Supporting Information

# Coordination Polymers of a Multipyridyl and Pyrazolyl Ligand with Conformational Flexibility: Syntheses, Structures and Luminescence

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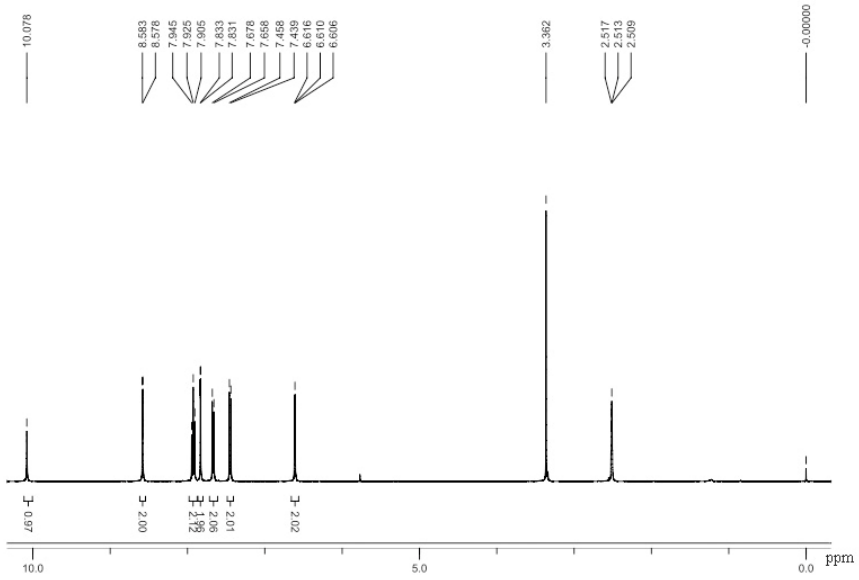


