Supporting Information

Ligand-Directed Construction of Zn(II) Complexes from 0D Metallomacrocycle to 1D, 2D and 3D Coordination Polymers Based on N-Donor and *β*-Diketone Bifunctional Ligands

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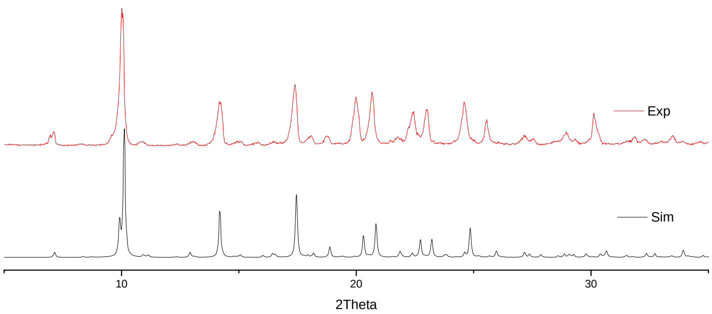

Figure S1. XRD patterns of **1** and the simulated pattern based on the single crystal **1**.

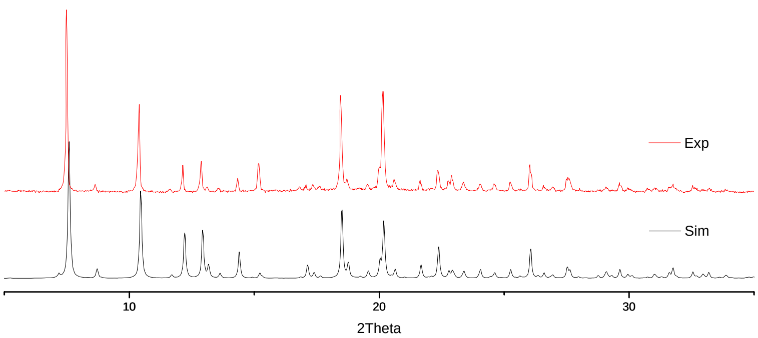

Figure S2. XRD patterns of **2** and the simulated pattern based on the single crystal **2**.

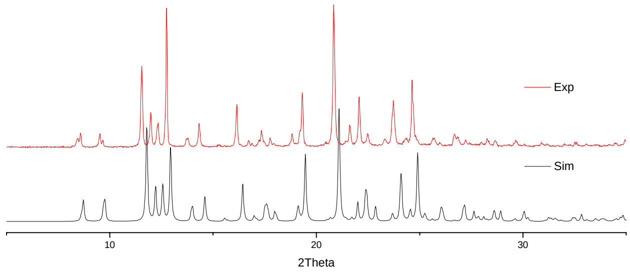

Figure S3. XRD patterns of **3** and the simulated pattern based on the single crystal **3**.

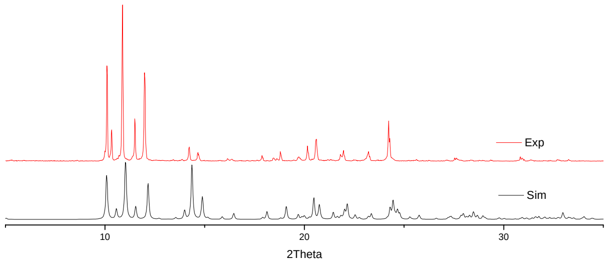

Figure S4. XRD patterns of **4** and the simulated pattern based on the single crystal **4**.

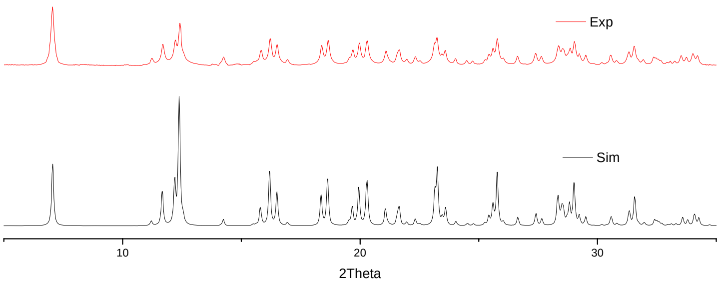

Figure S5. XRD patterns of **5** and the simulated pattern based on the single crystal **5**.

