Electronic Supplementary Information for Dalton Transactions


# $d^{10}$ Metal coordination polymers based on analogue di(pyridyl)imidazole derivatives and 4,4'-oxydibenzoic acid: influence of flexible and angular characters of neutral ligands on structural diversity

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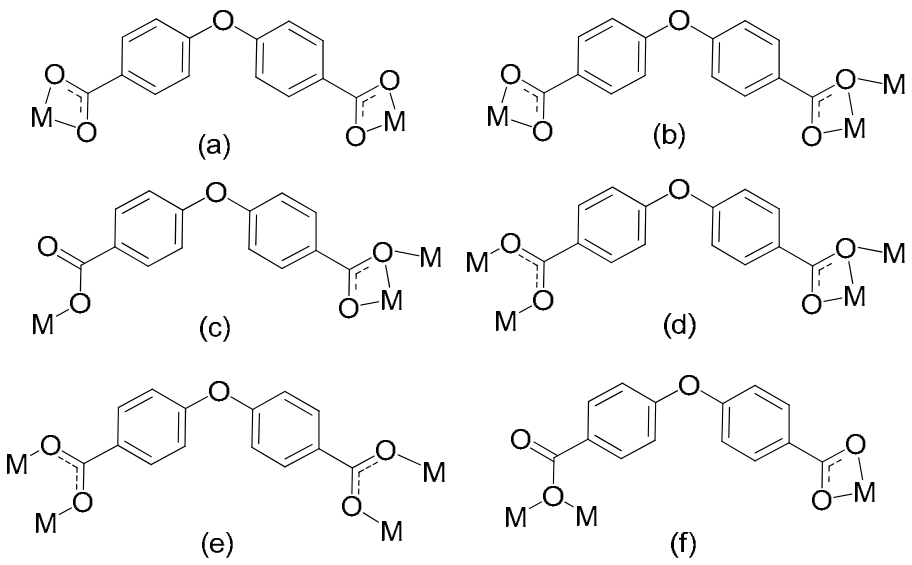



Chart S1. The coordination modes of $oba^{2-}$ anions in this case.

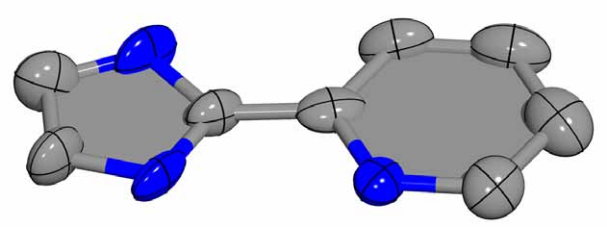
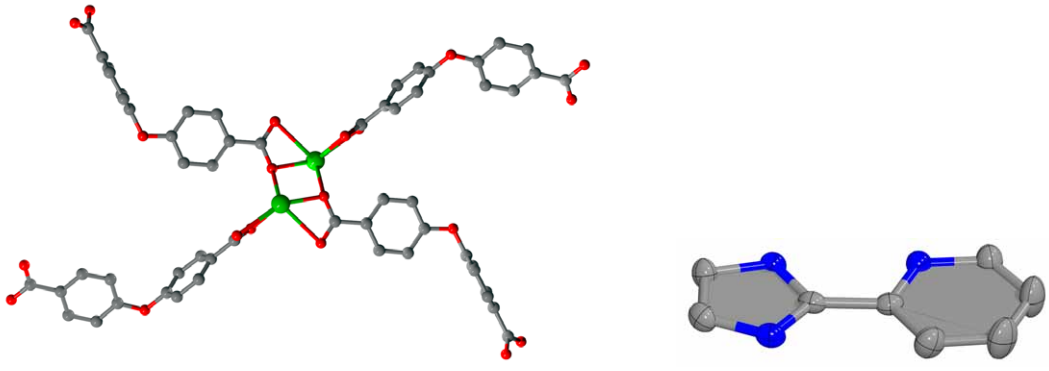
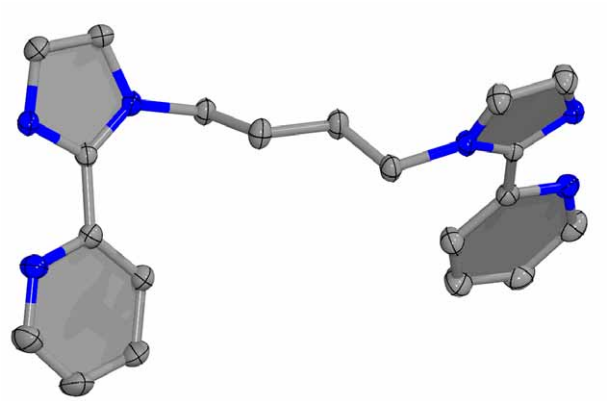


