# Syntheses, Structures and Properties of Nine $d^{10}$ or *p*-Block Coordination Polymers Based on Ligand Containing Both Terpyridyl and Sulfo Groups

**Li Zhang, Jia-Dan Zheng, Yi-Ting Chen, Sheng-Run Zheng,* Jun Fan, Wei-Guang Zhang ***

## Supporting information

Table S**1** Selected bond lengths [Å] and angles[°] for the compounds.[a]

| | | | |
|---|---|---|---|
| Complex **1** | | | |
| Zn(1)-N(3) | 2.114(6) | Zn(1)-O(2W) | 2.138(5) |
| Zn(1)-N(3)#1 | 2.114(6) | Zn(1)-O(1W) | 2.153(4) |
| Zn(1)-O(2W)#1 | 2.138(5) | Zn(1)-O(1W)#1 | 2.153(4) |
| N(3)-Zn(1)-N(3)#1 | 180.00 | O(2W)#1-Zn(1)-O(1W) | 88.1(2) |
| N(3)-Zn(1)-O(2W)#1 | 92.1(2) | O(2W)-Zn(1)-O(1W) | 91.9(2) |
| N(3)#1-Zn(1)-O(2W)#1 | 87.9(3) | N(3)-Zn(1)-O(1W)#1 | 88.84(19) |
| N(3)-Zn(1)-O(2W) | 87.9(3) | N(3)#1-Zn(1)-O(1W)#1 | 91.16(19) |
| N(3)#1-Zn(1)-O(2W) | 92.1(2) | O(2W)#1-Zn(1)-O(1W)#1 | 91.9(2) |
| O(2W)#1-Zn(1)-O(2W) | 180.000 | O(2W)-Zn(1)-O(1W)#1 | 88.1(2) |
| N(3)-Zn(1)-O(1W) | 91.16(19) | O(1W)-Zn(1)-O(1W)#1 | 180.000 |
| N(3)#1-Zn(1)-O(1W) | 88.84(19) | | |
| Complex **2** | | | |
| Cd(1)-N(3)#1 | 2.317(3) | Cd(1)-O(2W) | 2.353(3) |
| Cd(1)-N(1)#2 | 2.322(3) | Cd(1)-O(6)#3 | 2.415(3) |
| Cd(1)-O(3) | 2.331(2) | Cd(1)-O(1W) | 2.432(3) |
| N(3)#1-Cd(1)-N(1)#2 | 108.12(11) | O(3)-Cd(1)-O(6)#3 | 86.85(9) |
| N(3)#1-Cd(1)-O(3) | 85.16(10) | O(2W)-Cd(1)-O(6)#3 | 78.71(11) |
| N(1)#2-Cd(1)-O(3) | 166.48(10) | N(3)#1-Cd(1)-O(1W) | 77.50(11) |
| N(3)#1-Cd(1)-O(2W) | 147.53(11) | N(1)#2-Cd(1)-O(1W) | 84.24(11) |
| N(1)#2-Cd(1)-O(2W) | 89.04(11) | O(3)-Cd(1)-O(1W) | 101.55(9) |
| O(3)-Cd(1)-O(2W) | 80.50(10) | O(2W)-Cd(1)-O(1W) | 77.08(11) |
| N(3)#1-Cd(1)-O(6)#3 | 129.57(11) | O(6)#3-Cd(1)-O(1W) | 152.60(11) |
| N(1)#2-Cd(1)-O(6)#3 | 82.71(11) | | |
| Complex **3** | | | |
| Ag(1)-N(1) | 2.103(13) | Ag(2)-N(3) | 2.144(13) |
| Ag(1)-N(1)#1 | 2.103(13) | Ag(2)-N(3)#2 | 2.144(13) |
| N(1)-Ag(1)-N(1)#1 | 180.0 | N(3)-Ag(2)-N(3)#2 | 180.0 |
| Complex **4** | | | |
| Ag(1)-N(3) | 2.196(8) | N(3)-Ag(1)-O(1W) | 155.3(3) |

