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A series of coordination polymers assembled from d^{10} metals and a new multidentate N-donor ligand: syntheses, structures, and photoluminescent properties

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

Cd(1)-O(8)	2.211(3)	Cd(1)-O(1W)	2.305(3)
Cd(1)-O(7)#1	2.380(3)	Cd(1)-O(6)#1	2.394(3)
Cd(1)-N(8)#2	2.411(3)	Cd(1)-N(6)#3	2.411(3)
Cd(2)-N(2)	2.253(3)	Cd(2)-O(4)	2.325(3)
Cd(2)-N(5)#3	2.331(4)	Cd(2)-O(9)	2.341(3)
Cd(2)-O(5)	2.384(3)	Cd(2)-Cl(1)	2.5629(12)
Na(1)-O(2W)	1.935(6)	Na(1)-Cl(1)	2.5664(13)
Na(1)-O(10)	2.846(11)	O(8)-Cd(1)-O(1W)	100.43(12)
O(8)-Cd(1)-O(7)#1	100.50(12)	O(1W)-Cd(1)-O(7)#1	158.15(12)
O(8)-Cd(1)-O(6)#1	153.08(12)	O(1W)-Cd(1)-O(6)#1	103.49(12)
O(7)#1-Cd(1)-O(6)#1	54.73(11)	O(8)-Cd(1)-N(8)#2	84.40(12)
O(1W)-Cd(1)-N(8)#2	80.04(12)	O(7)#1-Cd(1)-N(8)#2	95.84(11)
O(6)#1-Cd(1)-N(8)#2	87.73(13)	O(8)-Cd(1)-N(6)#3	117.30(13)
O(1W)-Cd(1)-N(6)#3	83.28(12)	O(7)#1-Cd(1)-N(6)#3	92.65(12)
O(6)#1-Cd(1)-N(6)#3	77.94(14)	N(8)#2-Cd(1)-N(6)#3	154.81(13)
N(2)-Cd(2)-O(4)	110.34(12)	N(2)-Cd(2)-N(5)#3	107.31(13)
O(4)-Cd(2)-N(5)#3	139.99(11)	N(2)-Cd(2)-O(9)	83.27(12)
O(4)-Cd(2)-O(9)	88.72(11)	N(5)#3-Cd(2)-O(9)	82.64(11)
N(2)-Cd(2)-O(5)	164.62(13)	O(4)-Cd(2)-O(5)	55.69(10)
N(5)#3-Cd(2)-O(5)	85.14(12)	O(9)-Cd(2)-O(5)	89.62(11)
N(2)-Cd(2)-Cl(1)	91.05(10)	O(4)-Cd(2)-Cl(1)	99.16(9)
N(5)#3-Cd(2)-Cl(1)	93.14(9)	O(9)-Cd(2)-Cl(1)	171.54(9)
O(5)-Cd(2)-Cl(1)	97.35(8)	O(2W)-Na(1)-Cl(1)#4	92.4(2)

O(2W)#4-Na(1)-Cl(1)	87.6(2)	O(2W)-Na(1)-O(10)#4	102.2(3)
O(2W)#4-Na(1)-O(10)#4	77.8(3)	Cl(1)#4-Na(1)-O(10)#4	93.7(2)
Cl(1)-Na(1)-O(10)#4	86.3(2)		

Symmetry transformations used to generate equivalent atoms: [#1] x + 1, y, z; [#2] -x + 2, -y, - z + 2; [#3] x - 1, y, z - 1; [#4] -x, -y + 1, -z + 1; [#5] -x + 2, -y + 1, -z + 2; [#6] x - 1, y, z; [#7] -x, -y, -z + 2; [#8] -x + 1, -y + 1, -z + 1; [#9] x + 1, y, z + 1.

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

Cd(1)-O(8)	2.212(5)	Cd(1)-O(1W)	2.305(5)
Cd(1)-O(4)	2.375(5)	Cd(1)-O(5)	2.386(5)
Cd(1)-N(2)#1	2.404(6)	Cd(1)-N(5)	2.430(6)
Cd(2)-N(6)	2.317(6)	Cd(2)-N(8)#2	2.225(6)
Cd(2)-O(7)#3	2.332(5)	Cd(2)-O(9)	2.319(5)
Cd(2)-O(10)	2.510(12)	Cd(2)-O(6)#3	2.346(5)
O(8)-Cd(1)-O(1W)	100.5(2)	O(8)-Cd(1)-O(4)	153.1(2)
O(1W)-Cd(1)-O(4)	103.7(2)	O(8)-Cd(1)-O(5)	100.3(2)
O(1W)-Cd(1)-O(5)	158.4(2)	O(4)-Cd(1)-O(5)	54.79(19)
O(8)-Cd(1)-N(2)#1	84.6(2)	O(1W)-Cd(1)-N(2)#1	80.0(2)
O(4)-Cd(1)-N(2)#1	88.2(2)	O(5)-Cd(1)-N(2)#1	96.05(19)
O(8)-Cd(1)-N(5)	117.6(2)	O(1W)-Cd(1)-N(5)	82.5(2)
O(4)-Cd(1)-N(5)	77.4(2)	O(5)-Cd(1)-N(5)	93.1(2)
N(2)#1-Cd(1)-N(5)	154.1(2)	N(8)#2-Cd(2)-N(6)	106.2(2)
N(8)#2-Cd(2)-O(9)	84.6(2)	N(6)-Cd(2)-O(9)	84.18(19)
N(8)#2-Cd(2)-O(7)#3	110.3(2)	N(6)-Cd(2)-O(7)#3	142.5(2)
O(9)-Cd(2)-O(7)#3	90.92(19)	N(8)#2-Cd(2)-O(6)#3	165.4(2)

