N(1)	2.392(6)	Cd(1)–N(2)	2.284(6)
Cd(1)–O(1)	2.440(6)	Cd(1)–I(1)	2.714(6)
Cd(1)–I(1A)	2.711(4)	Cd(1)–I(2)	2.737(5)
Cd(1)–I(2A)	2.727(4)	Cd(2)–N(3)	2.367(6)
Cd(2)–N(5)	2.319(6)	Cd(2)–N(6)	2.438(6)
Cd(2)–O(2)	2.337(5)	Cd(2)–O(3)	2.455(6)
Cd(2)–I(3)	2.7323(10)		

Table S8. Selected bond angles (°) for compound **3**

bond angle	degree	bond angle	degree
N(1)–Cd(1)–N(2)	70.5(2)	N(1)–Cd(1)–O(1)	136.83(19)
N(1)–Cd(1)–I(1)	102.8(3)	N(1)–Cd(1)–I(1A)	103.1(2)
N(1)–Cd(1)–I(2)	104.8(2)	N(1)–Cd(1)–I(2A)	105.0(2)
N(2)–Cd(1)–O(1)	66.7(2)	N(2)–Cd(1)–I(1)	121.3(3)
N(2)–Cd(1)–I(2)	116.9(4)	O(1)–Cd(1)–I(1)	103.7(3)
O(1)–Cd(1)–I(2)	89.9(3)	I(1)–Cd(1)–I(2)	120.9(3)
N(3)–Cd(2)–N(5)	67.6(2)	N(3)–Cd(2)–N(6)	133.6(2)
N(5)–Cd(2)–N(6)	68.1(2)	N(3)–Cd(2)–O(2)	82.4(2)
N(3)–Cd(2)–O(3)	87.4(2)	N(5)–Cd(2)–O(2)	97.2(2)
N(5)–Cd(2)–O(3)	74.8(2)	N(6)–Cd(2)–O(2)	90.2(2)
N(6)–Cd(2)–O(3)	93.8(2)	N(3)–Cd(2)–I(3)	115.59(15)
N(5)–Cd(2)–I(3)	164.51(15)	N(6)–Cd(2)–I(3)	110.79(15)
O(2)–Cd(2)–I(3)	98.27(15)	O(3)–Cd(2)–I(3)	89.98(16)

Table S9. Hydrogen bond parameters (Å, °) of compound **3**

D-H···A	D(D—H)	d(H···A)	d(D···A)	∠(DHA)	Symmetry transformation for A
N(4)—H(4D)···O(1)	0.88	1.99	2.850(10)	166	2 — x, 1 — y, — z
O(2)—H(2)···O(4)	0.87	1.87	2.718(12)	166	
O(2)—H(2E)···O(4)	0.87	1.97	2.761(11)	150	1 — x, 1 — y, — z

Table S10. Selected bond lengths (Å) for compound **4**

bond	length	bond	length
Zn(1)–N(1)	2.204(4)	Zn(1)–N(2)	2.115(4)
Zn(1)–N(7)	2.300(4)	Zn(1)–N(8)	2.110(4)
Zn(1)–S(1)	2.5276(15)	Zn(1)–S(2)	2.5108(15)
Zn(2)–Cl(1)	2.2315(17)	Zn(2)–Cl(2)	2.2472(17)
Zn(2)–N(3)	2.230(4)	Zn(2)–N(5)	2.107(4)
Zn(2)–N(6)	2.272(4)	Zn(3)–Cl(3)	2.2681(15)
Zn(3)–Cl(4)	2.2385(16)	Zn(3)–N(9)	2.225(4)
Zn(3)–N(11)	2.090(4)	Zn(3)–N(12)	2.233(4)