Fig. S1. The $^{1}$H NMR spectrum of **D2** in DMSO-$d_6$

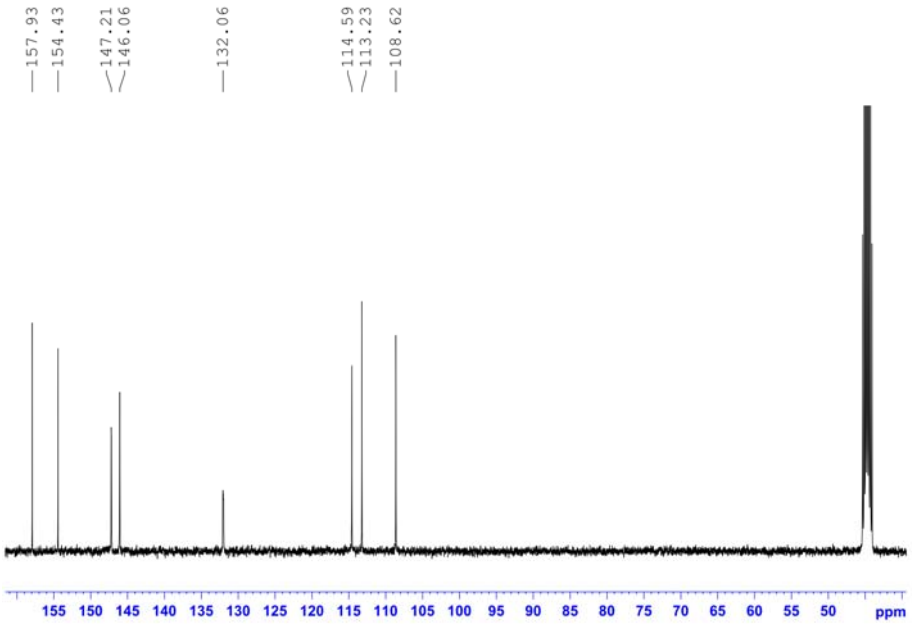


Fig. S2. The $^{13}$C NMR spectrum of **D2** in DMSO-$d_6$

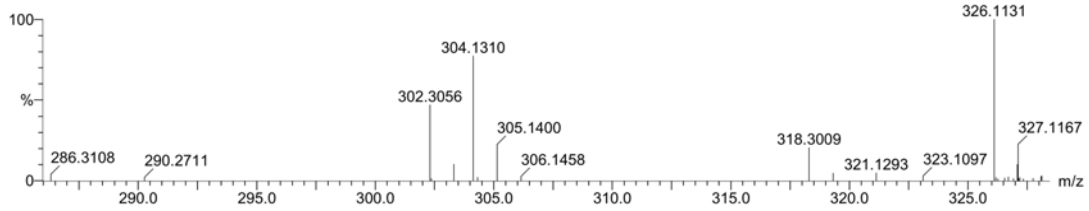


Fig. S3. HRMS of **D2** in MeOH

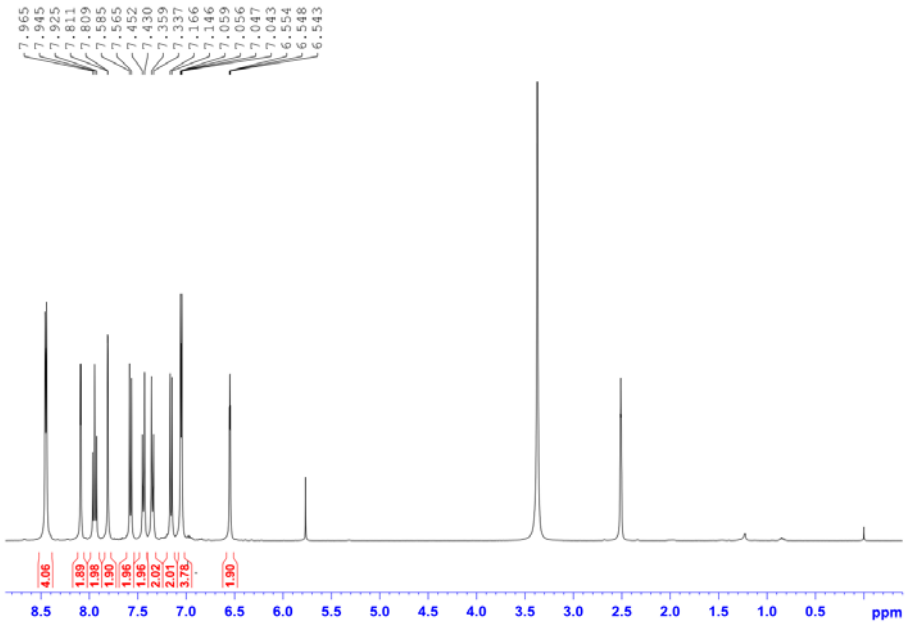


Fig. S4. The $^{1}$H NMR spectrum of **L** in DMSO-$d_6$

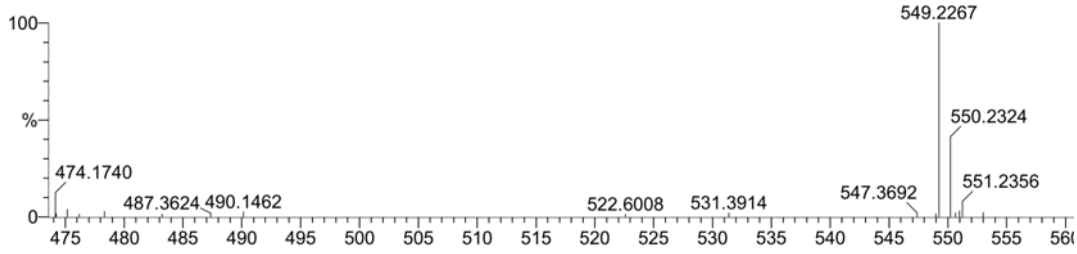


Fig. S5. HRMS of **L** in MeOH