| | | | |
|---|---|---|---|
| Ag(1)-O(1W) | 2.218(7) | | |
| Complex **5** | | | |
| Ag(1)-N(1)#1 | 2.127(7) | Ag(2)-O(3)#3 | 2.537(6) |
| Ag(1)-N(1) | 2.127(7) | Ag(2)-O(3)#4 | 2.599(7) |
| Ag(2)-N(3) | 2.192(7) | Ag(3)-O(1)#7 | 2.387(7) |
| Ag(2)-O(5)#2 | 2.205(7) | Ag(3)-Ag(3)#8 | 2.451(4) |
| N(1)#1-Ag(1)-N(1) | 180.000 | N(3)-Ag(2)-O(3)#4 | 97.6(3) |
| N(3)-Ag(2)-O(5)#2 | 154.2(3) | O(5)#2-Ag(2)-O(3)#4 | 96.8(3) |
| N(3)-Ag(2)-O(3)#3 | 93.7(3) | O(3)#3-Ag(2)-O(3)#4 | 82.7(2) |
| O(5)#2-Ag(2)-O(3)#3 | 109.3(3) | O(2)-S(1)-O(1) | 111.8(5) |
| Complex **6** | | | |
| Ag(3)-N(1) | 2.131(5) | Ag(2)-N(3)#3 | 2.193(6) |
| Ag(3)-N(6) | 2.134(5) | Ag(2)-O(3)#4 | 2.468(5) |
| Ag(1)-O(5)#1 | 2.272(5) | Ag(2)-O(6) | 2.551(6) |
| Ag(1)-O(2W) | 2.294(6) | Ag(4)-N(4) | 2.195(6) |
| Ag(1)-O(3)#2 | 2.361(5) | Ag(4)-O(1W) | 2.228(8) |
| Ag(1)-O(1) | 2.518(5) | | |
| N(1)-Ag(3)-N(6) | 172.4(2) | O(3)#2-Ag(1)-O(1) | 91.61(18) |
| O(5)#1-Ag(1)-O(2W) | 116.4(2) | N(3)#3-Ag(2)-O(3)#4 | 131.0(2) |
| O(5)#1-Ag(1)-O(3)#2 | 92.99(19) | N(3)#3-Ag(2)-O(6) | 126.7(2) |
| O(2W)-Ag(1)-O(3)#2 | 144.3(2) | O(3)#4-Ag(2)-O(6) | 100.89(19) |
| O(5)#1-Ag(1)-O(1) | 120.9(2) | N(4)-Ag(4)-O(1W) | 144.4(4) |
| O(2W)-Ag(1)-O(1) | 90.1(2) | | |
| Complex **7** | | | |
| Pb(1)-O(3) | 2.539(4) | Pb(1)-O(2W) | 2.634(5) |
| Pb(1)-O(1W) | 2.564(6) | Pb(1)-O(5)#3 | 2.661(4) |
| Pb(1)-N(3)#1 | 2.608(5) | Pb(1)-O(6)#3 | 2.689(4) |
| Pb(1)-N(1)#2 | 2.635(5) | | |
| O(3)-Pb(1)-O(1W) | 79.60(19) | O(1W)-Pb(1)-O(5)#3 | 80.66(19) |
| O(3)-Pb(1)-N(3)#1 | 86.93(15) | N(3)#1-Pb(1)-O(5)#3 | 131.06(15) |
| O(1W)-Pb(1)-N(3)#1 | 146.04(19) | N(1)#2-Pb(1)-O(5)#3 | 77.83(15) |
| O(3)-Pb(1)-N(1)#2 | 168.01(15) | O(2W)-Pb(1)-O(5)#3 | 151.45(14) |
| O(1W)-Pb(1)-N(1)#2 | 93.5(2) | O(3)-Pb(1)-O(6)#3 | 75.63(13) |
| N(3)#1-Pb(1)-N(1)#2 | 103.95(17) | O(1W)-Pb(1)-O(6)#3 | 125.84(18) |
| O(3)-Pb(1)-O(2W) | 106.02(14) | N(3)#1-Pb(1)-O(6)#3 | 79.46(13) |
| O(1W)-Pb(1)-O(2W) | 80.38(19) | N(1)#2-Pb(1)-O(6)#3 | 101.11(16) |
| N(3)#1-Pb(1)-O(2W) | 73.59(15) | O(2W)-Pb(1)-O(6)#3 | 152.80(14) |
| N(1)#2-Pb(1)-O(2W) | 82.24(17) | O(5)#3-Pb(1)-O(6)#3 | 52.99(12) |
| O(3)-Pb(1)-O(5)#3 | 91.28(13) | | |
| Complex **8** | | | |
| Pb(1)-O(3W) | 2.462(7) | Pb(1)-N(1) | 2.645(9) |
| Pb(1)-O(2W) | 2.511(9) | Pb(1)-N(3)#1 | 2.673(9) |