Table S11. Selected bond angles (°) for compound **4**

bond angle	degree	bond angle	degree
N(1)–Zn(1)–N(2)	75.52(16)	N(1)–Zn(1)–N(7)	92.11(15)
N(1)–Zn(1)–N(8)	112.29(15)	N(2)–Zn(1)–N(7)	105.97(15)
N(2)–Zn(1)–N(8)	172.19(16)	N(7)–Zn(1)–N(8)	74.66(15)
S(1)–Zn(1)–N(1)	152.75(11)	S(1)–Zn(1)–N(2)	77.85(12)
S(1)–Zn(1)–N(7)	89.68(11)	S(1)–Zn(1)–N(8)	94.40(11)
S(2)–Zn(1)–N(1)	89.82(11)	S(2)–Zn(1)–N(2)	101.60(12)
S(2)–Zn(1)–N(7)	151.96(11)	S(2)–Zn(1)–N(8)	78.74(11)
S(1)–Zn(1)–S(2)	101.14(5)	N(3)–Zn(2)–N(5)	71.91(16)
N(3)–Zn(2)–N(6)	144.94(17)	N(5)–Zn(2)–N(6)	73.58(16)
Cl(1)–Zn(2)–N(3)	100.15(12)	Cl(1)–Zn(2)–N(5)	116.01(13)
Cl(1)–Zn(2)–N(6)	100.28(14)	Cl(2)–Zn(2)–N(3)	95.57(12)
Cl(2)–Zn(2)–N(5)	124.45(13)	Cl(2)–Zn(2)–N(6)	98.75(13)
Cl(1)–Zn(2)–Cl(2)	119.46(8)	N(9)–Zn(3)–N(11)	72.06(14)
N(9)–Zn(3)–N(12)	146.59(15)	N(11)–Zn(3)–N(12)	74.55(15)
Cl(3)–Zn(3)–N(9)	95.41(11)	Cl(3)–Zn(3)–N(11)	121.33(12)
Cl(3)–Zn(3)–N(12)	101.14(11)	Cl(4)–Zn(3)–N(9)	100.43(11)
Cl(4)–Zn(3)–N(11)	122.70(13)	Cl(4)–Zn(3)–N(12)	98.11(12)

Table S12. Hydrogen bond parameters (Å, °) of compound **4**

D-H···A	D(D—H)	d(H···A)	d(D···A)	∠(DHA)	Symmetry transformation for A
N(4)—H(4)···O(4)	0.86	1.96	2.786(6)	162.2	
N(10)—H(10)···O(3)	0.86	2.06	2.788(6)	141.9	
O(4)—H(4)···O(1)	0.85	1.93	2.781(10)	173.1	
O(4)—H(4)···O(1A)	0.85	2.06	2.784(15)	141.8	
O(4)—H(4E)···O(5)	0.85	1.96	2.738(7)	150.9	1 + x, y, z
O(5)—H(5)···O(2)	0.85	1.90	2.731(8)	166.8	
O(5)—H(5)···Cl(3)	0.85	2.45	3.245(7)	155	

Table S13. Selected bond lengths (Å) for compound **5**

bond	length	bond	length
Zn(1)–N(1)	2.248(5)	Zn(1)–N(2)	2.120(5)
Zn(1)–N(7)	2.202(5)	Zn(1)–N(8)	2.128(5)
Zn(1)–S(1)	2.5032(18)	Zn(1)–S(2)	2.4958(18)
Zn(2)–Cl(1)	2.243(2)	Zn(2)–N(3)	2.202(5)
Zn(2)–N(5)	2.100(5)	Zn(2)–N(6)	2.236(5)
Zn(2)–N(13)	1.975(6)	Zn(3)–N(9)	2.220(5)
Zn(3)–N(11)	2.087(6)	Zn(3)–N(12)	2.227(5)
Zn(3)–N(14)	1.960(6)	Zn(3)–N(15)	1.961(6)

Table S14. Selected bond angles (°) for compound **5**

bond angle	degree	bond angle	degree
N(1)–Zn(1)–N(2)	74.96(19)	N(1)–Zn(1)–N(7)	87.47(18)
N(1)–Zn(1)–N(8)	111.33(19)	N(2)–Zn(1)–N(7)	115.32(19)
N(2)–Zn(1)–N(8)	168.6(2)	N(7)–Zn(1)–N(8)	75.17(19)
S(1)–Zn(1)–N(1)	150.59(14)	S(1)–Zn(1)–N(2)	78.28(14)
S(1)–Zn(1)–N(7)	93.14(14)	S(1)–Zn(1)–N(8)	97.17(14)
S(2)–Zn(1)–N(1)	92.23(13)	S(2)–Zn(1)–N(2)	91.43(14)

Table S14. (continued)

bond angle	degree	bond angle	degree
S(2)–Zn(1)–N(7)	152.07(14)	S(2)–Zn(1)–N(8)	78.99(15)
S(1)–Zn(1)–S(2)	100.46(6)	N(3)–Zn(2)–N(5)	72.3(2)
N(3)–Zn(2)–N(6)	146.9(2)	N(3)–Zn(2)–N(13)	96.1(2)
N(5)–Zn(2)–N(6)	74.9(2)	N(5)–Zn(2)–N(13)	127.3(3)
N(6)–Zn(2)–N(13)	100.6(2)	Cl(1)–Zn(2)–N(3)	101.33(16)
Cl(1)–Zn(2)–N(5)	115.19(16)	Cl(1)–Zn(2)–N(6)	96.03(16)
Cl(1)–Zn(2)–N(13)	117.5(2)	N(9)–Zn(3)–N(11)	72.5(2)
N(9)–Zn(3)–N(12)	147.0(2)	N(9)–Zn(3)–N(14)	96.6(2)
N(9)–Zn(3)–N(15)	94.7(2)	N(11)–Zn(3)–N(12)	74.5(2)
N(11)–Zn(3)–N(14)	121.7(2)	N(11)–Zn(3)–N(15)	116.6(2)
N(12)–Zn(3)–N(14)	100.2(2)	N(12)–Zn(3)–N(15)	100.4(2)
N(14)–Zn(3)–N(15)	121.3(3)		