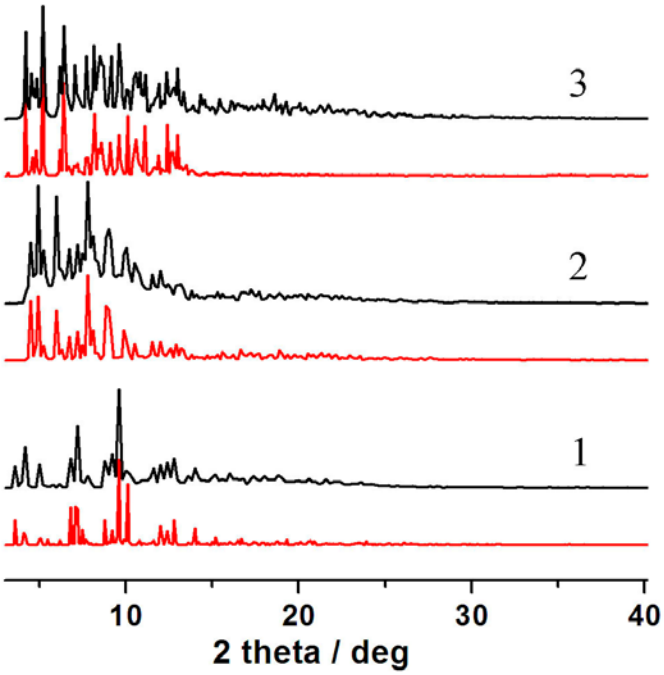


Fig. S6. Stimulated (red) and experimental (black) XRPD patterns of complexes **1**-**3**.

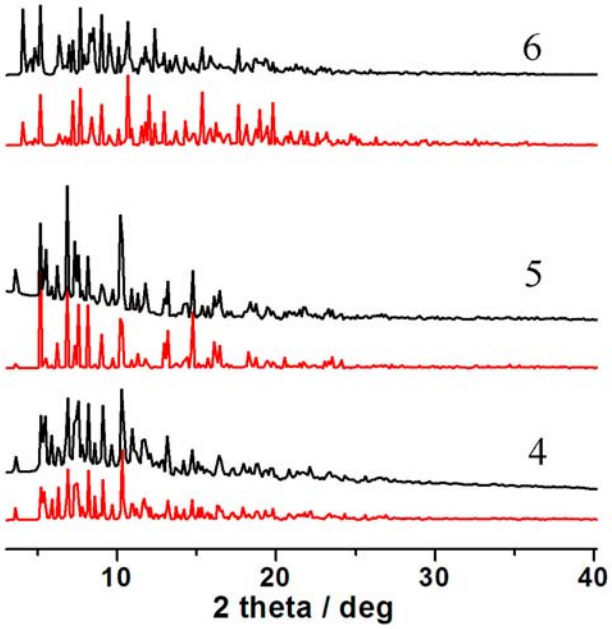


Fig. S7. Stimulated (red) and experimental (black) XRPD patterns of complexes **4**-**6**.

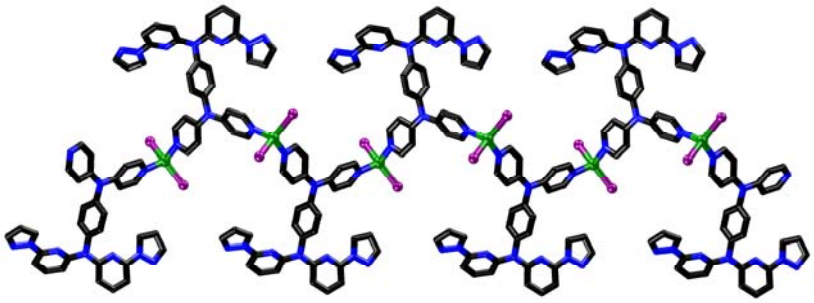

Fig. S8. 1D zigzag chain of complex **3**.

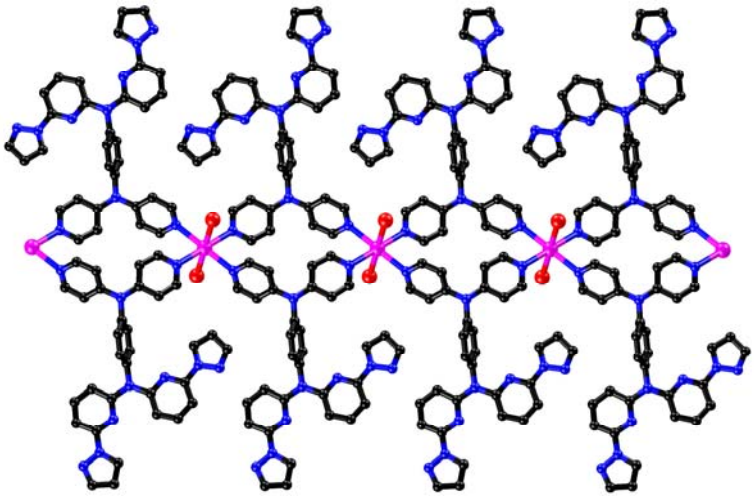

Fig. S9. 1D chain of complex **5**.