| | | | |
|---|---|---|---|
| Pb(1)-O(1W) | 2.580(8) | | |
| O(3W)-Pb(1)-O(2W) | 79.3(3) | O(1W)-Pb(1)-N(1) | 156.1(3) |
| O(3W)-Pb(1)-O(1W) | 81.3(3) | O(3W)-Pb(1)-N(3)#1 | 75.0(3) |
| O(2W)-Pb(1)-O(1W) | 81.1(3) | O(2W)-Pb(1)-N(3)#1 | 152.4(3) |
| O(3W)-Pb(1)-N(1) | 81.2(3) | O(1W)-Pb(1)-N(3)#1 | 85.2(3) |
| O(2W)-Pb(1)-N(1) | 79.7(3) | N(1)-Pb(1)-N(3)#1 | 105.8(3) |
| Complex **9** | | | |
| Pb(1)-N(1) | 2.536(10) | K(1)-O(3W) | 2.13(4) |
| Pb(1)-O(1W) | 2.557(15) | K(1)-N(3) | 2.390(15) |
| Pb(1)-O(3)#1 | 2.580(10) | K(1)-O(2)#3 | 2.651(13) |
| Pb(1)-O(7) | 2.64(2) | K(1)-O(2W) | 3.27(3) |
| Pb(1)-O(5)#2 | 2.667(16) | | |
| N(1)-Pb(1)-O(1W) | 78.7(5) | O(3)#1-Pb(1)-O(5)#2 | 143.4(4) |
| N(1)-Pb(1)-O(3)#1 | 78.2(3) | O(7)-Pb(1)-O(5)#2 | 116.9(7) |
| O(1W)-Pb(1)-O(3)#1 | 75.2(4) | O(3W)-K(1)-N(3) | 80.2(7) |
| N(1)-Pb(1)-O(7) | 80.1(6) | O(3W)-K(1)-O(2)#3 | 67.2(5) |
| O(1W)-Pb(1)-O(7) | 156.6(6) | N(3)-K(1)-O(2)#3 | 147.2(6) |
| O(3)#1-Pb(1)-O(7) | 90.9(6) | O(3W)-K(1)-O(2W) | 160.7(9) |
| N(1)-Pb(1)-O(5)#2 | 83.3(4) | N(3)-K(1)-O(2W) | 84.9(4) |
| O(1W)-Pb(1)-O(5)#2 | 70.3(5) | O(2)#3-K(1)-O(2W) | 127.8(3) |

[a]Symmetry transformations used to generate equivalentatoms: #1 –x + 1/2, -y + 3/2, -z + 1 for complex **1**; #1 x, y - 1, z, #2 x - 1, y - 1, z - 1, #3 x - 1, y, z, #4 x + 1, y, z, #5 x + 1, y + 1, z + 1, #6 x, y + 1, z for complex **2**; #1 -x, -y, -z - 1, #2 –x + 1/2, -y - 1/2, -z + 1 for complex **3**; #1 –x + 3, -y + 3, -z + 2, #2 –x + 2, -y + 1, -z + 2, #3 x, y, z + 1, #4 –x + 3, -y + 1, -z + 2, #5 x + 1, y, z, #6 x, y, z - 1, #7 x - 1, y, z, #8 –x + 1, -y + 2, -z + 1 for complex **5**; #1 x + 1, y, z, #2 -x, -y, -z - 1 #3 x - 1, y - 1, z, #4 –x - 1, -y, -z - 1, #5 x + 1, y + 1, z, #6 x - 1, y, z for complex **6**; #1 x, y + 1, z, #2 x + 1, y + 1, z + 1, #3 x + 1, y, z, #4 x - 1, y - 1, z - 1, #5 x - 1, y, z, #6 x, y - 1, z for complex **7**; #1 x, y, z - 1, #2 x, y, z + 1 for complex **8**; #1 x, y + 1/2, -z + 2, #2 y + 1/4, -x + 5/4, z + 1/4, #3 x + 1, y, z, #4 x - 1, y, z, #5 x, y - 1/2, -z + 2, #6 –y + 5/4, x - 1/4, z-1/4 for complex **9**.