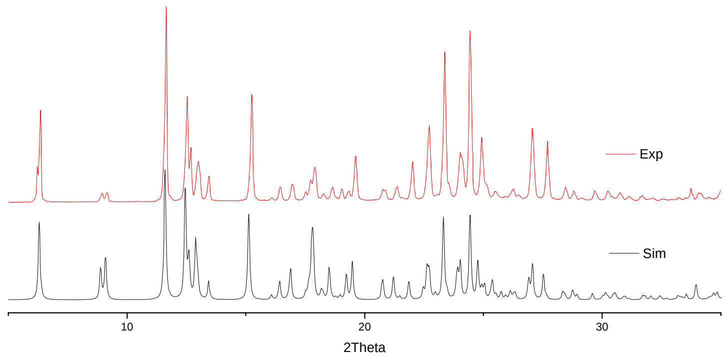

Figure S6. XRD patterns of **6** and the simulated pattern based on the single crystal **6**.

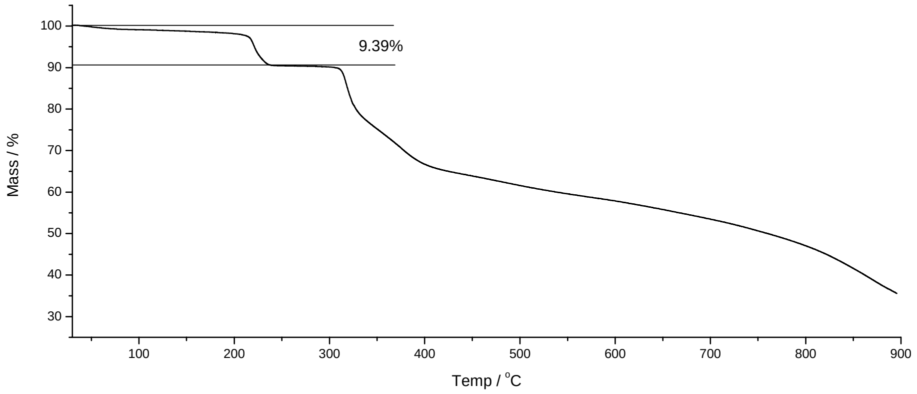

Figure S7. TGA of complex **1**.

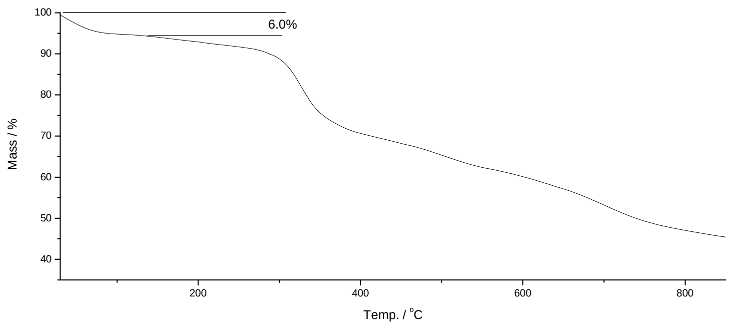

Figure S8. TGA of complex **2**.

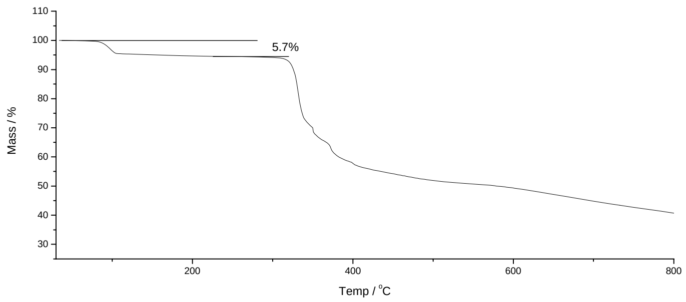

Figure S9. TGA of complex **4**.