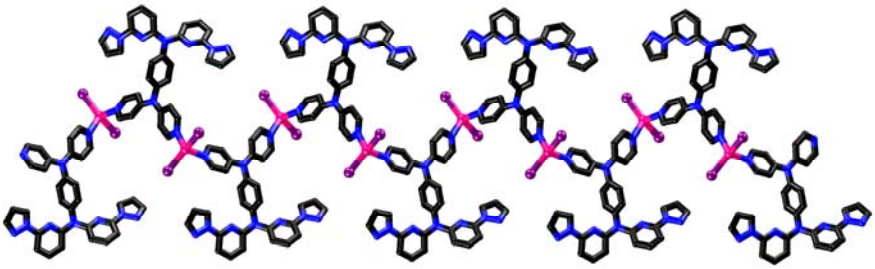

Fig. S10. 1D chain of complex **6**.

Table S1. Selected Bond lengths (Å) and Angles (°) for complexes **1**~ **8**.

Complex **1**

| | | |
|---|---|---|
| Zn(1)-N(9) 2.019(9) | N(9)-Zn(1)-N(10) 109.6(4) | N(9)-Zn(1)-Cl(2) 102.9(3) |
| Zn(1)-N(10) 2.035(10) | N(9)-Zn(1)-Cl(1) 109.6(3) | N(10)-Zn(1)-Cl(2) 102.0(3) |
| Zn(1)-Cl(1) 2.208(3) | N(10)-Zn(1)-Cl(1) 108.9(3) | Cl(1)-Zn(1)-Cl(2) 123.13(16) |
| Zn(1)-Cl(2) 2.246(4) | | |

Complex **2**

| | | |
|---|---|---|
| Zn(1)-N(10)#1 2.031(9) | N(10)#1-Zn(1)-N(9) 108.0(4) | N(10)#1-Zn(1)-Br(2) 108.2(3) |
| Zn(1)-N(9) 2.037(8) | N(10)#1-Zn(1)-Br(1) 108.6(3) | N(9)-Zn(1)-Br(2) 104.7(3) |
| Zn(1)-Br(1) 2.367(2) | N(9)-Zn(1)-Br(1) 103.6(2) | Br(1)-Zn(1)-Br(2) 122.92(8) |
| Zn(1)-Br(2) 2.3699(18) | | |

Symmetry transformations used to generate equivalent atoms: #1 -x+3/2, y+1/2, -z+3/2

Complex **3**

| | | |
|---|---|---|
| Zn(1)-N(10)#1 2.055(8) | N(10)#1-Zn(1)-N(9) 100.0(3) | N(10)#1-Zn(1)-I(1) 109.7(3) |
| Zn(1)-N(9) 2.067(8) | N(10)#1-Zn(1)-I(2) 110.1(2) | N(9)-Zn(1)-I(1) 104.3(3) |
| Zn(1)-I(2) 2.5362(16) | N(9)-Zn(1)-I(2) 109.7(2) | I(2)-Zn(1)-I(1) 120.83(6) |
| Zn(1)-I(1) 2.5583(18) | | |

Symmetry transformations used to generate equivalent atoms: #1 -x+1/2, y-1/2, -z+1/2

Complex **4**

| | | |
|---|---|---|
| Cd(1)-N(10)#1 2.436(5) | N(10)#1-Cd(1)-N(9) 96.55(18) | N(10)#1-Cd(1)-Cl(1) 90.05(14) |
| Cd(1)-N(9) 2.499(6) | N(10)#2-Cd(1)-N(9) 83.45(18) | N(9)-Cd(1)-Cl(1) 89.19(16) |
| Cd(1)-Cl(1) 2.532(3) | N(9)-Cd(1)-N(9)#3 180.0(2) | N(9)#3-Cd(1)-Cl(1) 90.81(16) |
| N(10)#1-Cd(1)-N(10)#2 180.00(18) | N(10)#1-Cd(1)-Cl(1)#3 89.95(14) | Cl(1)#3-Cd(1)-Cl(1) 180.0 |

Symmetry transformations used to generate equivalent atoms: #1 x, y, z-1 #2 -x+3, -y+1, -z+1 #3 -x+3, -y+1, -z