N(6)-Cd(2)-O(6)#3	87.1(2)	O(9)-Cd(2)-O(6)#3	90.82(19)
O(7)#3-Cd(2)-O(6)#3	55.80(18)	N(8)#2-Cd(2)-O(10)	86.2(3)
N(6)-Cd(2)-O(10)	90.7(3)	O(9)-Cd(2)-O(10)	167.8(3)
O(7)#3-Cd(2)-O(10)	99.7(3)	O(6)#3-Cd(2)-O(10)	100.0(3)

Symmetry transformations used to generate equivalent atoms: [#1] -x + 2, -y, -z + 1; [#2] x + 1, y, z + 1; [#3] x - 1, y, z; [#4] -x + 1,-y + 1, -z; [#5] x + 1, y, z; [#6] -x + 1, -y, -z + 2; [#7] x - 1, y, z - 1.

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

Zn(1)-O(7)	1.9494(18)	Zn(1)-O(5)	1.950(2)
Zn(1)-N(2)	2.004(2)	Zn(1)-N(8)#1	2.014(3)
O(7)-Zn(1)-O(5)	111.17(9)	O(7)-Zn(1)-N(2)	104.80(8)
O(5)-Zn(1)-N(2)	115.12(10)	O(7)-Zn(1)-N(8)#1	115.95(10)
O(5)-Zn(1)-N(8)#1	106.80(10)	N(2)-Zn(1)-N(8)#1	103.02(10)

Symmetry transformations used to generate equivalent atoms: [#1] x + 1, y, z + 1; [#2] -x - 1, -y, -z; [#3] -x + 2, -y, -z + 1; [#4] -x + 1, -y - 1, -z; [#5] -x, -y - 1, -z + 1; [#6] x - 1, y, z - 1; [#7] -x + 1, -y, -z + 1.

Table S4. Selected bond distances (Å) and angles (°) for **4**.

Zn(1)-O(6)	1.912(5)	Zn(1)-O(4)	1.957(5)
Zn(1)-N(9)#1	1.999(6)	Zn(1)-N(2)	2.022(6)
O(6)-Zn(1)-O(4)	95.0(3)	O(6)-Zn(1)-N(9)#1	117.6(2)
O(4)-Zn(1)-N(9)#1	115.5(3)	O(6)-Zn(1)-N(2)	117.9(2)
O(4)-Zn(1)-N(2)	108.8(3)	N(9)#1-Zn(1)-N(2)	102.4(3)

Symmetry transformations used to generate equivalent atoms: [#1] x - 1, y, z - 1; [#2] -x + 2, -y + 1, -z + 2; [#3] -x + 3, -y + 1, -z + 1; [#4] -x + 2, -y, -z; [#5] x + 1, y, z + 1.

Table S5. Selected bond distances (Å) and angles (°) for **5**.

Zn(1)-O(7)	1.956(5)	Zn(1)-O(4)	2.001(6)
Zn(1)-N(6)	2.019(4)	Zn(1)-N(2)#1	2.021(4)
Zn(1)-O(5)	2.248(19)	O(7)-Zn(1)-O(4)	89.9(3)
O(7)-Zn(1)-N(6)	120.1(2)	O(4)-Zn(1)-N(6)	103.2(2)
O(7)-Zn(1)-N(2)#1	109.55(19)	O(4)-Zn(1)-N(2)#1	131.1(3)
N(6)-Zn(1)-N(2)#1	104.24(17)	O(7)-Zn(1)-O(5)	130.1(5)
O(4)-Zn(1)-O(5)	48.5(6)	N(6)-Zn(1)-O(5)	98.5(5)
N(2)#1-Zn(1)-O(5)	87.9(6)		

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ -x, -y, -z + 2; $^{\#2}$ -x + 1, -y + 1, -z + 2.

Table S6. Selected bond distances (Å) and angles (°) for **6**.

Zn(1)-O(4)	1.950(4)	Zn(1)-O(6)	1.966(4)
Zn(1)-N(5)	2.015(4)	Zn(1)-N(3)#1	2.022(4)
O(4)-Zn(1)-O(6)	95.73(17)	O(4)-Zn(1)-N(5)	110.19(17)
O(6)-Zn(1)-N(5)	119.52(18)	O(4)-Zn(1)-N(3)#1	119.52(17)
O(6)-Zn(1)-N(3)#1	107.16(17)	N(5)-Zn(1)-N(3)#1	105.38(15)

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ -x + 2, -y, -z; $^{\#2}$ -x + 3, -y, -z + 1.