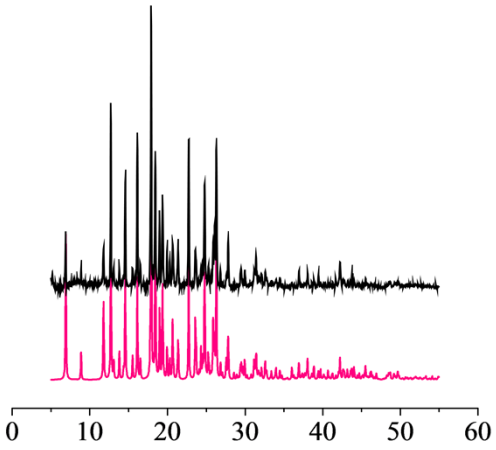


**Figure S1.** PXRD patterns of simulated based on the X-ray single-crystal diffraction data of **1** (lower) and for as-synthesized **1**(upper).

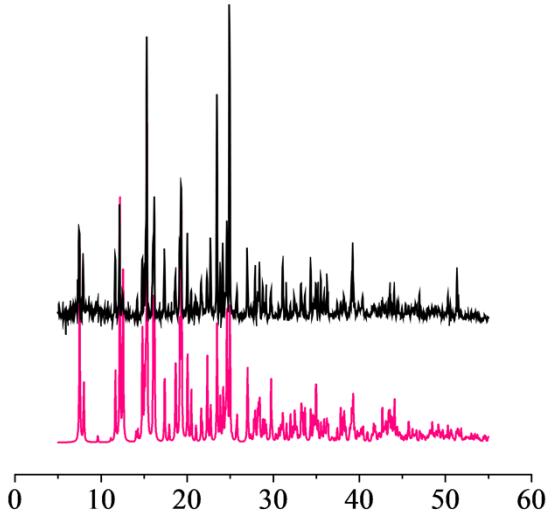


**Figure S2.** PXRD patterns of simulated based on the X-ray single-crystal diffraction data of **2** (lower) and for as-synthesized **2**(upper).

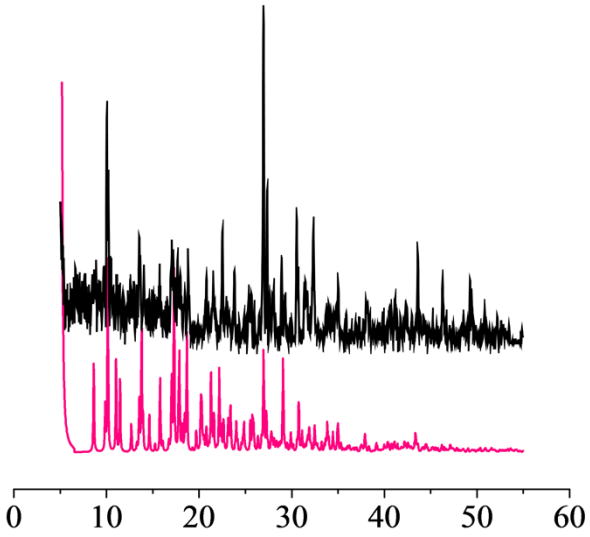


**Figure S3.** PXRD patterns of simulated based on the X-ray single-crystal diffraction data of **3** (lower) and for as-synthesized **3**(upper).