Complex **5**

| | | |
|---|---|---|
| Cd(1)-N(9) 2.487(4) | N(9)#1-Cd(1)-N(10)#2 95.82(15) | N(10)#2-Cd(1)-Br(1)#1 90.84(11) |
| Cd(1)-N(10)#2 2.496(5) | N(9)-Cd(1)-Br(1)#1 89.75(10) | N(10)#3-Cd(1)-Br(1)#1 89.16(11) |
| Cd(1)-Br(1) 2.6646(6) | N(9)#1-Cd(1)-Br(1)#1 90.25(10) | N(9)-Cd(1)-Br(1) 90.25(10) |
| N(9)-Cd(1)-N(10)#2 84.18(15) | | |

Symmetry transformations used to generate equivalent atoms: #1 -x+1, -y+1, -z+3 #2 -x, -y+1, -z+2 #3 x+1, y, z+1

Complex **6**

| | | |
|---|---|---|
| Cd(1)-N(10)#1 2.270(5) | N(10)#1-Cd(1)-N(9) 93.87(19) | N(10)#1-Cd(1)-I(1) 106.08(14) |
| Cd(1)-N(9) 2.301(5) | N(10)#1-Cd(1)-I(2) 111.83(15) | N(9)-Cd(1)-I(1) 103.82(14) |

| | | | | | |
|---|---|---|---|---|---|
| Cd(1)-I(2) | 2.6708(9) | N(9)-Cd(1)-I(2) | 107.62(14) | I(2)-Cd(1)-I(1) | 128.01(3) |
| Cd(1)-I(1) | 2.7038(8) | | | | |

Symmetry transformations used to generate equivalent atoms: #1 -x+3/2, y-1/2, -z+3/2

Complex **7**

| | | | | | |
|---|---|---|---|---|---|
| Co(1)-N(5) | 2.085(4) | N(8)-Co(1)-N(11) | 92.89(16) | N(8)-Co(1)-N(9) | 84.92(14) |
| Co(1)-N(8) | 2.094(4) | N(6)-Co(1)-N(11) | 92.01(16) | N(6)-Co(1)-N(9) | 88.18(14) |
| Co(1)-N(6) | 2.100(4) | N(5)-Co(1)-N(3) | 79.49(14) | N(11)-Co(1)-N(9) | 177.72(15) |
| Co(1)-N(11) | 2.103(5) | N(8)-Co(1)-N(3) | 168.21(15) | N(3)-Co(1)-N(9) | 93.06(13) N(5)-Co(1)-N(6) 167.32(14) |
| Co(1)-N(3) | 2.105(3) | N(6)-Co(1)-N(3) | 88.97(14) | N(8)-Co(1)-N(6) | 79.37(15) |
| Co(1)-N(9) | 2.244(4) | N(11)-Co(1)-N(3) | 89.22(15) | N(5)-Co(1)-N(11) | 93.04(16) |
| N(5)-Co(1)-N(8) | 111.96(15) | N(5)-Co(1)-N(9) | 87.23(14) | | |

Complex **8**

| | | | | | |
|---|---|---|---|---|---|
| Cu(1)-N(3) | 1.971(3) | N(3)-Cu(1)-N(2) | 173.39(13) | N(3)-Cu(1)-N(8)#1 | 88.91(13) |
| Cu(1)-N(2) | 1.972(3) | N(3)-Cu(1)-N(4) | 82.56(12) | N(2)-Cu(1)-N(8)#1 | 88.92(13) |
| Cu(1)-N(4) | 1.978(3) | N(2)-Cu(1)-N(4) | 91.45(12) | N(4)-Cu(1)-N(8)#1 | 95.88(12) |
| Cu(1)-N(1) | 1.990(3) | N(3)-Cu(1)-N(1) | 103.22(14) | N(1)-Cu(1)-N(8)#1 | 84.83(13) |
| Cu(1)-N(8)#1 | 2.433(3) | N(2)-Cu(1)-N(1) | 82.79(13) | N(3)-Cu(1)-N(14) | 95.39(17) |
| Cu(1)-N(14) | 2.546(5) | N(4)-Cu(1)-N(1) | 174.20(13) | N(2)-Cu(1)-N(14) | 87.07(16) |
| N(1)-Cu(1)-N(14) | 91.82(16) | N(8)#1-Cu(1)-N(14) | 175.07(14) | N(4)-Cu(1)-N(14) | 87.10(16) |

Symmetry transformations used to generate equivalent atoms: #1 x,-y+1,z+1/2