Electronic supplementary information (ESI)

Syntheses, structures and luminescent properties of zinc(II) and cadmium(II) coordination complexes based on new bis(imidazolyl)ether and different carboxylate ligands

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

Zn(1)-O(3)	1.9307(17)	Zn(1)-O(1)	1.9546(18)
Zn(1)-N(4)$^{\#1}$	1.993(2)	Zn(1)-N(1)	2.0139(18)
O(3)-Zn(1)-O(1)	103.30(8)	O(3)-Zn(1)-N(4)$^{\#1}$	118.83(8)
O(1)-Zn(1)-N(4)$^{\#1}$	112.09(7)	O(3)-Zn(1)-N(1)	101.06(7)
O(1)-Zn(1)-N(1)	114.21(8)	N(4)$^{\#1}$-Zn(1)-N(1)	107.14(8)

Symmetry codes for **1**: $^{\#1}$ -x+1,-y,-z+1

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

Zn(1)-O(2)$^{\#2}$	2.086(3)	Zn(1)-O(4)	2.102(3)
Zn(1)-O(3)	2.164(3)	Zn(1)-O(1)	2.191(3)
Zn(1)-N(4)$^{\#1}$	2.085(4)	Zn(1)-N(1)	2.098(4)
N(4)$^{\#1}$-Zn(1)-O(2)$^{\#2}$	93.13(14)	N(4)$^{\#1}$-Zn(1)-N(1)	95.83(16)
O(2)$^{\#2}$-Zn(1)-N(1)	101.57(16)	N(4)$^{\#1}$-Zn(1)-O(4)	96.07(14)
O(2)$^{\#2}$-Zn(1)-O(4)	164.94(13)	N(1)-Zn(1)-O(4)	89.35(14)
N(4)$^{\#1}$-Zn(1)-O(3)	93.71(13)	O(2)$^{\#2}$-Zn(1)-O(3)	89.71(13)
N(1)-Zn(1)-O(3)	164.78(15)	O(4)-Zn(1)-O(3)	77.84(12)
N(4)$^{\#1}$-Zn(1)-O(1)	171.20(14)	O(2)$^{\#2}$-Zn(1)-O(1)	78.20(12)
N(1)-Zn(1)-O(1)	87.50(15)	O(4)-Zn(1)-O(1)	92.10(12)
O(3)-Zn(1)-O(1)	84.82(14)		

Symmetry codes for **2**: $^{\#1}$ -x+1/2, y, -z+1/2; $^{\#2}$ -x,-y+1,-z; $^{\#3}$ -x-1/2, y, -z+1/2

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

Zn(1)-O(1)	1.9401(18)	Zn(1)-O(4)$^{\#1}$	1.9768(17)
Zn(1)-N(1)	2.006(3)	Zn(1)-N(4)$^{\#2}$	2.015(2)
O(1)-Zn(1)-O(4)$^{\#1}$	115.88(8)	O(1)-Zn(1)-N(1)	116.32(9)
O(4)$^{\#1}$-Zn(1)-N(1)	104.55(8)	O(1)-Zn(1)-N(4)$^{\#2}$	111.86(9)
O(4)$^{\#1}$-Zn(1)-N(4)$^{\#2}$	95.78(8)	N(1)-Zn(1)-N(4)$^{\#2}$	110.42(10)

Symmetry codes for **3**: $^{\#1}$ x, y-1, z; $^{\#2}$ x+1/2, y+1/2, z

Table S4. Selected bond distances (Å) and angles (^{o}) for **4**.

Cd(1)-O(4)$^{\#1}$	2.266(3)	Cd(1)-O(1)	2.375(3)
Cd(1)-O(3)$^{\#3}$	2.395(3)	Cd(1)-O(2)	2.513(3)
Cd(1)-N(1)	2.267(3)	Cd(1)-N(4)$^{\#2}$	2.272(3)
O(4)$^{\#1}$-Cd(1)-N(1)	110.01(12)	O(4)$^{\#1}$-Cd(1)-N(4)$^{\#2}$	90.57(12)
N(1)-Cd(1)-N(4)$^{\#2}$	158.60(12)	O(4)$^{\#1}$-Cd(1)-O(1)	86.18(10)
N(1)-Cd(1)-O(1)	88.33(11)	N(4)$^{\#2}$-Cd(1)-O(1)	99.20(11)
O(4)$^{\#1}$-Cd(1)-O(3)$^{\#3}$	118.30(10)	N(1)-Cd(1)-O(3)$^{\#3}$	83.66(11)
N(4)$^{\#2}$-Cd(1)-O(3)$^{\#3}$	81.28(11)	O(1)-Cd(1)-O(3)$^{\#3}$	155.52(9)
O(4)$^{\#1}$-Cd(1)-O(2)	138.08(10)	N(1)-Cd(1)-O(2)	83.95(10)
N(4)$^{\#2}$-Cd(1)-O(2)	84.41(10)	O(1)-Cd(1)-O(2)	53.97(9)
O(3)$^{\#3}$-Cd(1)-O(2)	102.05(9)		

Symmetry codes for **4**: $^{\#1}$ x, y+1, z; $^{\#2}$ x-1, y, z-1; $^{\#3}$ -x+1, -y, -z+1

Table S5. Selected bond distances (Å) and angles (^{o}) for **5**.

Cd(1)-O(2)$^{\#1}$	2.216(2)	Cd(1)-O(1)	2.2600(19)
Cd(1)-O(4)$^{\#3}$	2.362(2)	Cd(1)-O(3)$^{\#3}$	2.515(2)

Cd(1)-N(1)	2.282(3)	Cd(1)-N(4)$^{\#2}$	2.294(3)
O(2)$^{\#1}$-Cd(1)-O(1)	108.39(8)	O(2)$^{\#1}$-Cd(1)-N(1)	97.82(10)
O(1)-Cd(1)-N(1)	93.72(9)	O(2)$^{\#1}$-Cd(1)-N(4)$^{\#2}$	92.57(10)
O(1)-Cd(1)-N(4)$^{\#2}$	86.01(9)	N(1)-Cd(1)-N(4)$^{\#2}$	169.13(9)
O(2)$^{\#1}$-Cd(1)-O(4)$^{\#3}$	145.43(7)	O(1)-Cd(1)-O(4)$^{\#3}$	105.99(7)
N(1)-Cd(1)-O(4)$^{\#3}$	83.32(8)	N(4)$^{\#2}$-Cd(1)-O(4)$^{\#3}$	86.30(9)
O(2)$^{\#1}$-Cd(1)-O(3)$^{\#3}$	91.53(7)	O(1)-Cd(1)-O(3)$^{\#3}$	158.37(7)
N(1)-Cd(1)-O(3)$^{\#3}$	91.74(8)	N(4)$^{\#2}$-Cd(1)-O(3)$^{\#3}$	84.73(8)
O(4)$^{\#3}$-Cd(1)-O(3)$^{\#3}$	53.93(6)		

Symmetry codes for **5**: $^{\#1}$ -x+1, -y+2, -z+1; $^{\#2}$ x-1, y, z+1; $^{\#3}$ -x+1, -y+1, -z+1

Table S6. Selected bond distances (Å) and angles (^{o}) for **6**.

Zn(1)-O(3)$^{\#1}$	1.9678(17)	Zn(1)-O(1)	1.9978(16)
Zn(1)-N(4)$^{\#2}$	2.0164(19)	Zn(1)-N(1)	2.026(2)
O(3)$^{\#1}$-Zn(1)-O(1)	109.73(7)	O(3)$^{\#1}$-Zn(1)-N(4)$^{\#2}$	100.62(8)
O(1)-Zn(1)-N(4)$^{\#2}$	115.19(8)	O(3)$^{\#1}$-Zn(1)-N(1)	110.20(9)
O(1)-Zn(1)-N(1)	108.18(8)	N(4)$^{\#2}$-Zn(1)-N(1)	112.69(8)

Symmetry codes for **6**: $^{\#1}$ x+1, y, z; $^{\#2}$ -x+3/2, y+1/2, -z+5/2

Table S7. Selected bond distances (Å) and angles (^{o}) for **7**.

Zn(1)-O(3)	1.921(4)	Zn(1)-O(1)	1.941(4)
Zn(1)-N(4)$^{\#1}$	1.977(5)	Zn(1)-N(1)	1.992(5)
O(3)-Zn(1)-O(1)	102.7(2)	O(3)-Zn(1)-N(4)$^{\#1}$	118.4(2)
O(1)-Zn(1)-N(4)$^{\#1}$	113.4(2)	O(3)-Zn(1)-N(1)	112.53(19)

O(1)-Zn(1)-N(1)	97.9(2)	N(4)$^{\#1}$-Zn(1)-N(1)	109.9(2)

Symmetry codes for **7**: $^{\#1}$ -x, y, -z+3/2; $^{\#2}$ -x, -y+1, -z+1; $^{\#3}$ -x+1/2, -y-1/2, -z+1

Table S8. Selected bond distances (Å) and angles (^{o}) for **8**.