Fig. S1. View of the $L^1$ ligand in **1**.

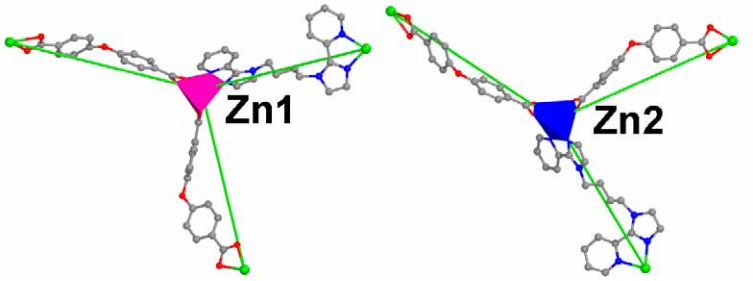


(a) (b)

Fig. S2. (a) Ball-and stick representation of the $[Cd_2(CO_2)_4]$ unit. (b) View of the $L^1$ ligand in **2**.

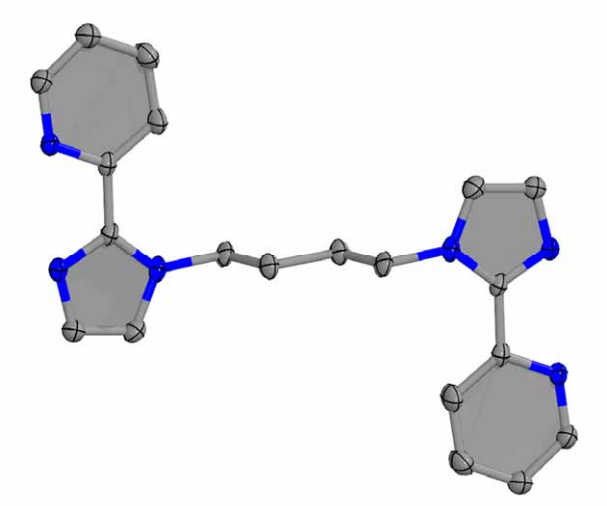


(a)

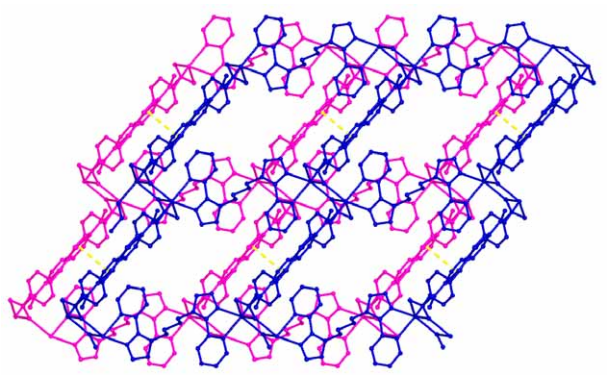



(b)

Fig. S3. (a) View of the $L^2$ ligand in **3**. (b) Ball-and-stick and polyhedral representation of the 3-connected node.