Table S15. Hydrogen bond parameters (Å, °) of compound **5**

D-H···A	D(D—H)	d(H···A)	d(D···A)	∠(DHA)	Symmetry transformation for A
N(4)—H(4)···O(1)	0.88	1.88	2.689(7)	152.3	
N(10)—H(10)···O(2)	0.88	1.80	2.669(8)	170.1	

Table S16. Selected bond lengths (Å) for compound **6**

bond	length	bond	length
Zn(1)–Cl(1)	2.293(3)	Zn(1)–N(1)	2.266(6)
Zn(1)–N(2)	2.114(6)	Zn(1)–O(1A)	2.017(5)
Zn(1)–S(1)	2.526(3)	Zn(2)–Cl(2)	2.267(3)
Zn(2)–N(3)	2.191(6)	Zn(2)–N(5)	2.096(7)
Zn(2)–N(6)	2.280(7)	Zn(2)–O(1)	1.994(6)

Symmetry transformations used to generate equivalent atoms: A: 2 — x, 1 — y, 1 — z.

Table 17. Selected bond angles (°) for compound **6**

bond angle	degree	bond angle	degree

Cl(1)–Zn(1)–N(1)	97.46(19)	Cl(1)–Zn(1)–N(2)	116.2(2)
Cl(1)–Zn(1)–O(1A)	115.66(16)	Cl(1)–Zn(1)–S(1)	99.75(9)
N(1)–Zn(1)–N(2)	75.3(2)	N(1)–Zn(1)–O(1A)	94.3(2)
N(1)–Zn(1)–S(1)	152.90(17)	N(2)–Zn(1)–O(1A)	128.0(2)
N(2)–Zn(1)–S(1)	78.4(2)	O(1A)–Zn(1)–S(1)	96.86(18)
Cl(2)–Zn(2)–N(3)	99.83(19)	Cl(2)–Zn(2)–N(5)	123.9(2)
Cl(2)–Zn(2)–N(6)	96.0(2)	Cl(2)–Zn(2)–O(1)	111.41(18)
N(3)–Zn(2)–N(5)	72.8(3)	N(3)–Zn(2)–N(6)	146.5(3)
N(5)–Zn(2)–N(6)	73.8(3)	N(3)–Zn(2)–O(1)	99.8(2)
N(5)–Zn(2)–O(1)	124.7(3)	N(6)–Zn(2)–O(1)	101.5(2)

Symmetry transformations used to generate equivalent atoms: A: 2 — x, 1 — y, 1 — z.

Table S18. Hydrogen bond parameters (Å, °) of compound **6**

D-H···A	D(D—H)	d(H···A)	d(D···A)	∠(DHA)	Symmetry transformation for A
O(1)—H(1)···O(2)	0.98	2.16	3.043(16)	149	
O(2)—H(2)···Cl(2)	0.87	2.45	3.284(12)	161	
N(4)—H(4C)···O(3)	0.88	1.90	2.739(8)	159.3	2 — x, — y,1 — z

Table S19. Selected bond lengths (Å) for compound **7**

bond	length	bond	length
Cd(1)–I(1)	2.745(3)	Cd(1)–I(2A)	2.8793(7)
Cd(1)–N(1)	2.418(5)	Cd(1)–N(2)	2.324(5)
Cd(1)–S(1)	2.6005(17)	Cd(2)–I(2)	2.8292(7)
Cd(2)–I(3)	2.7203(7)	Cd(2)–N(3)	2.410(5)
Cd(2)–N(5)	2.304(5)	Cd(2)–N(6)	2.456(5)

Symmetry transformations used to generate equivalent atoms: A: 1 — x, 1 — y, 1 — z.