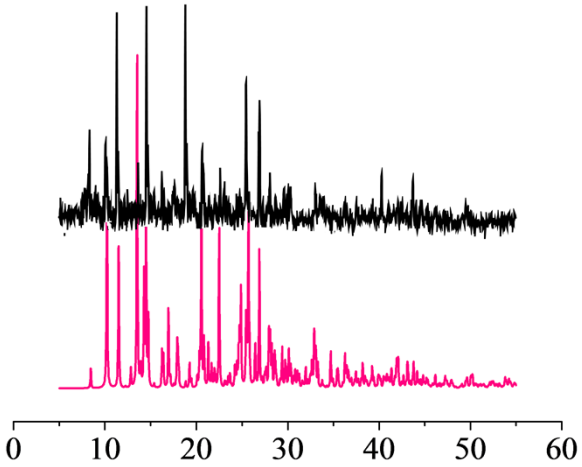


**Figure S4.** PXRD patterns of simulated based on the X-ray single-crystal diffraction data of **4** (lower) and for as-synthesized **4**(upper).

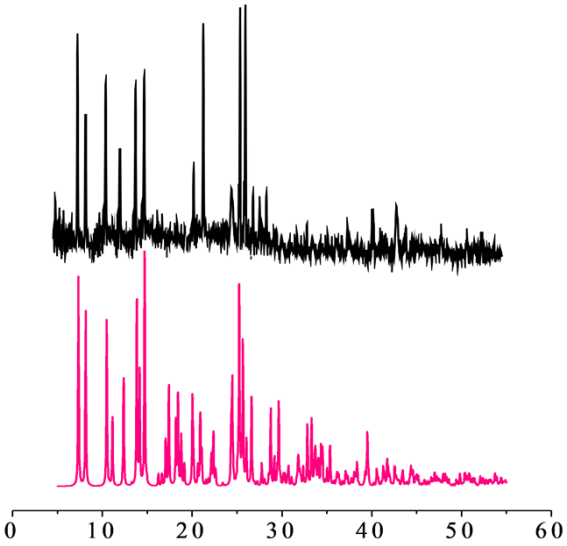


**Figure S5.** PXRD patterns of simulated based on the X-ray single-crystal diffraction data of **5** (lower) and for as-synthesized **5**(upper).

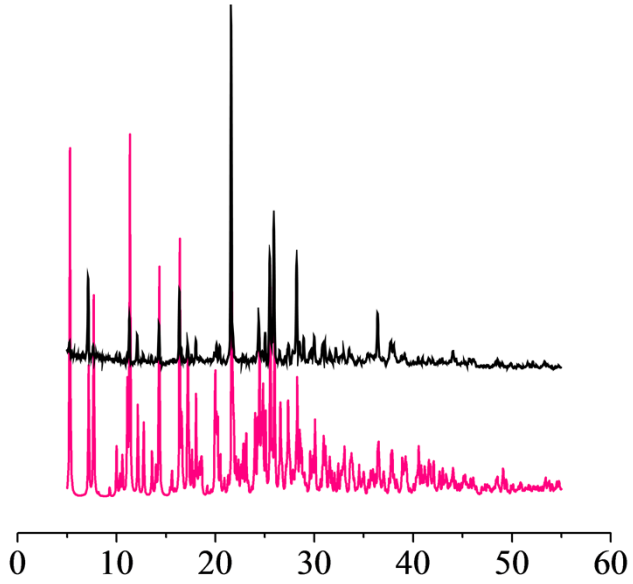


**Figure S6.** PXRD patterns of simulated based on the X-ray single-crystal diffraction data of **6** (lower) and for as-synthesized **6**(upper).