Cd(1)-O(1)$^{\#1}$	2.262(5)	Cd(1)-O(6)	2.298(5)
Cd(1)-O(4)$^{\#2}$	2.332(4)	Cd(1)-O(4)	2.379(4)
Cd(1)-O(3)	2.497(4)	Cd(1)-O(5)	2.577(5)
Cd(2)-O(2)$^{\#1}$	2.226(4)	Cd(2)-O(5)	2.281(4)
Cd(2)-O(3)	2.383(4)	Cd(1)-N(1)	2.261(7)
N(1)-Cd(1)-O(1)$^{\#1}$	173.0(2)	N(1)-Cd(1)-O(6)	91.6(3)
O(1)$^{\#1}$-Cd(1)-O(6)	84.9(2)	N(1)-Cd(1)-O(4)$^{\#2}$	97.1(2)
O(1)$^{\#1}$-Cd(1)-O(4)$^{\#2}$	89.62(18)	O(6)-Cd(1)-O(4)$^{\#2}$	102.60(16)
N(1)-Cd(1)-O(4)	97.5(2)	O(1)$^{\#1}$-Cd(1)-O(4)	86.24(18)
O(6)-Cd(1)-O(4)	170.7(2)	O(4)$^{\#2}$-Cd(1)-O(4)	74.34(17)
N(1)-Cd(1)-O(3)	92.6(2)	O(1)$^{\#1}$-Cd(1)-O(3)	84.89(18)
O(6)-Cd(1)-O(3)	128.74(16)	O(4)$^{\#2}$-Cd(1)-O(3)	127.39(14)
O(4)-Cd(1)-O(3)	53.12(14)	N(1)-Cd(1)-O(5)	86.3(2)
O(1)$^{\#1}$-Cd(1)-O(5)	86.67(17)	O(6)-Cd(1)-O(5)	53.51(15)
O(4)$^{\#2}$-Cd(1)-O(5)	156.05(14)	O(4)-Cd(1)-O(5)	128.88(14)
O(3)-Cd(1)-O(5)	75.83(14)	O(2)$^{\#1}$-Cd(2)-O(2)$^{\#3}$	101.7(3)
O(2)$^{\#1}$-Cd(2)-O(5)	86.76(18)	O(2)$^{\#3}$-Cd(2)-O(5)	169.74(19)
O(5)-Cd(2)-O(5)$^{\#4}$	85.5(3)	O(2)$^{\#1}$-Cd(2)-O(3)	94.57(17)
O(2)$^{\#3}$-Cd(2)-O(3)	89.53(17)	O(5)-Cd(2)-O(3)	83.90(15)
O(5)$^{\#4}$-Cd(2)-O(3)	91.33(16)	O(3)-Cd(2)-O(3)$^{\#4}$	173.5(2)

Symmetry codes for **8**: $^{\#1}$ x, -y+2, z+1/2; $^{\#2}$ -x+1/2, -y+3/2, -z+1; $^{\#3}$ -x+1, -y+2, -z+1; $^{\#4}$ -x+1, y, -z+3/2; $^{\#5}$ -x+1, -y+1, -z+2

Table S9. Selected bond distances (Å) and angles (°) for **9**.

Cd(1)-O(12)$^{\#1}$	2.247(4)	Cd(1)-O(3)$^{\#2}$	2.250(3)
Cd(1)-O(2)	2.278(4)	Cd(1)-O(5)$^{\#3}$	2.385(3)
Cd(1)-O(7)	2.403(3)	Cd(1)-O(6)$^{\#3}$	2.450(4)
Cd(2)-O(4)$^{\#2}$	2.261(4)	Cd(2)-O(10)$^{\#5}$	2.275(4)
Cd(2)-O(8)	2.341(4)	Cd(2)-O(7)	2.525(4)
Cd(3)-O(11)$^{\#1}$	2.267(3)	Cd(3)-O(1)	2.285(4)
Cd(3)-O(9)	2.322(4)	Cd(3)-O(5)$^{\#3}$	2.337(3)
O(3)-Cd(1)$^{\#2}$	2.250(3)	O(4)-Cd(2)$^{\#2}$	2.261(4)
O(10)-Cd(2)$^{\#4}$	2.275(4)	O(11)-Cd(3)$^{\#1}$	2.267(3)
Cd(2)-N(8)$^{\#4}$	2.262(5)	Cd(2)-N(5)	2.295(5)
Cd(3)-N(1)	2.293(4)	N(4)-Cd(3)$^{\#6}$	2.304(5)
O(12)$^{\#1}$-Cd(1)-O(3)$^{\#2}$	94.73(14)	O(12)$^{\#1}$-Cd(1)-O(2)	102.73(15)
O(3)$^{\#2}$-Cd(1)-O(2)	84.71(13)	O(12)$^{\#1}$-Cd(1)-O(5)$^{\#3}$	106.55(12)
O(3)$^{\#2}$-Cd(1)-O(5)$^{\#3}$	158.25(12)	O(2)-Cd(1)-O(5)$^{\#3}$	86.25(13)
O(12)$^{\#1}$-Cd(1)-O(7)	81.73(14)	O(3)$^{\#2}$-Cd(1)-O(7)	102.46(13)
O(2)-Cd(1)-O(7)	171.34(14)	O(5)$^{\#3}$-Cd(1)-O(7)	85.35(12)
O(12)$^{\#1}$-Cd(1)-O(6)$^{\#3}$	158.33(13)	O(3)$^{\#2}$-Cd(1)-O(6)$^{\#3}$	105.67(13)
O(2)-Cd(1)-O(6)$^{\#3}$	86.63(15)	O(5)$^{\#3}$-Cd(1)-O(6)$^{\#3}$	54.00(11)
O(7)-Cd(1)-O(6)$^{\#3}$	86.72(13)	O(4)$^{\#2}$-Cd(2)-N(8)$^{\#4}$	88.06(15)
O(4)$^{\#2}$-Cd(2)-O(10)$^{\#5}$	129.93(13)	N(8)$^{\#4}$-Cd(2)-O(10)$^{\#5}$	96.37(16)
O(4)$^{\#2}$-Cd(2)-N(5)	85.43(17)	N(8)$^{\#4}$-Cd(2)-N(5)	172.24(18)
O(10)$^{\#5}$-Cd(2)-N(5)	84.63(16)	O(4)$^{\#2}$-Cd(2)-O(8)	132.95(13)
N(8)$^{\#4}$-Cd(2)-O(8)	98.58(16)	O(10)$^{\#5}$-Cd(2)-O(8)	95.76(13)
N(5)-Cd(2)-O(8)	88.96(17)	O(4)$^{\#2}$-Cd(2)-O(7)	81.01(12)
N(8)$^{\#4}$-Cd(2)-O(7)	84.65(15)	O(10)$^{\#5}$-Cd(2)-O(7)	149.03(12)
N(5)-Cd(2)-O(7)	98.47(15)	O(8)-Cd(2)-O(7)	53.73(11)

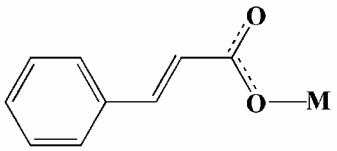
O(11)$^{\#1}$-Cd(3)-O(1)	88.03(15)	O(11)$^{\#1}$-Cd(3)-N(1)	170.96(16)
O(1)-Cd(3)-N(1)	83.27(15)	O(11)$^{\#1}$-Cd(3)-N(4)$^{\#6}$	81.41(16)
O(1)-Cd(3)-N(4)$^{\#6}$	94.45(18)	N(1)-Cd(3)-N(4)$^{\#6}$	96.78(16)
O(11)$^{\#1}$-Cd(3)-O(9)	96.85(14)	O(1)-Cd(3)-O(9)	172.17(14)
N(1)-Cd(3)-O(9)	92.06(14)	N(4)$^{\#6}$-Cd(3)-O(9)	92.34(17)
O(11)$^{\#1}$-Cd(3)-O(5)$^{\#3}$	87.98(13)	O(1)-Cd(3)-O(5)$^{\#3}$	88.52(13)
N(1)-Cd(3)-O(5)$^{\#3}$	94.23(14)	N(4)$^{\#6}$-Cd(3)-O(5)$^{\#3}$	168.86(14)
O(9)-Cd(3)-O(5)$^{\#3}$	85.55(13)		

Symmetry codes for **9**: $^{\#1}$ -x+1, -y+1, -z+1; $^{\#2}$ -x, -y+1, -z+1; $^{\#3}$ -x, y-1/2, -z+1/2; $^{\#4}$ x, -y+1/2, z-1/2; $^{\#5}$ x, -y+1/2, z+1/2; $^{\#6}$ -x, -y+1, -z; $^{\#7}$ -x, y+1/2, -z+1/2

Table S10. Selected bond distances (Å) and angles (^{o}) for **10**.