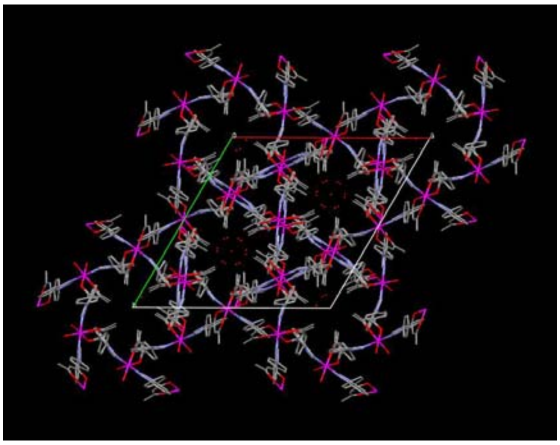

Figure S10. View of the 1D channel along the *c* axis in **2**.

Table S1. Bond lengths (Å) and angles (°) for **1** to **6**.

		Complex **1**			
N(1)–Zn(1)	2.135(3)	O(1)–Zn(1)	2.113(3)	O(5)–Zn(2)	2.122(4)
N(3)–Zn(1)	2.135(3)	O(2)–Zn(1)	2.060(2)	O(6)–Zn(2)	2.063(3)
N(5)–Zn(2)	2.147(3)	O(3)–Zn(1)	2.111(3)	O(7)–Zn(2)	2.095(3)
N(7)–Zn(2)	2.144(3)	O(4)–Zn(1)	2.059(2)	O(8)–Zn(2)	2.052(3)
O(2)–Zn(1)–O(4)	179.8(1)	O(2)–Zn(1)–N(1)	90.6(1)	O(6)–Zn(2)–O(5)	88.2(1)
O(2)–Zn(1)–O(3)	91.08(10)	O(4)–Zn(1)–N(1)	89.3(1)	O(8)–Zn(2)–N(5)	90.6(1)
O(4)–Zn(1)–O(3)	89.0(1)	O(3)–Zn(1)–N(1)	90.8(1)	O(7)–Zn(2)–N(5)	91.7(1)
O(2)–Zn(1)–O(1)	88.8(1)	O(1)–Zn(1)–N(1)	89.1(1)	O(6)–Zn(2)–N(5)	90.5(1)
O(4)–Zn(1)–O(1)	91.1(1)	N(3)–Zn(1)–N(1)	179.1(1)	O(5)–Zn(2)–N(5)	86.4(1)
O(3)–Zn(1)–O(1)	179.8(1)	O(8)–Zn(2)–O(7)	89.1(1)	O(8)–Zn(2)–N(7)	90.8(1)
O(2)–Zn(1)–N(3)	89.6(1)	O(8)–Zn(2)–O(6)	178.7(1)	O(7)–Zn(2)–N(7)	91.4(1)
O(4)–Zn(1)–N(3)	90.6(1)	O(7)–Zn(2)–O(6)	91.6(1)	O(6)–Zn(2)–N(7)	88.1(1)
O(3)–Zn(1)–N(3)	90.1(1)	O(8)–Zn(2)–O(5)	91.2(1)	O(5)–Zn(2)–N(7)	90.4(1)
O(1)–Zn(1)–N(3)	90.0(1)	O(7)–Zn(2)–O(5)	178.1(1)	N(5)–Zn(2)–N(7)	176.6(1)
		Complex **2**			