Table S20. Selected bond angles (°) for compound **7**

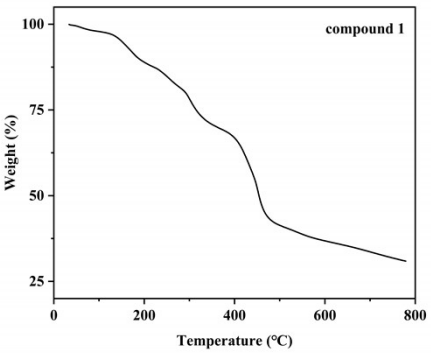
bond angle	degree	bond angle	degree

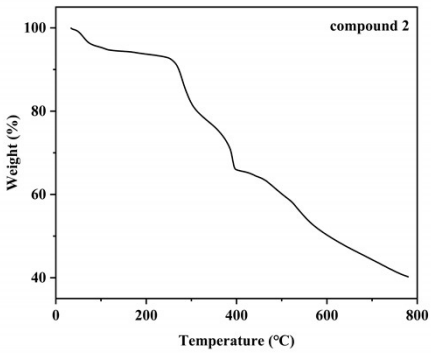
I(1)–Cd(1)–I(2A)	117.77(7)	I(1)–Cd(1)–N(1)	102.08(14)
I(1)–Cd(1)–N(2)	107.81(14)	I(1)–Cd(1)–S(1)	104.86(12)
I(2A)–Cd(1)–N(1)	101.41(12)	I(2A)–Cd(1)–N(2)	134.36(12)
I(2A)–Cd(1)–S(1)	92.30(4)	N(1)–Cd(1)–N(2)	69.87(17)
N(1)–Cd(1)–S(1)	139.38(13)	N(2)–Cd(1)–S(1)	73.23(12)
I(2)–Cd(2)–I(3)	109.01(2)	I(2)–Cd(2)–N(3)	103.77(12)
I(2)–Cd(2)–N(5)	111.98(11)	I(2)–Cd(2)–N(6)	95.85(12)
I(3)–Cd(2)–N(3)	103.80(12)	I(3)–Cd(2)–N(5)	139.00(11)
I(3)–Cd(2)–N(6)	106.32(12)	N(3)–Cd(2)–N(5)	67.20(17)
N(3)–Cd(2)–N(6)	136.03(16)	N(5)–Cd(2)–N(6)	69.02(17)

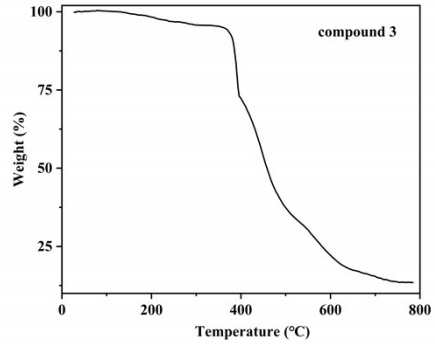
Symmetry transformations used to generate equivalent atoms: A: 1 — x, 1 — y, 1 — z.

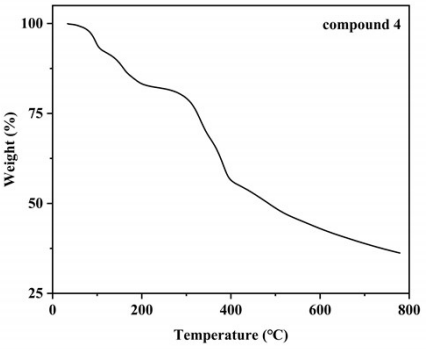
Table S21. Hydrogen bond parameters (Å, °) of compound **7**

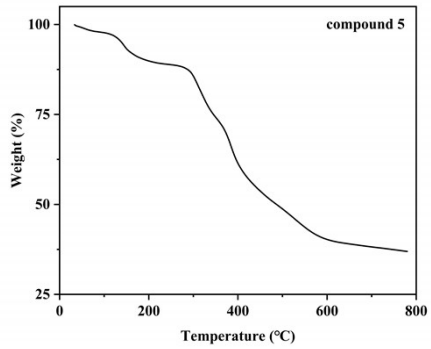
D-H···A	D(D—H)	d(H···A)	d(D···A)	∠(DHA)	Symmetry transformation for A
N(4)—H(4)···O(1)	0.88	1.90	2.750(7)	163.3	

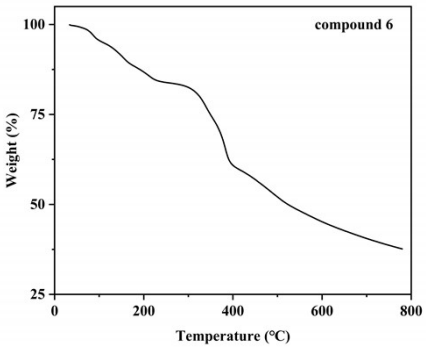












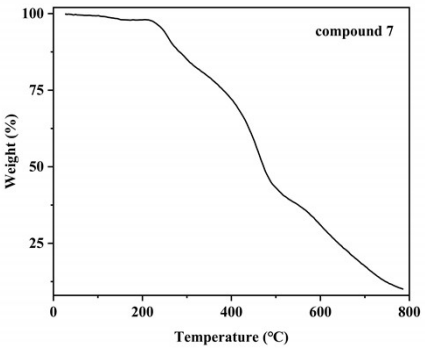


Figure S1. TGA curves for compounds **1**–**7**.