Zn(1)-O(1)	1.952(6)	Zn(1)-O(4)	2.068(14)
Zn(1)-N(4)$^{\#1}$	1.999(5)	Zn(1)-N(1)	2.007(6)
O(1)-Zn(1)-N(4)$^{\#1}$	104.6(2)	O(1)-Zn(1)-N(1)	123.8(3)
N(4)$^{\#1}$-Zn(1)-N(1)	112.9(2)	O(1)-Zn(1)-O(4)	109.7(4)
N(4)$^{\#1}$-Zn(1)-O(4)	95.4(4)	N(1)-Zn(1)-O(4)	106.9(4)

Symmetry codes for **10**: $^{\#1}$ -x+1,-y,-z+1; $^{\#2}$ -x,-y+1,-z+1; $^{\#3}$ x,-y+1/2, z+1/2; $^{\#4}$ x,-y+1/2, z-1/2



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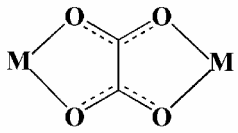

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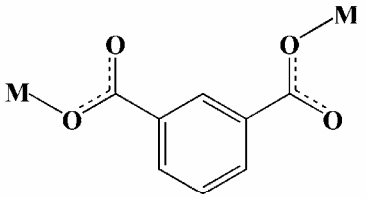

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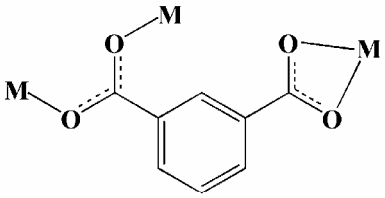

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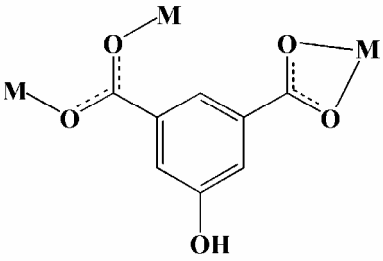

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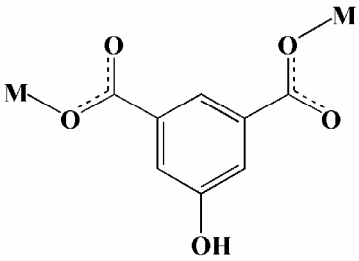

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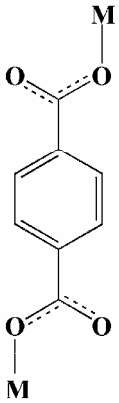

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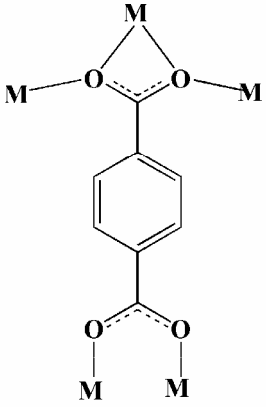

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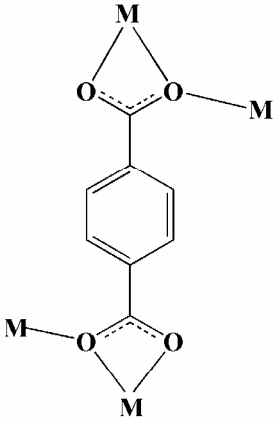

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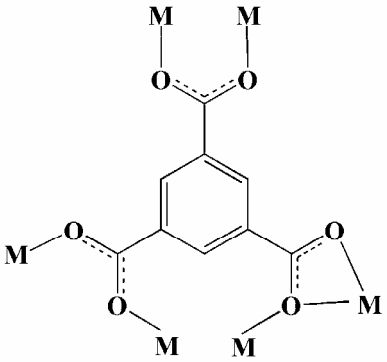

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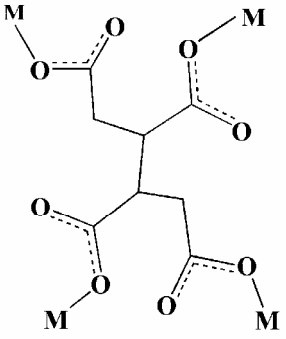


XI

Scheme S1. Coordination Modes of the carboxylate ligands in 1–10.

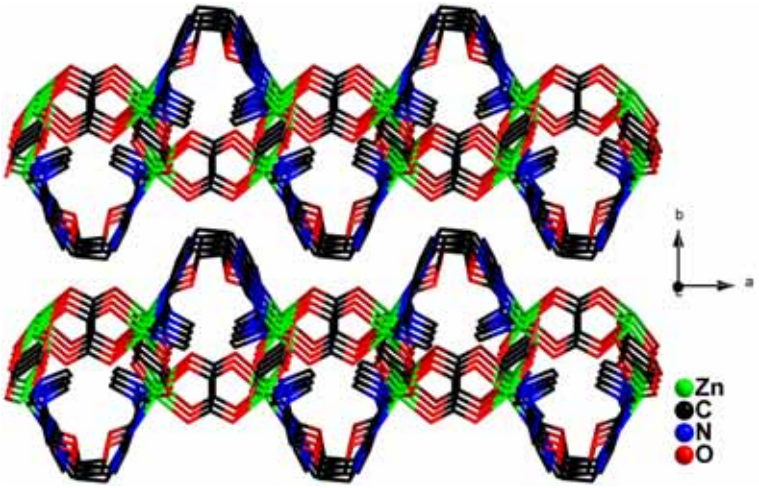


Fig. S1. Interdigitation of adjacent grids in **2** as viewed down the *c* axis.

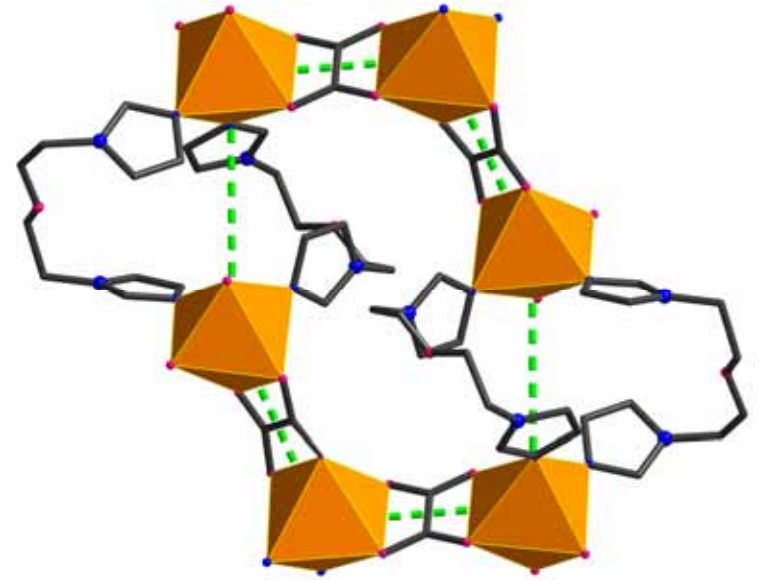


Fig. S2. One 6-membered ring is shown in yellow polyhedron for each net shortest closed circuits, and the **hcb** net of compound **2**.

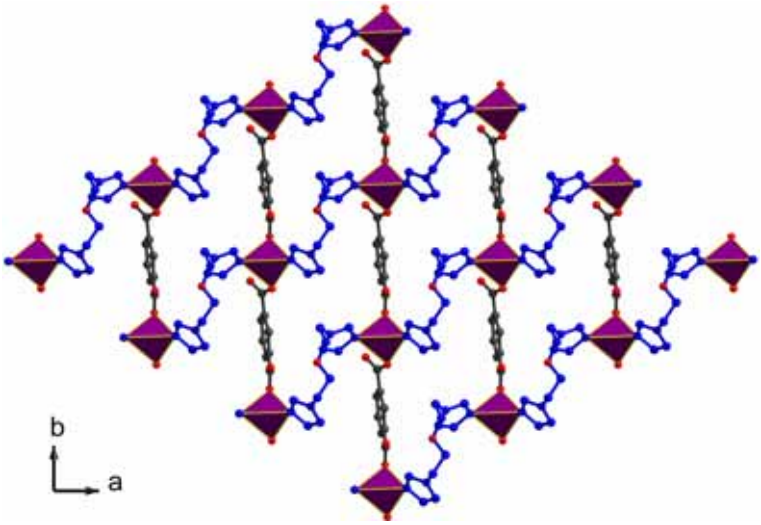


Fig. S3. View of the 2D rhombohedral grid **sql** structure of **3** along *c* axis.