N(1)–Zn(1)	2.157(5)	O(1)–Zn(2)#1	2.073(5)	O(5)–Zn(1)	2.097(5)
N(3)–Zn(1)	2.175(5)	O(2)–Zn(2)#1	2.062(4)	O(6)–Zn(1)	2.076(4)
N(5)–Zn(2)	2.172(6)	O(3)–Zn(2)#2	2.093(5)	O(7)–Zn(1)#3	2.080(5)
N(7)–Zn(2)	2.189(5)	O(4)–Zn(2)#2	2.064(4)	O(8)–Zn(1)#3	2.071(4)
O(8)#4–Zn(1)–O(6)	177.4(2)	O(8)#4–Zn(1)–N(3)	92.55(19)	O(1)#5–Zn(2)–O(3)#6	179.01(19)
O(8)#4–Zn(1)–O(7)#4	88.49(18)	O(6)–Zn(1)–N(3)	89.33(19)	O(2)#5–Zn(2)–N(5)	93.20(18)
O(6)–Zn(1)–O(7)#4	89.76(19)	O(7)#4–Zn(1)–N(3)	90.3(2)	O(4)#6–Zn(2)–N(5)	88.46(18)
O(8)#4–Zn(1)–O(5)	93.08(18)	O(5)–Zn(1)–N(3)	89.3(2)	O(1)#5–Zn(2)–N(5)	91.0(2)
O(6)–Zn(1)–O(5)	88.68(18)	N(1)–Zn(1)–N(3)	177.3(2)	O(3)#6–Zn(2)–N(5)	89.6(2)
O(7)#4–Zn(1)–O(5)	178.41(16)	O(2)#5–Zn(2)–O(4)#6	177.83(19)	O(2)#5–Zn(2)–N(7)	86.82(17)
O(8)#4–Zn(1)–N(1)	86.61(18)	O(2)#5–Zn(2)–O(1)#5	88.71(17)	O(4)#6–Zn(2)–N(7)	91.58(18)
O(6)–Zn(1)–N(1)	91.59(19)	O(4)#6–Zn(2)–O(1)#5	89.86(18)	O(1)#5–Zn(2)–N(7)	91.3(2)
O(7)#4–Zn(1)–N(1)	92.2(2)	O(2)#5–Zn(2)–O(3)#6	92.05(17)	O(3)#6–Zn(2)–N(7)	88.1(2)
O(5)–Zn(1)–N(1)	88.1(2)	O(4)#6–Zn(2)–O(3)#6	89.35(18)	N(5)–Zn(2)–N(7)	177.7(2)
			Complex **3**		
N(2)–Zn(2)	2.274(3)	O(3)–Zn(2)	2.008(3)	O(6)–Zn(1)	1.977(2)
N(6)–Zn(1)	2.093(3)	O(4)–Zn(2)	2.045(3)	Zn(2)–O(4)#7	2.007(2)
O(1)–Zn(1)	2.045(2)	O(5)–Zn(1)	2.047(3)	Zn(2)–O(3)#7	2.086(3)
O(2)–Zn(1)	2.007(2)				
O(6)–Zn(1)–O(2)	151.30(11)	O(2)–Zn(1)–N(6)	97.18(10)	O(3)–Zn(2)–O(3)#7	154.07(6)
O(6)–Zn(1)–O(1)	87.67(10)	O(1)–Zn(1)–N(6)	104.66(11)	O(4)–Zn(2)–O(3)#7	84.84(11)
O(2)–Zn(1)–O(1)	87.68(10)	O(5)–Zn(1)–N(6)	94.20(11)	O(4)#7–Zn(2)–N(2)	97.31(11)
O(6)–Zn(1)–O(5)	88.44(10)	O(4)#7–Zn(2)–O(3)	87.92(11)	O(3)–Zn(2)–N(2)	98.51(14)
O(2)–Zn(1)–O(5)	86.77(10)	O(4)#7–Zn(2)–O(4)	153.73(6)	O(4)–Zn(2)–N(2)	108.97(11)
O(1)–Zn(1)–O(5)	160.86(11)	O(3)–Zn(2)–O(4)	88.35(11)	O(3)#7–Zn(2)–N(2)	107.37(14)
O(6)–Zn(1)–N(6)	111.39(10)	O(4)#7–Zn(2)–O(3)#7	87.24(11)		
			Complex **4**		
N(1)–Zn(2)	2.1603(18)	O(1)–Zn(1)	2.1106(14)	O(3)–Zn(2)	2.0808(14)
N(3)–Zn(1)	2.1740(18)	O(2)–Zn(1)	2.0582(14)	O(4)–Zn(2)	2.0769(14)
O(2)–Zn(1)–O(2)#8	180.0	O(2)–Zn(1)–N(3)	88.79(6)	O(3)#9–Zn(2)–O(3)	180.00(6)
O(2)–Zn(1)–O(1)	88.34(6)	O(2)#8–Zn(1)–N(3)	91.21(6)	O(4)–Zn(2)–N(1)	89.35(6)
O(2)#8–Zn(1)–O(1)	91.66(6)	O(1)–Zn(1)–N(3)	89.18(6)	O(4)#9–Zn(2)–N(1)	90.65(6)
O(2)–Zn(1)–O(1)#8	91.66(6)	O(1)#8–Zn(1)–N(3)	90.82(6)	O(3)#9–Zn(2)–N(1)	91.02(6)
O(2)#8–Zn(1)–O(1)#8	88.34(6)	N(3)#8–Zn(1)–N(3)	180.00(8)	O(3)–Zn(2)–N(1)	88.98(6)
O(1)–Zn(1)–O(1)#8	180.0	O(4)–Zn(2)–O(4)#9	180.00(6)	O(4)–Zn(2)–N(1)#9	90.65(6)
O(2)–Zn(1)–N(3)#8	91.21(6)	O(4)–Zn(2)–O(3)#9	89.85(6)	O(4)#9–Zn(2)–N(1)#9	89.35(6)
O(2)#8–Zn(1)–N(3)#8	88.79(6)	O(4)#9–Zn(2)–O(3)#9	90.15(6)	O(3)#9–Zn(2)–N(1)#9	88.98(6)
O(1)–Zn(1)–N(3)#8	90.82(6)	O(4)–Zn(2)–O(3)	90.15(6)	O(3)–Zn(2)–N(1)#9	91.02(6)