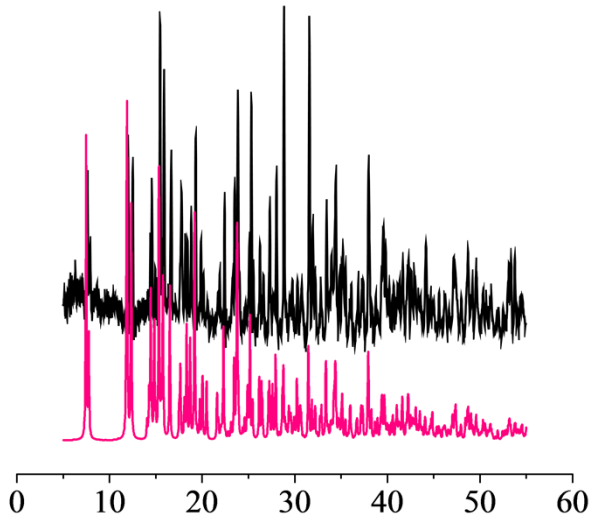


**Figure S7.** PXRD patterns of simulated based on the X-ray single-crystal diffraction data of **7** (lower) and for as-synthesized **7**(upper).

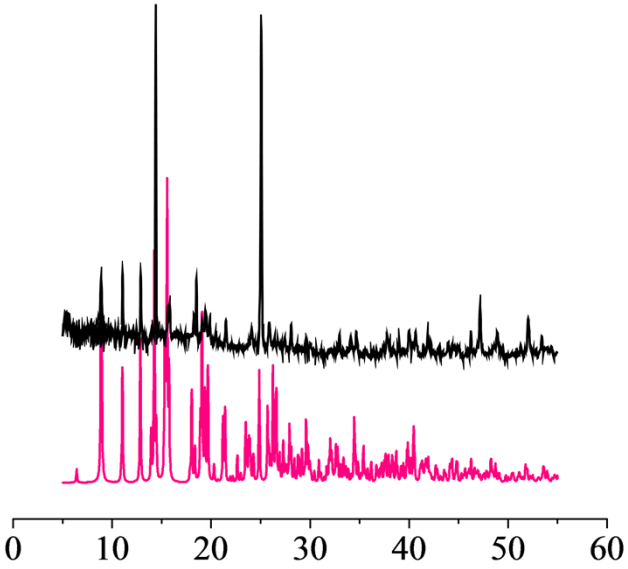


**Figure S8.** PXRD patterns of simulated based on the X-ray single-crystal diffraction data of **8** (lower) and for as-synthesized **8**(upper).

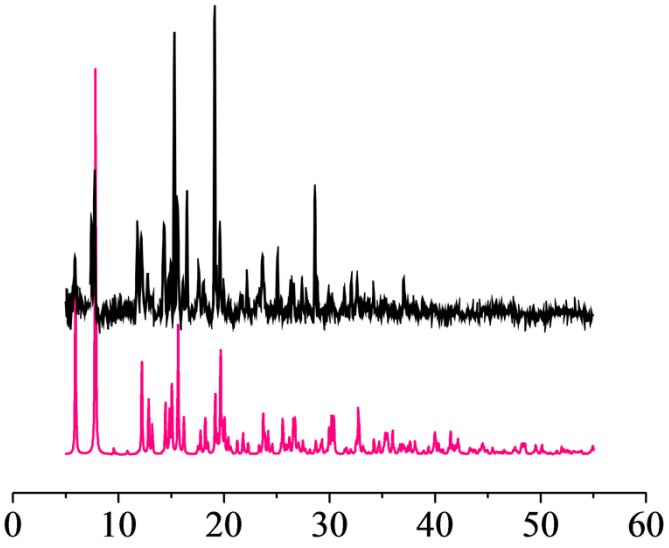


**Figure S9.** PXRD patterns of simulated based on the X-ray single-crystal diffraction data of **9** (lower) and for as-synthesized **9**(upper).