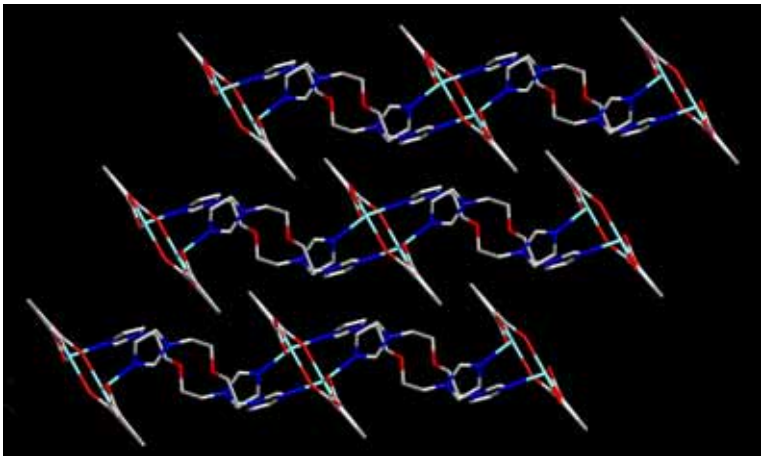


Fig. S4. Packing diagram showing the interdigitating arrangement of the 2D arrays in **4**.

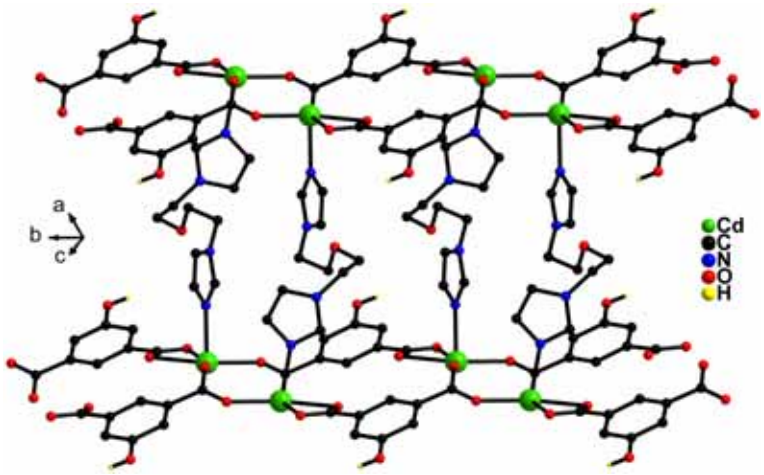


Fig. S5. View of the 2D layer of **5** formed by carboxylate-bridged bicadmium coordination polymer chain and BIE connector.

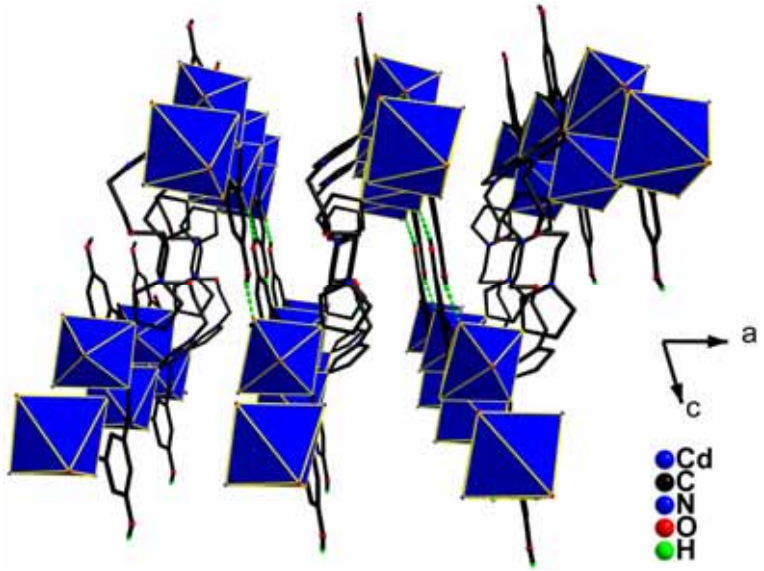


Fig. S6. View of the 3D supramolecular framework of **5** formed through hydrogen bonds between the 2D layers.

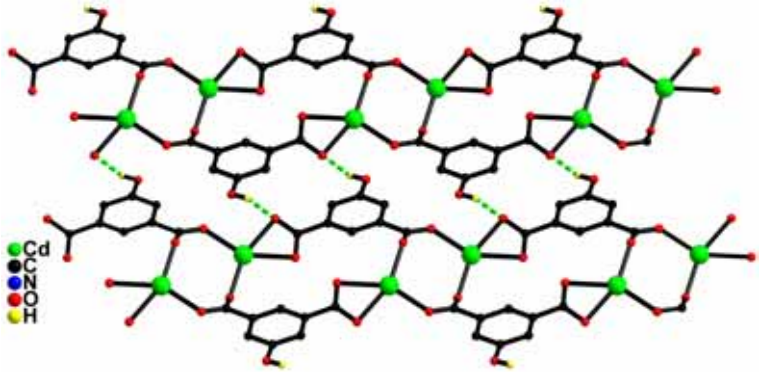


Fig. S7. Hydrogen bonding interaction between the bicadmium coordination polymeric chains in **5**.

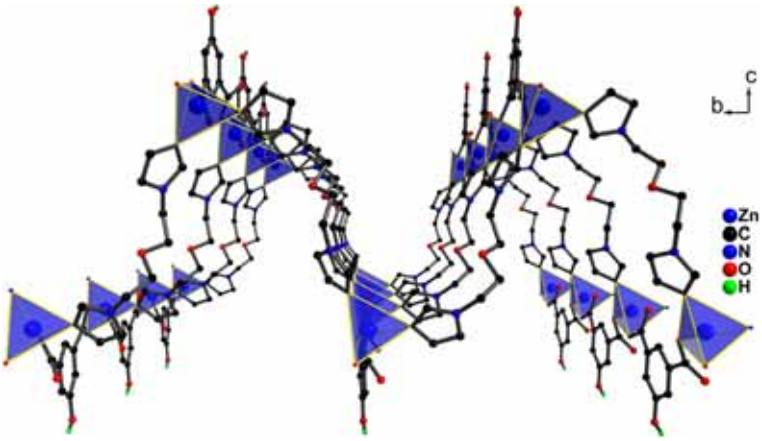


Fig. S8. The BIE further extended the Zn–carboxylate chains in a linear fashion in perpendicular direction, resulting in 2D sinusoidal-like **sql** plane network of **6**.

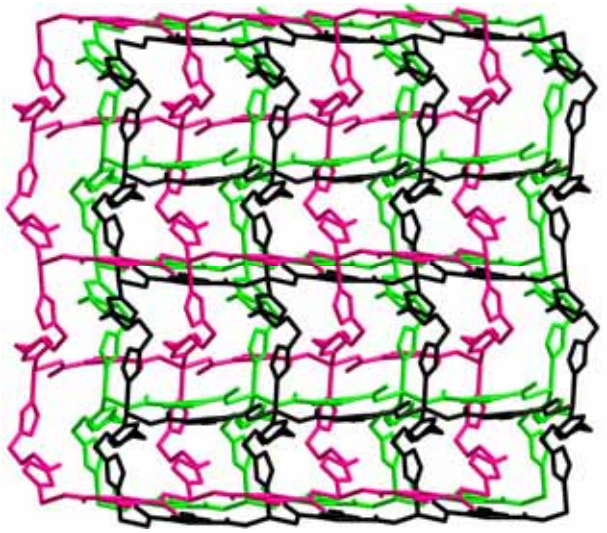


Fig. S9. Three parallel polycatenating **sql** net in the structure of **6**.