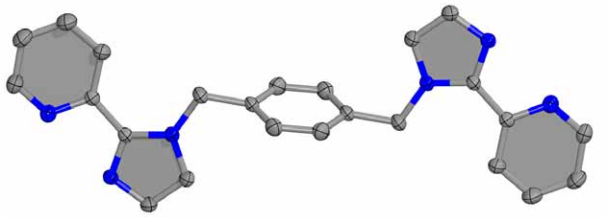


(a)

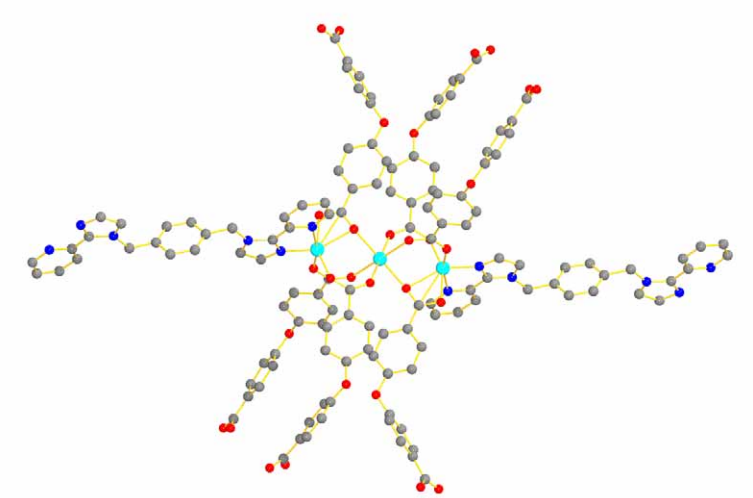


(b)

Fig. S4. (a) View of the $L^2$ ligand in **4**. (b) Ball-and-stick representation of the 3D supramolecular structure of **4**.



(a)



(b)

Fig. S5. (a) View of the $L^3$ ligand in **5**. (b) Ball-and-stick representation of the 8-connected node in **5**.

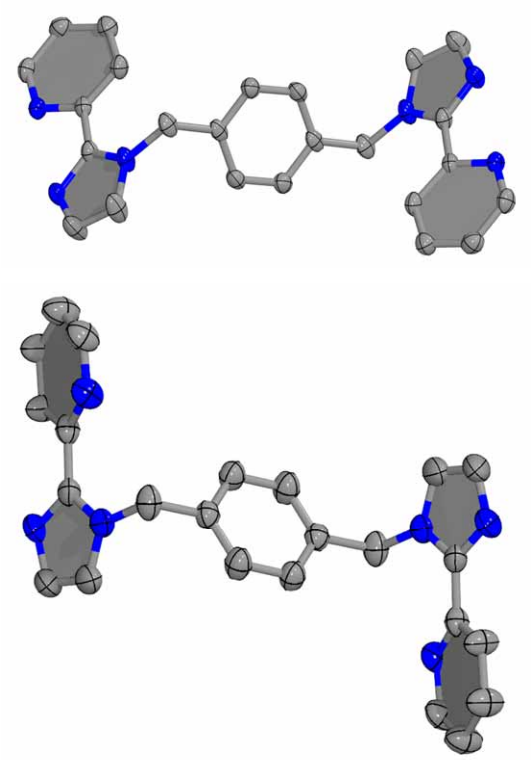
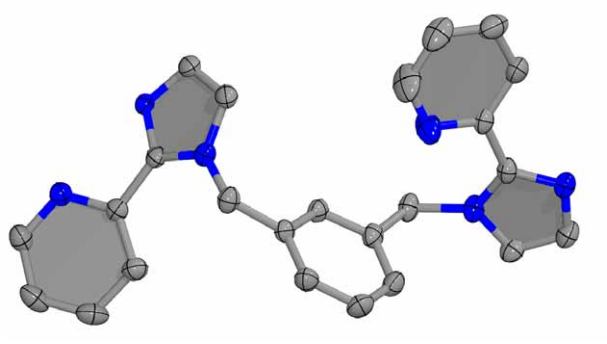
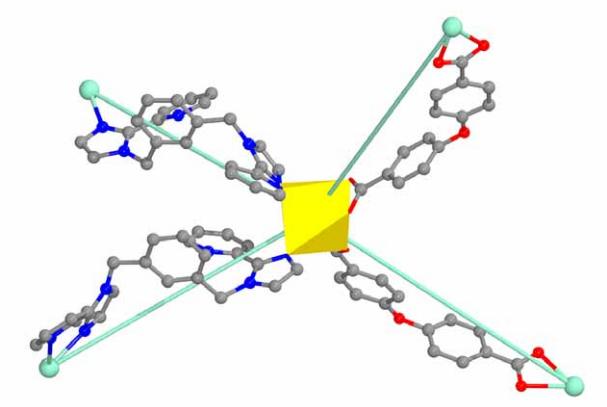