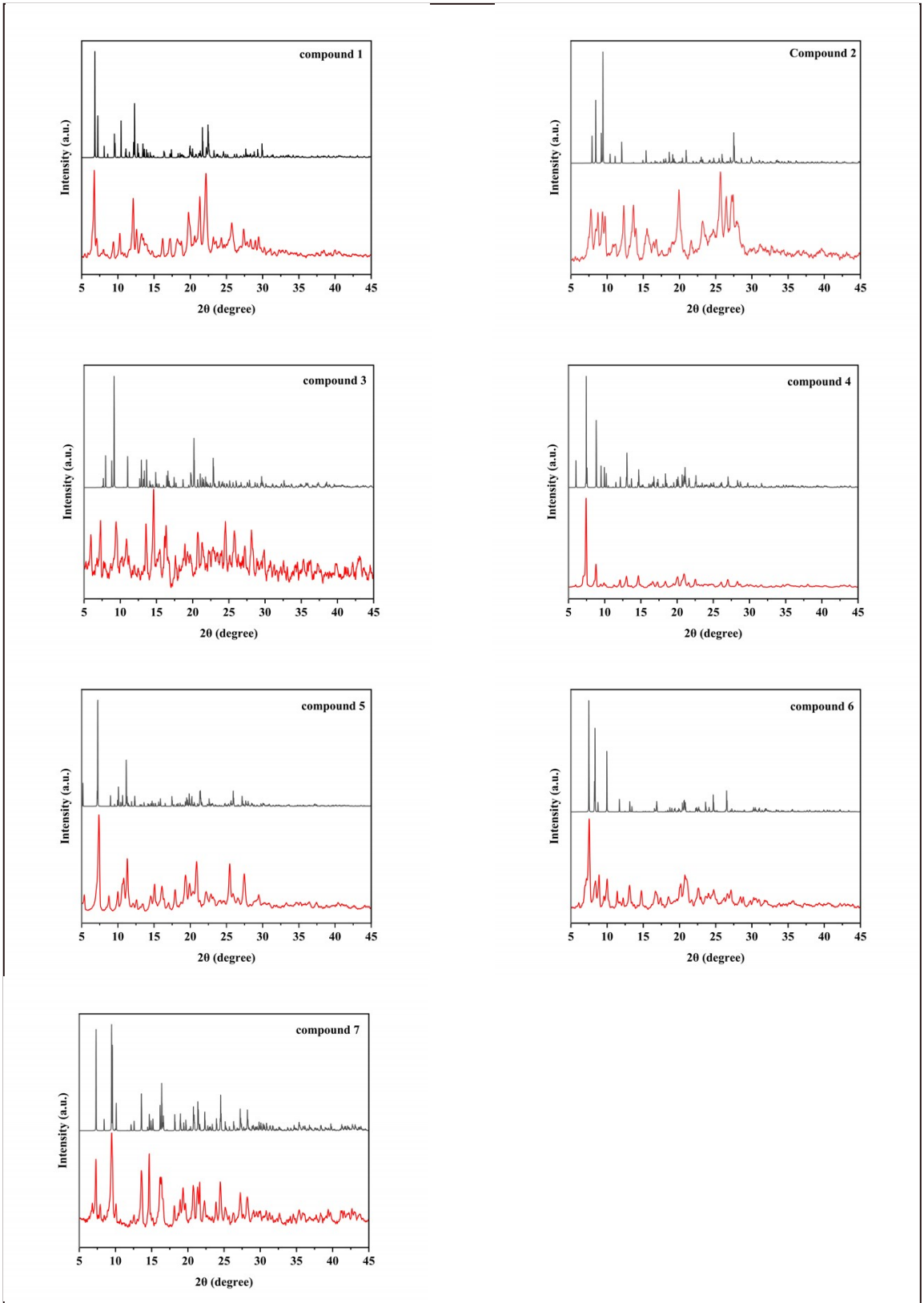


Figure S2. The X-ray powder diffraction (XRD) patterns of the bulk samples (bottom) and those calculated from the single-crystal diffraction data (top) for **1**–**7**.