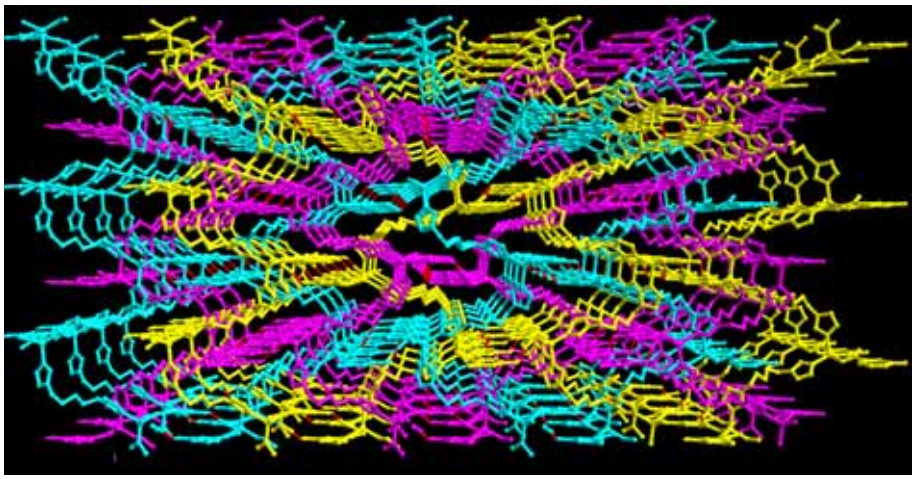


Fig. S10. Hydrogen bonds enhance the 3D supramolecular architecture in **6**.

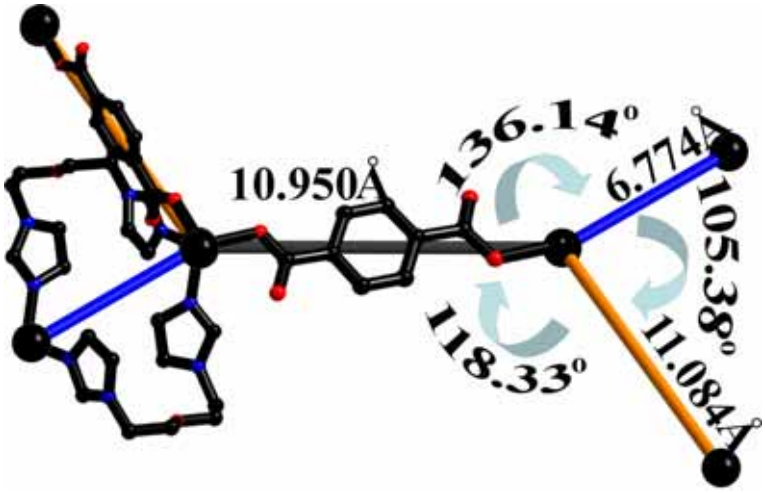


Fig. S11. Three different node-node distances and the angles in **7**.

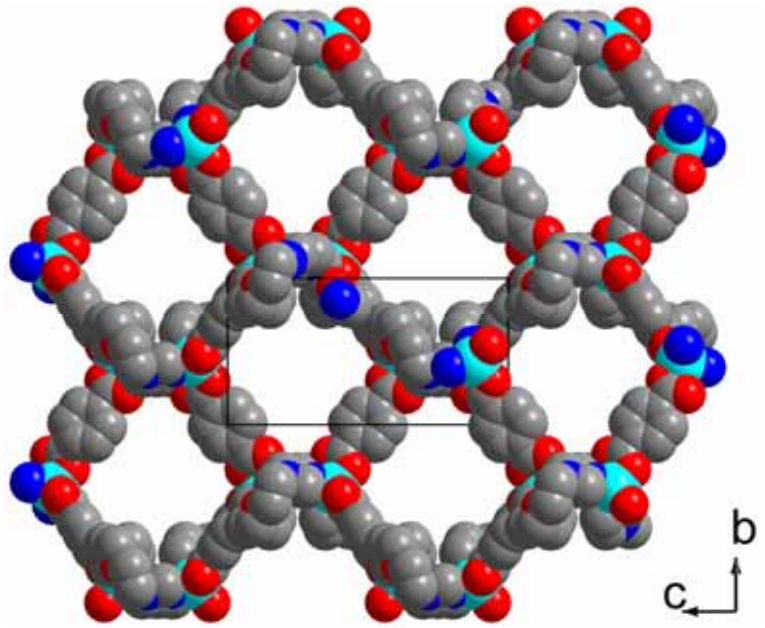


Fig. S12. Space-filling view of the single coordination network with honeycomb hexagonal channels along *a* axis.

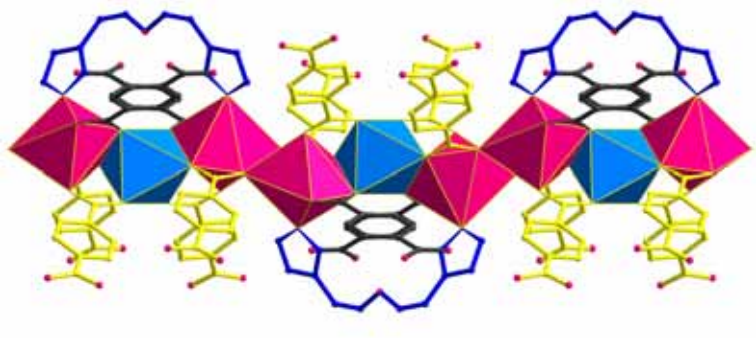


Fig. S13. Polyhedral representation of 1D edge-sharing rod constructed by cadmium clusters in **8**. ({CdO_6N} pentagonal bipyramidal is pink and {CdO_6} octahedron is blue).

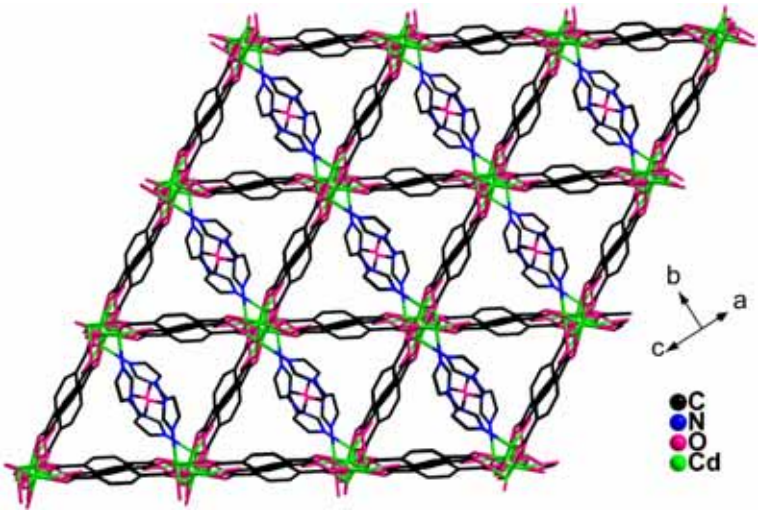


Fig. S14. The overall 3D framework structure of **8**, which is composed of 1D rods, showing each rod is connected covalently linked by *p*-BDC bridges to four adjacent rods.

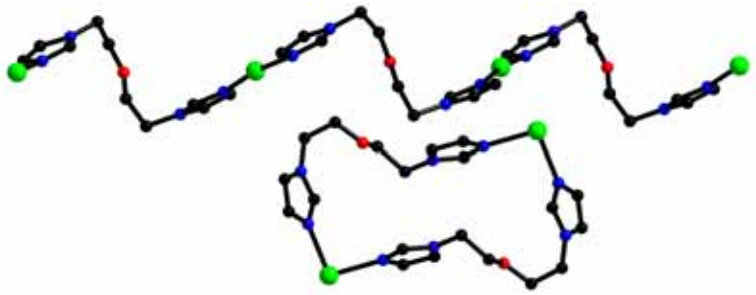


Fig. S15. The different conformations of two BIE ligands in **9**.