Fig. S6. View of two kinds of $L^3$ ligands in **6**.



(a)



(b)

Fig. S7. (a) View of the $L^4$ ligand in **7**. (b) Ball-and-stick and polyhedral representation of the 4-connected node in **7**.

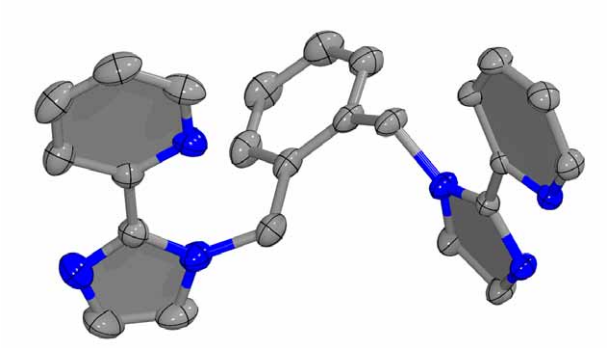


Fig. S8. (a) View of the $L^5$ ligand in **8**.

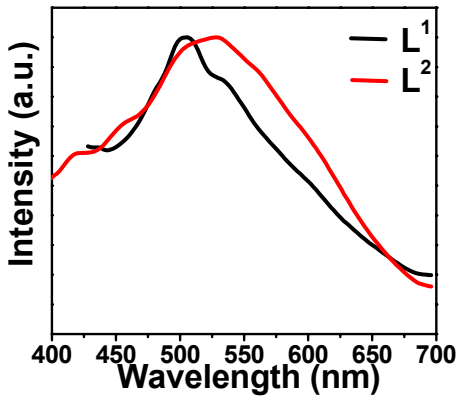
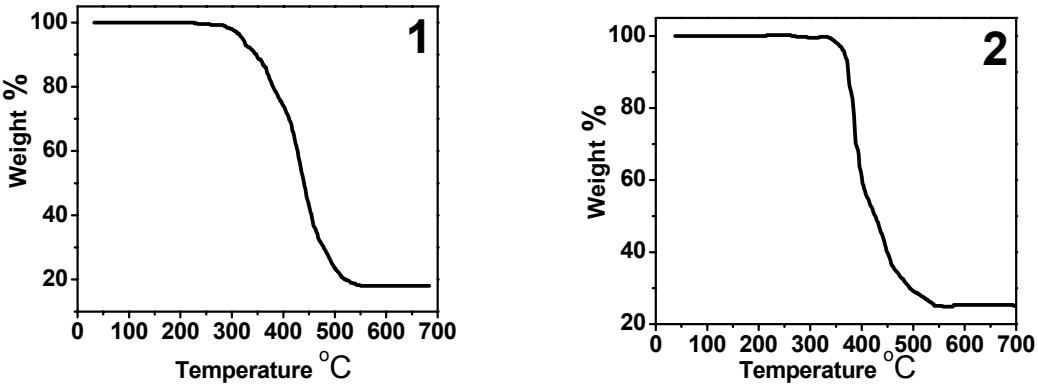



Fig. S9. Solid-state photoluminescent spectra of free ligands $L^1$-$L^2$ at room temperature.