O(1)#8–Zn(1)–N(3)#8	89.18(6)	O(4)#9–Zn(2)–O(3)	89.85(6)	N(1)–Zn(2)–N(1)#9	180.00(8)
		Complex **5**			
N(1)–Zn(1)	2.2467(19)	O(1)–Zn(1)	2.0654(15)	O(2)–Zn(1)	2.0382(15)
O(2)–Zn(1)–O(2)#10	180.00(5)	O(1)#10–Zn(1)–O(1)	180.00(7)	O(2)–Zn(1)–N(1)	89.79(6)
O(2)–Zn(1)–O(1)#10	89.97(6)	O(2)–Zn(1)–N(1)#10	90.21(6)	O(2)#10–Zn(1)–N(1)	90.21(6)
O(2)#10–Zn(1)–O(1)#10	90.03(6)	O(2)#10–Zn(1)–N(1)#10	89.79(6)	O(1)#10–Zn(1)–N(1)	93.42(6)
O(2)–Zn(1)–O(1)	90.03(6)	O(1)#10–Zn(1)–N(1)#10	86.58(6)	O(1)–Zn(1)–N(1)	86.58(6)
O(2)#10–Zn(1)–O(1)	89.97(6)	O(1)–Zn(1)–N(1)#10	93.42(6)	N(1)#10–Zn(1)–N(1)	180.0
		Complex **6**			
O(1)–Zn(1)	2.048(8)	O(3)–Zn(1)	2.001(7)	Zn(1)–N(4)#11	2.085(9)
O(2)–Zn(1)	2.073(7)	O(4)–Zn(1)	2.036(8)		
O(3)–Zn(1)–O(4)	89.6(3)	O(4)–Zn(1)–O(2)	165.5(2)	O(4)–Zn(1)–N(4)#11	104.1(2)
O(3)–Zn(1)–O(1)	145.6(3)	O(1)–Zn(1)–O(2)	87.4(3)	O(1)–Zn(1)–N(4)#11	103.9(3)
O(4)–Zn(1)–O(1)	84.5(3)	O(3)–Zn(1)–N(4)#11	110.4(3)	O(2)–Zn(1)–N(4)#11	89.5(3)
O(3)–Zn(1)–O(2)	90.3(3)				

Symmetry transformations used to generate equivalent atoms:

#1 $-y+4/3$, $x-y-1/3$, $z-1/3$; #2 $-y+1$, $x-y-1$, z; #3 $x+2/3$, $y+1/3$, $z+1/3$; #4 $x-2/3$, $y-1/3$, $z-1/3$; #5 $-x+y+5/3$, $-x+4/3$, $z+1/3$; #6 $-x+y+2$, $-x+1$, z; #7 $-x$, $-y+1$, $-z$; #8 $-x$, $-y+1$, $-z+1$; #9 $-x$, $-y+1$, $-z$; #10 $-x$, $-y$, $-z$; #11 $-x+1$, $-y+1$, $-z+1$.