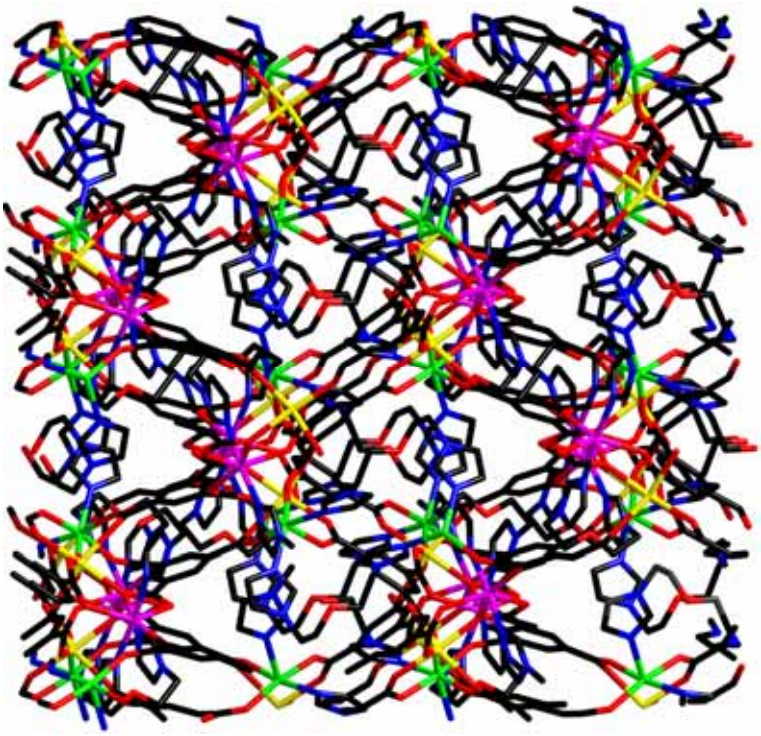


Fig. S16. The complicated 3D framework of **9**.

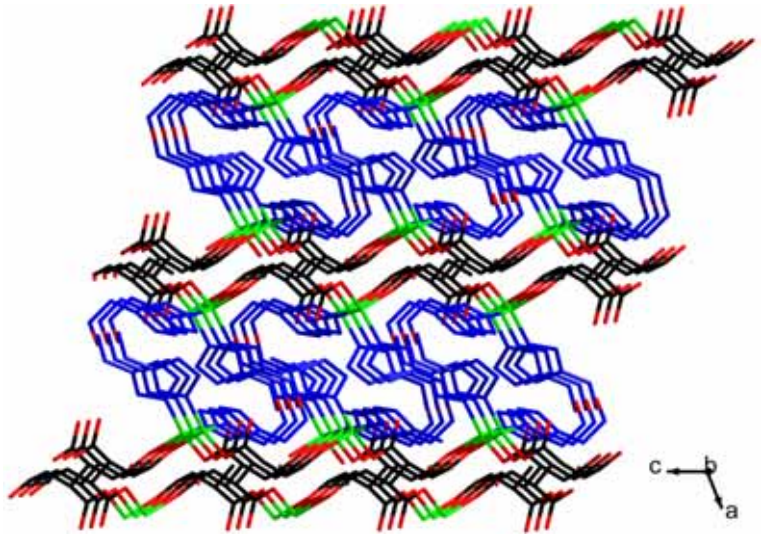


Fig. S17. The representation of the 3D metal-organic framework of **10** (blue represent the BIE ligands bonded to two adjacent BTCA layers).

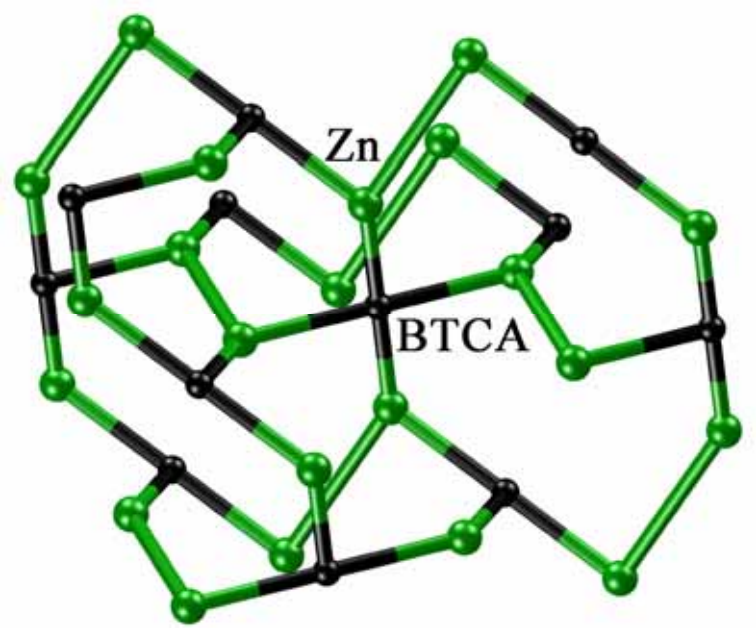


Fig. S18. Schematic diagram (OLEX) showing the $(8^3)_2(8^5\cdot10)$ network of **10**.

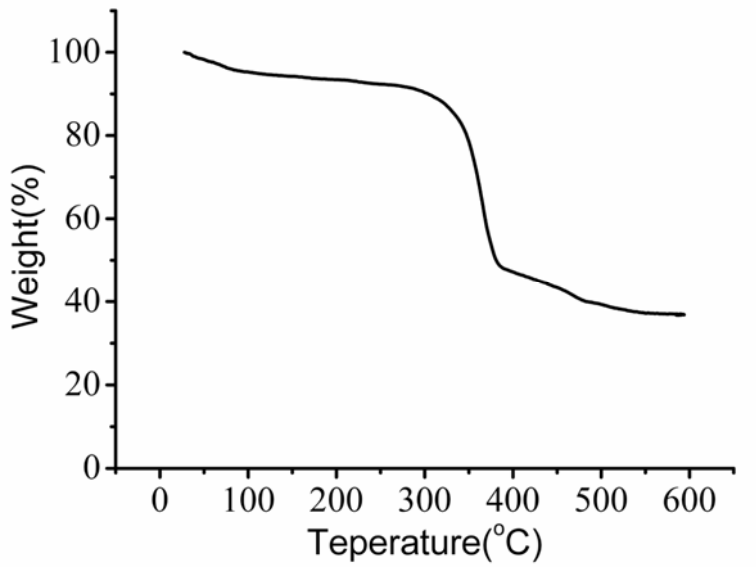


Fig. S19. TGA curve of **2**.

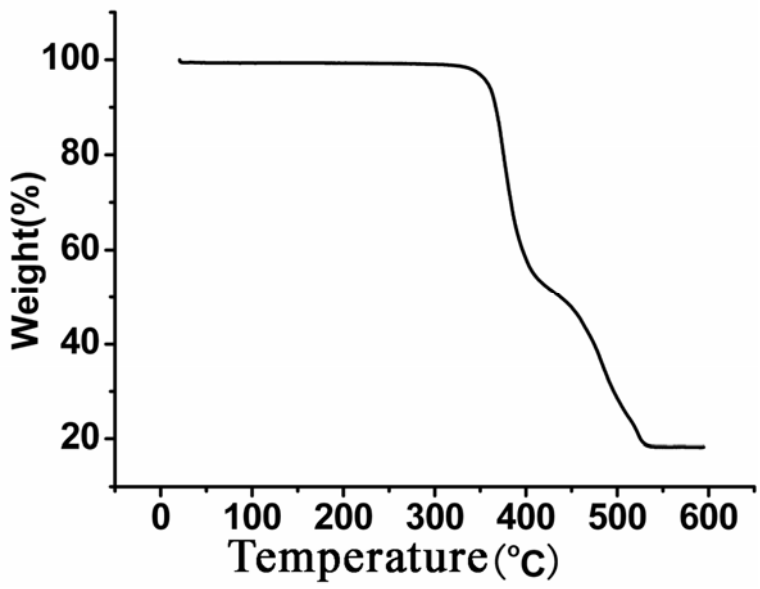


Fig. S20. TGA curve of **6**.

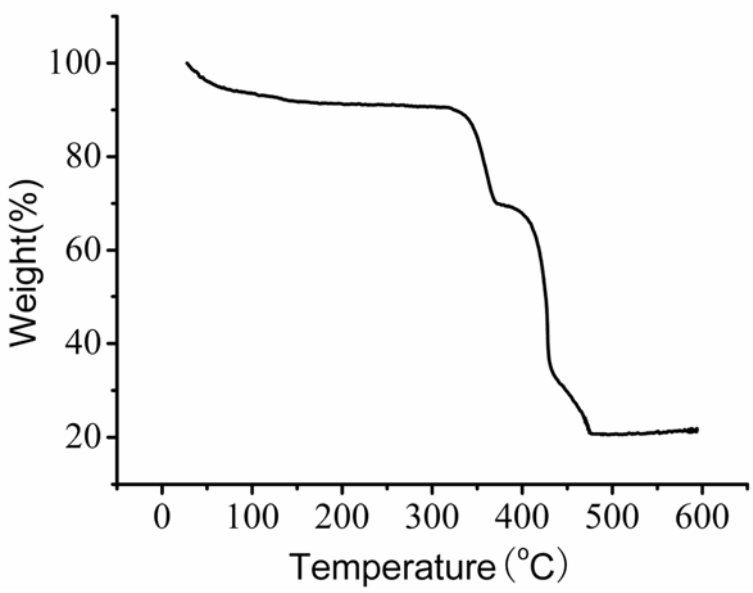


Fig. S21. TGA curve of **7**.