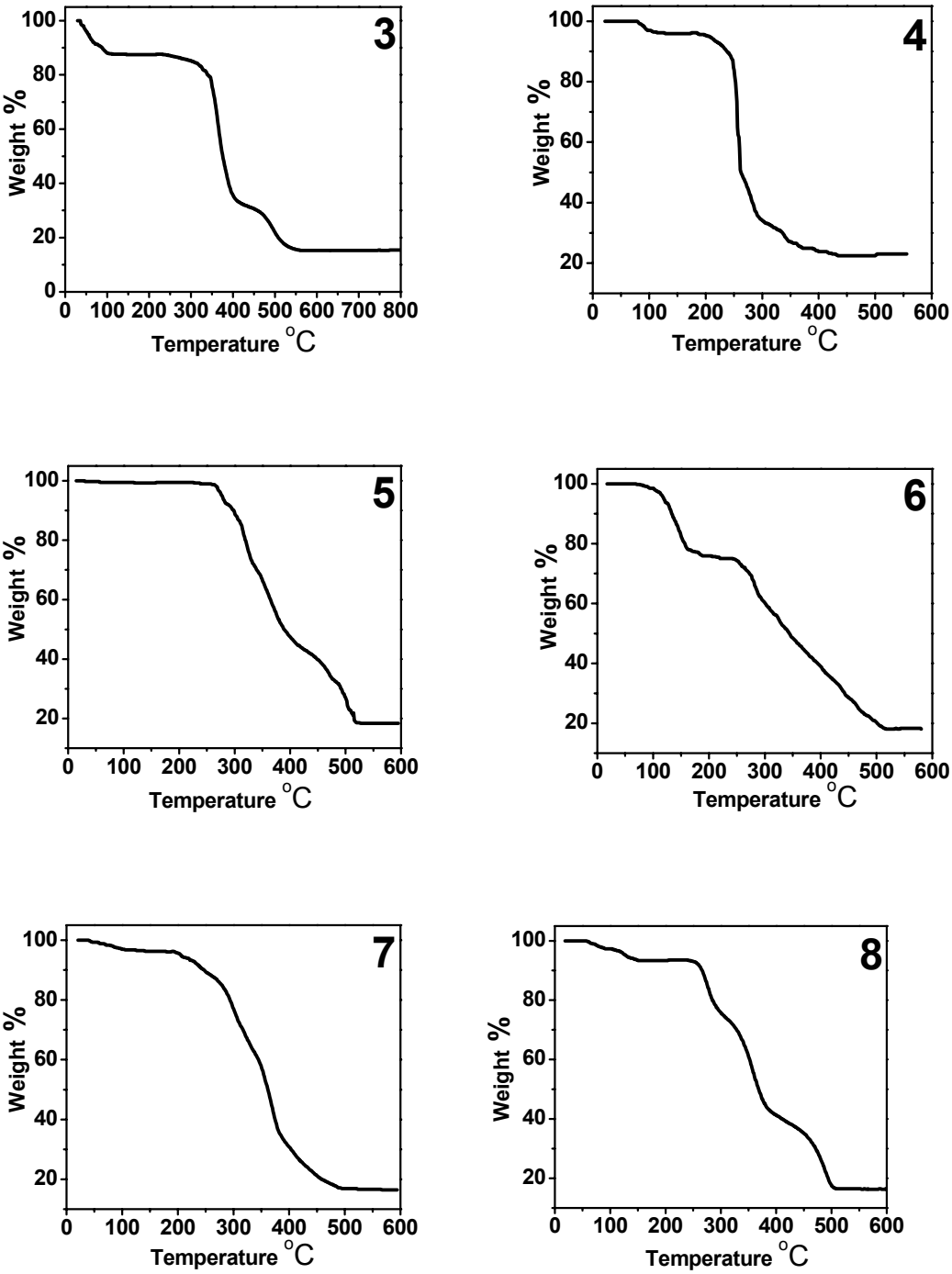



Fig. S10. TGA of compounds **1**-**8**.