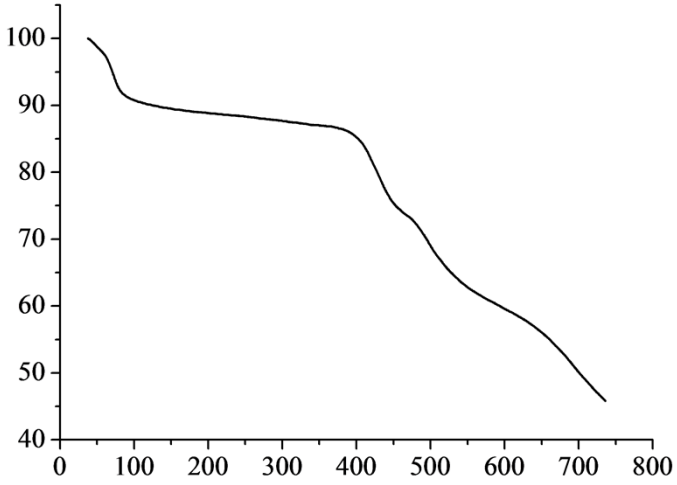


**Figure S10.** TG curve for **1**.

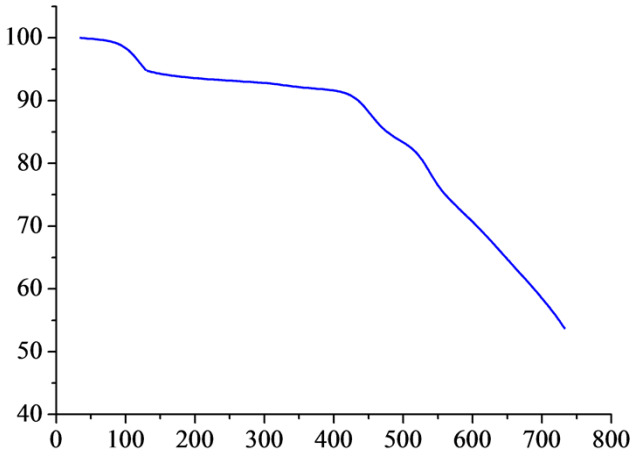


**Figure S11.** TG curve for **3**.

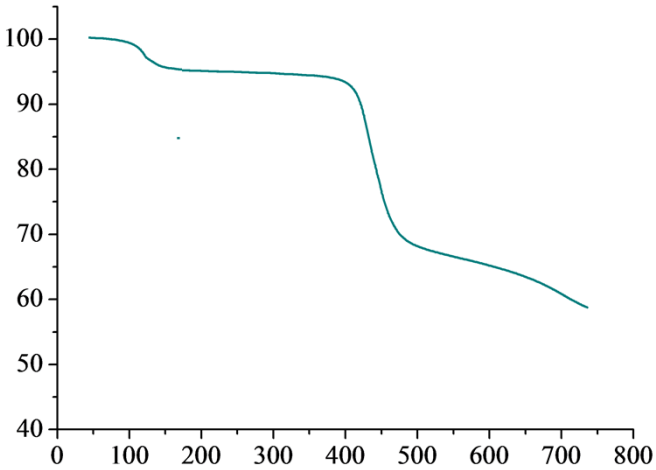


**Figure S12.** TG curve for **4**.

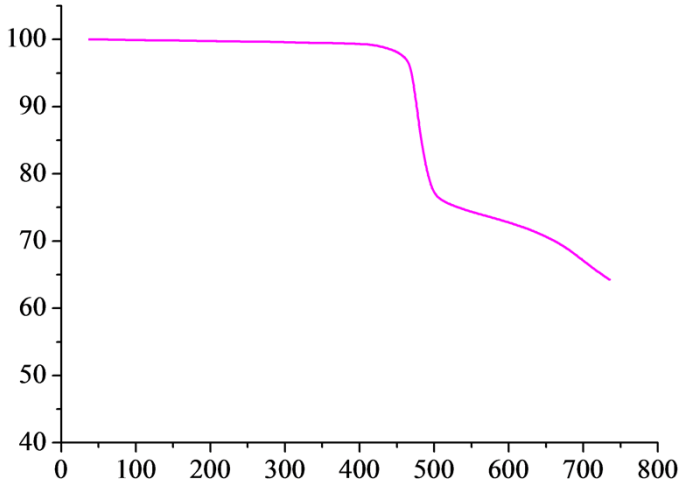