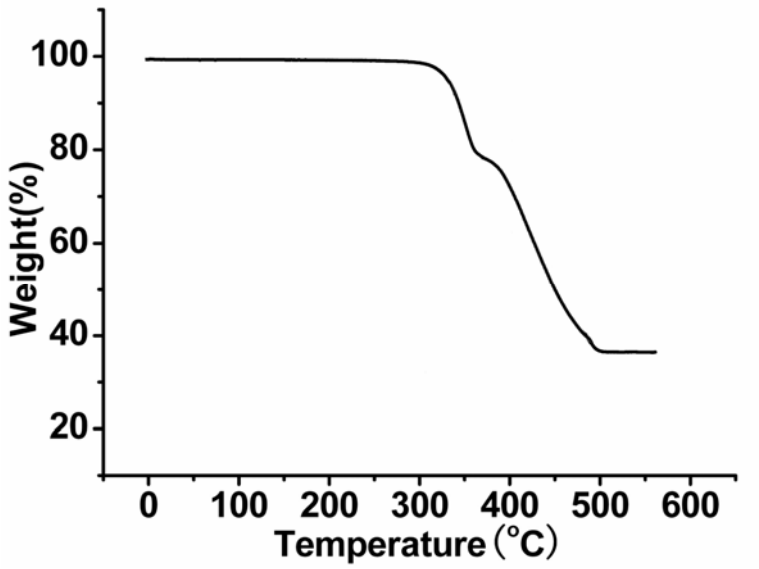


Fig. S22. TGA curve of **8**.

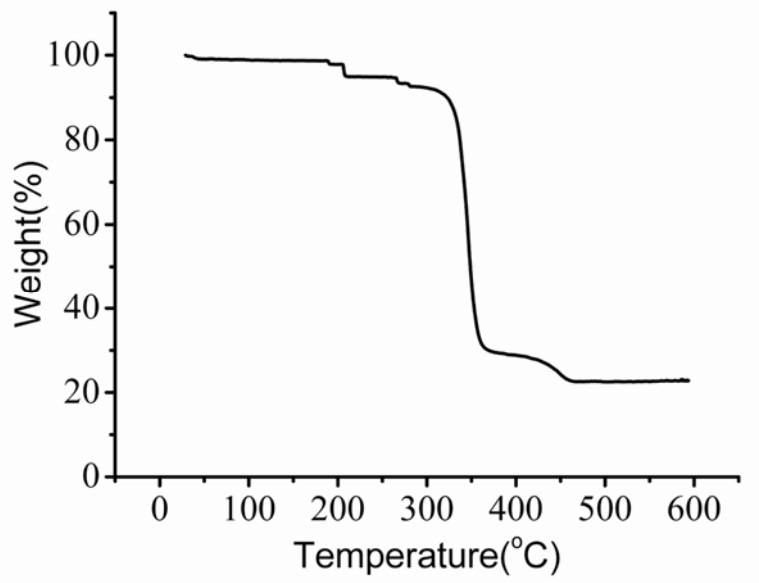


Fig. S23. TGA curve of **9**.

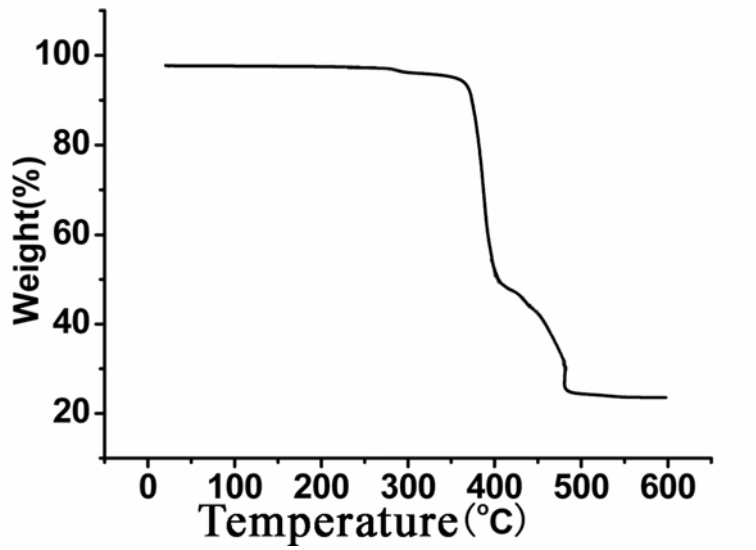


Fig. S24. TGA curve of **10**.

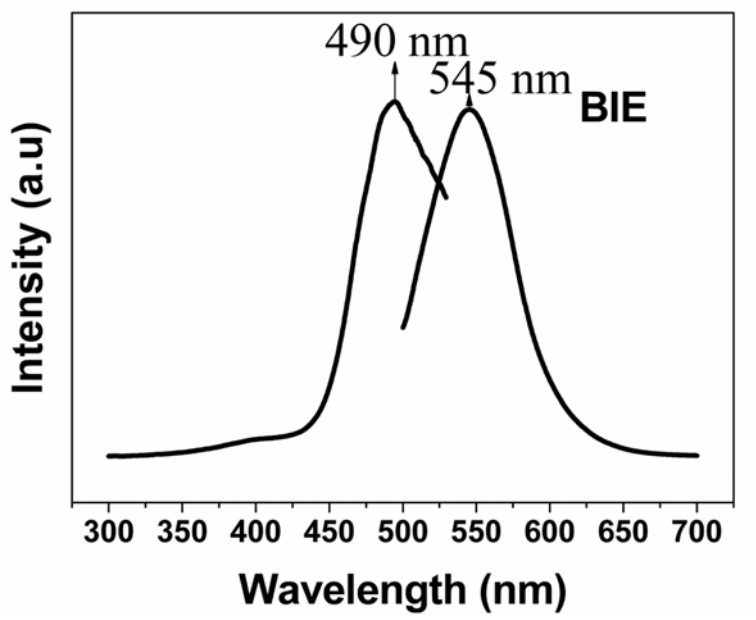
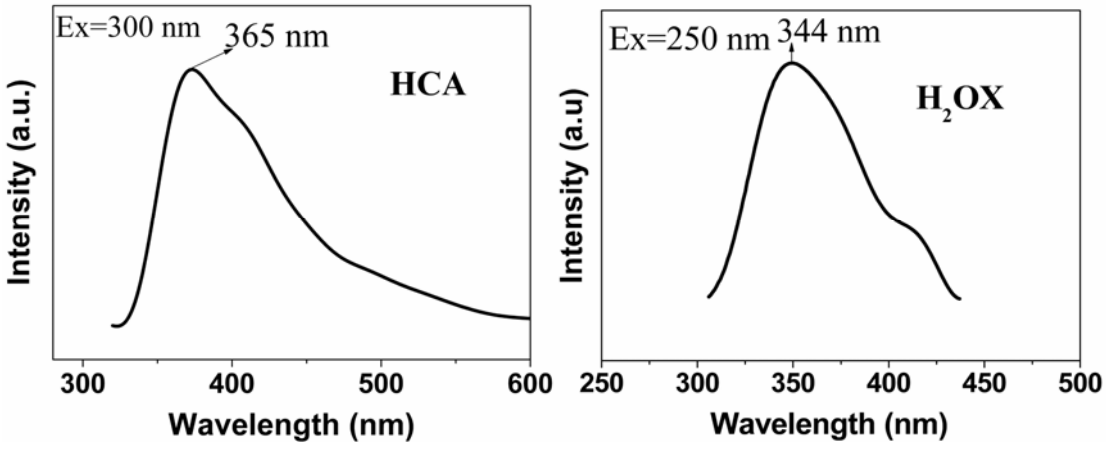


Fig. S 25. Free liquid photoluminescent spectra of BIE ligand at room temperature.