**Table S1**. Selected Hydrogen-Bonding Geometry for **1**, **2**, **3**, **4**, **7** and **8** (in Å and deg)

| D-H…A | d(D-H) | d(H...A) | d(D…A) | ∠(D-H...A) |
|---|---|---|---|---|
| Compound **1** | | | | |
| N(1)-H(1A)...O(5)#3 | 0.86 | 2.36 | 3.116(7) | 146.4 |

| | | | | |
|---|---|---|---|---|
| Compound **2** | | | | |
| N(2)-H(1N)...O(4)#5 | 0.87(3) | 1.92(3) | 2.767(2) | 164(3) |
| Compound **3** | | | | |
| O(2W)-H(2A)...O(1W)#5 | 0.80(8) | 2.00(9) | 2.787(5) | 169(12) |
| O(1W)-H(1A)...O(8W) | 0.81(7) | 2.13(8) | 2.770(8) | 136(10) |
| O(1W)-H(1B)...O(7) | 0.79(10) | 2.12(7) | 2.854(5) | 152(13) |
| O(2W)-H(2B)...O(6W) | 0.81(8) | 2.09(7) | 2.878(6) | 165(11) |
| O(3W)-H(3A)...O(5W)#6 | 0.81(9) | 2.22(8) | 2.854(6) | 136(11) |
| O(3W)-H(3B)...O(6) | 0.79(8) | 2.12(7) | 2.840(5) | 150(12) |
| O(4W)-H(4A)...O(3W)#7 | 0.81(10) | 2.11(10) | 2.895(7) | 163(12) |
| O(4W)-H(4B)...O(2) | 0.80(10) | 2.38(6) | 3.124(6) | 155(13) |
| O(5W)-H(5A)...O(2W)#8 | 0.80(9) | 2.09(10) | 2.882(6) | 172(12) |
| O(5W)-H(5B)...O(4W)#4 | 0.80(10) | 2.11(9) | 2.910(6) | 175(13) |
| O(6W)-H(6A)...O(7W)#9 | 0.81(6) | 1.93(3) | 2.722(6) | 168(15) |
| O(6W)-H(6B)...O(4)#10 | 0.81(10) | 2.07(10) | 2.857(6) | 164(10) |
| O(7W)-H(7A)...O(3W)#7 | 0.80(9) | 2.00(10) | 2.769(6) | 162(13) |
| O(7W)-H(7B)...O(2) | 0.80(10) | 2.07(9) | 2.861(6) | 168(12) |
| O(8W)-H(8B)...O(10)#2 | 0.82(9) | 2.22(10) | 2.889(7) | 130(13) |
| Compound **4** | | | | |
| O(1W)-H(1B)...O(3) | 0.85(6) | 1.99(5) | 2.825(5) | 167(6) |
| Compound **7** | | | | |
| O(1W)-H(1A)...O(1) | 0.77(4) | 2.09(4) | 2.859(3) | 173(5) |
| O(1W)-H(1B)...O(5)#5 | 0.77(4) | 2.15(4) | 2.920(3) | 176(5) |
| Compound **8** | | | | |
| O(1W)-H(1A)...N(5)#4 | 0.81(4) | 2.22(3) | 2.950(5) | 151(5) |
| O(1W)-H(1B)...O(4)#1 | 0.81(4) | 2.08(4) | 2.870(3) | 163(5) |
| O(2W)-H(2A)...O(1W) | 0.82(4) | 2.00(5) | 2.804(5) | 167(5) |
| O(2W)-H(2B)...O(3W) | 0.81(4) | 2.26(3) | 2.958(9) | 144(4) |

Symmetry transformations used to generate equivalent atoms for **1**: #3 -x+3/2 ,y-1/2, -z+3/2; for **2**: #5 -x+1, -y+1, -z+1; for **3**: #2 x+1/2, -y-1/2, z-1/2; #4 x+1/2, -y+3/2,

z+1/2; #5 -x+1/2, y+1/2, -z+1/2; #6 x, y-1, z-1; #7 -x+1/2, y+1/2, -z+3/2; #8 -x+1, -y+1, -z+2; #9 x+1/2, -y+1/2, z-1/2; #10 -x+3/2, y-1/2, -z+3/2; for **7**: #5 -x+3/2, y-1/2, -z+3/2; for **8**: #1 x, y, z-1; #4 -x+1, -y, -z.