**Figure S13.** TG curve for **5**.

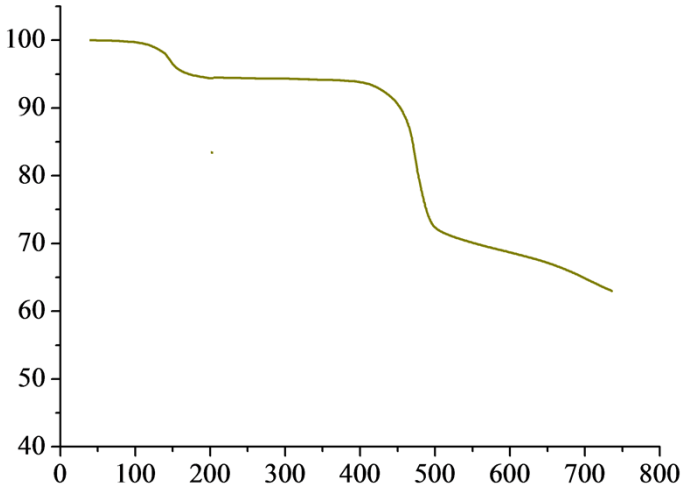


**Figure S14.** TG curve for **6**.

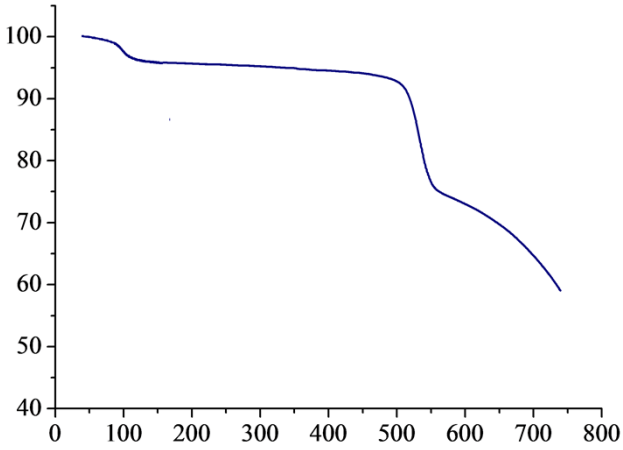


**Figure S15.** TG curve for **7**.

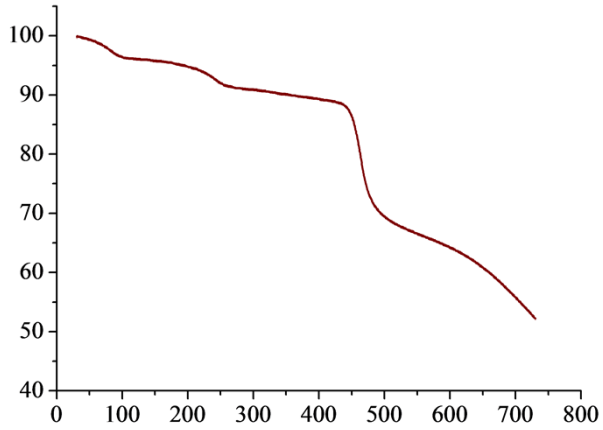


**Figure S16.** TG curve for **8**.

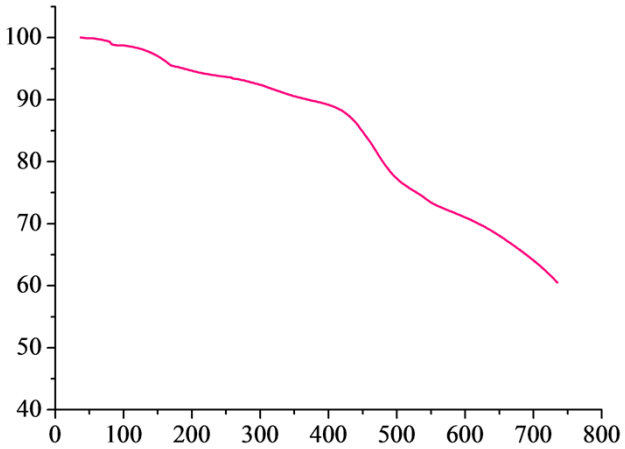


**Figure S17.** TG curve for **9**.