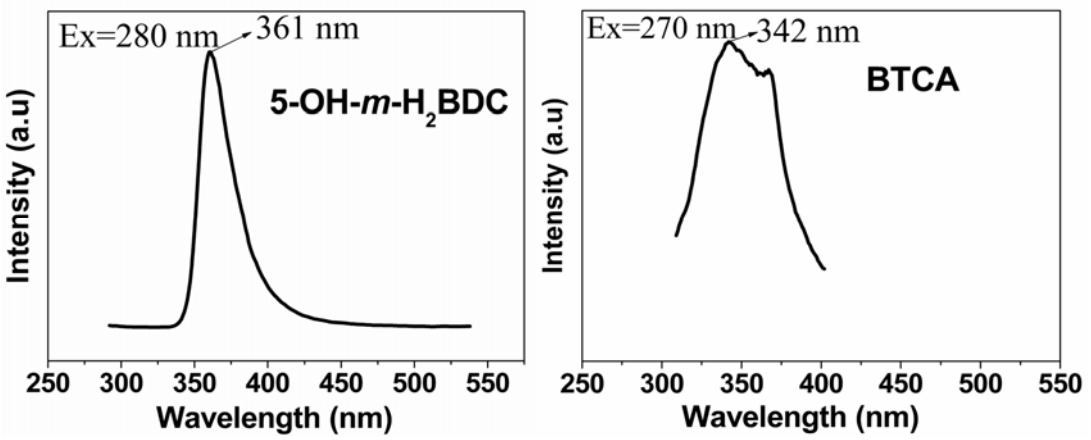
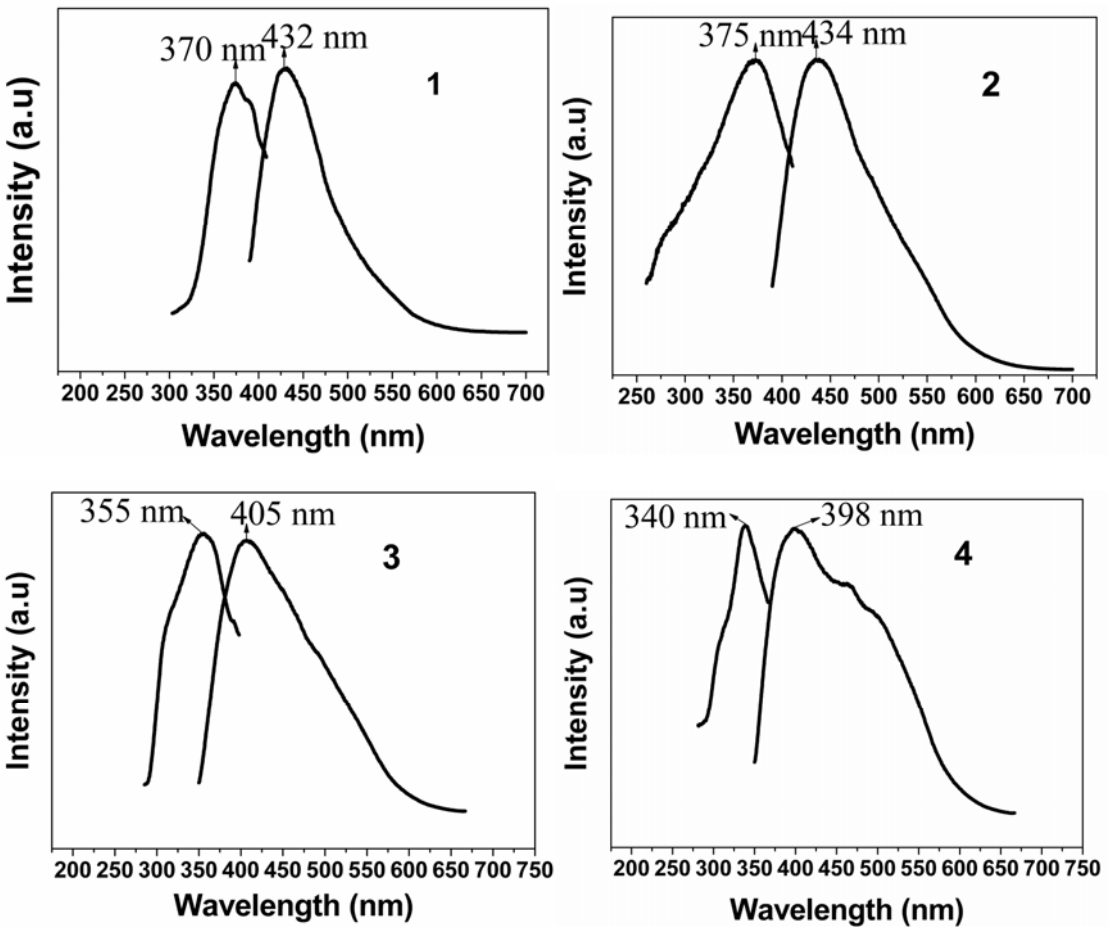


Fig. S26. Solid-state photoluminescent spectra of HCA, H_2OX, 5-OH-*m*-H_2BDC and H_4BTCA ligands.



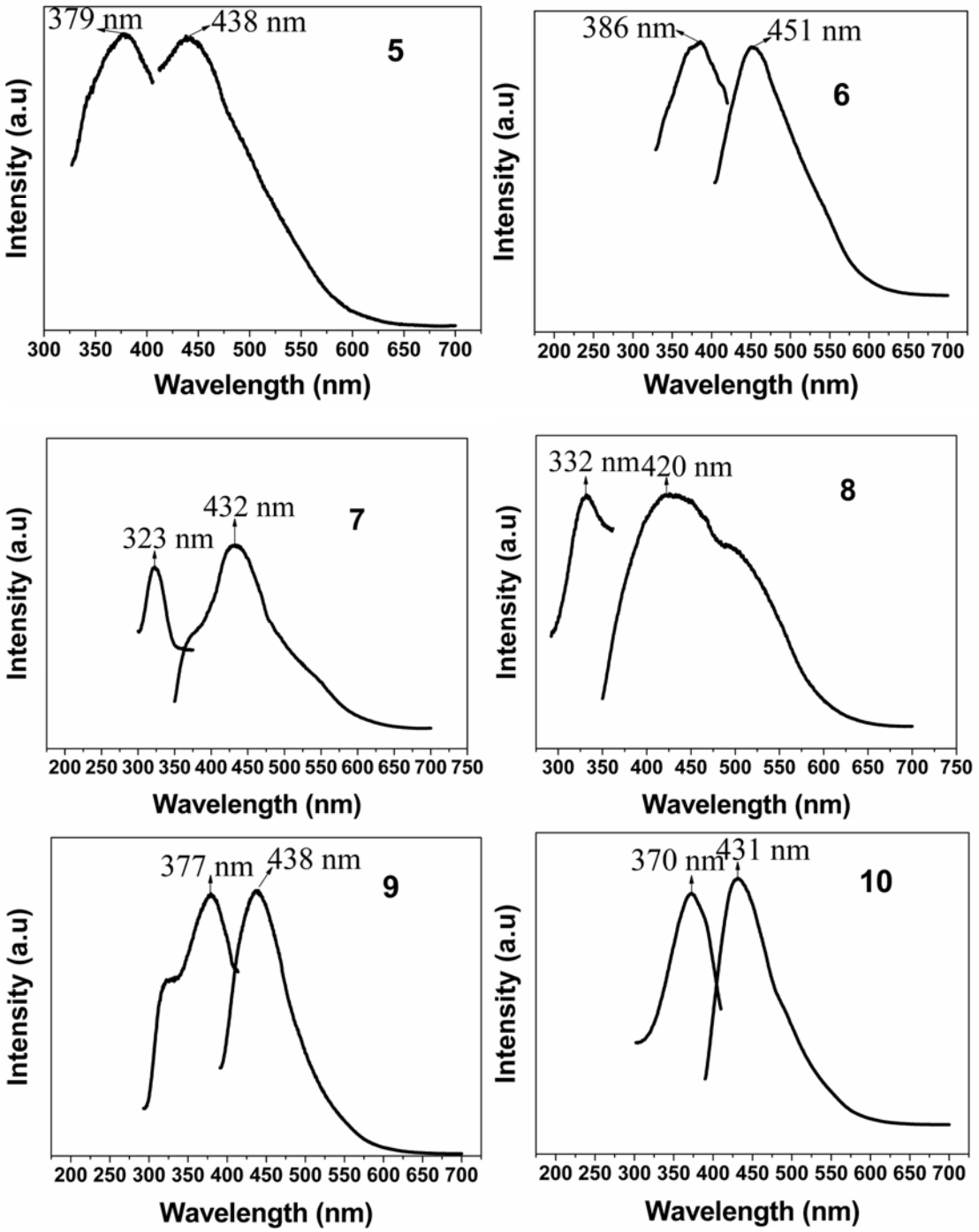


Fig. S27. Solid-state excitation and emission spectra for compounds **1**–**10**.