Table S7. Selected bond distances (Å) and angles (°) for **7**.

Cd(1)-O(9)	2.266(4)	Cd(1)-O(9)#1	2.298(4)
Cd(1)-O(7)#2	2.322(4)	Cd(1)-O(1W)	2.342(4)
Cd(1)-N(5)	2.348(5)	Cd(1)-N(9)#1	2.356(5)
Cd(2)-O(9)	2.221(4)	Cd(2)-O(5)	2.232(5)

Cd(2)-O(3W)	2.279(14)	Cd(2)-O(2W)	2.283(5)
Cd(2)-O(12W)	2.35(3)	Cd(2)-N(8)	2.373(6)
Cd(2)-N(6)	2.526(6)	O(9)-Cd(1)-O(9)#1	82.18(15)
O(9)-Cd(1)-O(7)#2	94.00(15)	O(9)#1-Cd(1)-O(7)#2	175.35(13)
O(9)-Cd(1)-O(1W)	168.24(14)	O(9)#1-Cd(1)-O(1W)	90.23(13)
O(7)#2-Cd(1)-O(1W)	93.96(14)	O(9)-Cd(1)-N(5)	86.97(15)
O(9)#1-Cd(1)-N(5)	94.90(16)	O(7)#2-Cd(1)-N(5)	87.51(17)
O(1W)-Cd(1)-N(5)	84.73(16)	O(9)-Cd(1)-N(9)#1	103.16(15)
O(9)#1-Cd(1)-N(9)#1	87.32(15)	O(7)#2-Cd(1)-N(9)#1	90.99(16)
O(1W)-Cd(1)-N(9)#1	85.35(16)	N(5)-Cd(1)-N(9)#1	169.84(17)
O(9)-Cd(2)-O(5)	105.19(18)	O(9)-Cd(2)-O(3W)	166.2(4)
O(5)-Cd(2)-O(3W)	85.9(4)	O(9)-Cd(2)-O(2W)	89.59(17)
O(5)-Cd(2)-O(2W)	90.1(2)	O(3W)-Cd(2)-O(2W)	98.7(3)
O(9)-Cd(2)-O(12W)	161.5(6)	O(5)-Cd(2)-O(12W)	92.9(7)
O(3W)-Cd(2)-O(12W)	14.1(5)	O(2W)-Cd(2)-O(12W)	86.5(6)
O(9)-Cd(2)-N(8)	89.86(16)	O(5)-Cd(2)-N(8)	108.98(19)
O(3W)-Cd(2)-N(8)	78.7(3)	O(2W)-Cd(2)-N(8)	160.4(2)
O(12W)-Cd(2)-N(8)	87.8(7)	O(9)-Cd(2)-N(6)	85.38(15)
O(5)-Cd(2)-N(6)	167.0(2)	O(3W)-Cd(2)-N(6)	84.9(4)
O(2W)-Cd(2)-N(6)	82.3(2)	O(12W)-Cd(2)-N(6)	76.1(6)
N(8)-Cd(2)-N(6)	78.1(2)		

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ -x + 3/2, -y + 1/2, -z; $^{\#2}$ -x + 2, y, -z + 1/2; $^{\#3}$ -x + 1, y, -z - 1/2; $^{\#4}$ -x + 2, y, -z - 1/2.

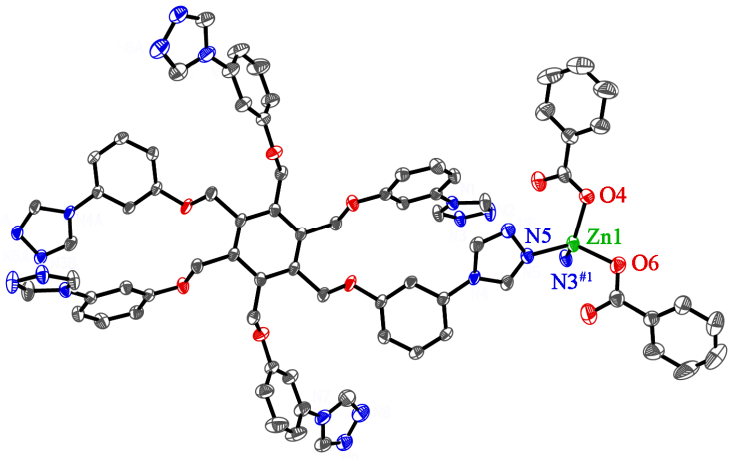

Fig. S1 (a) ORTEP view of **6** showing the local coordination environment of Zn(II) ion with hydrogen atoms omitted for clarity (30% probability displacement ellipsoids). Symmetry codes: #1 -x + 2, -y, -z.

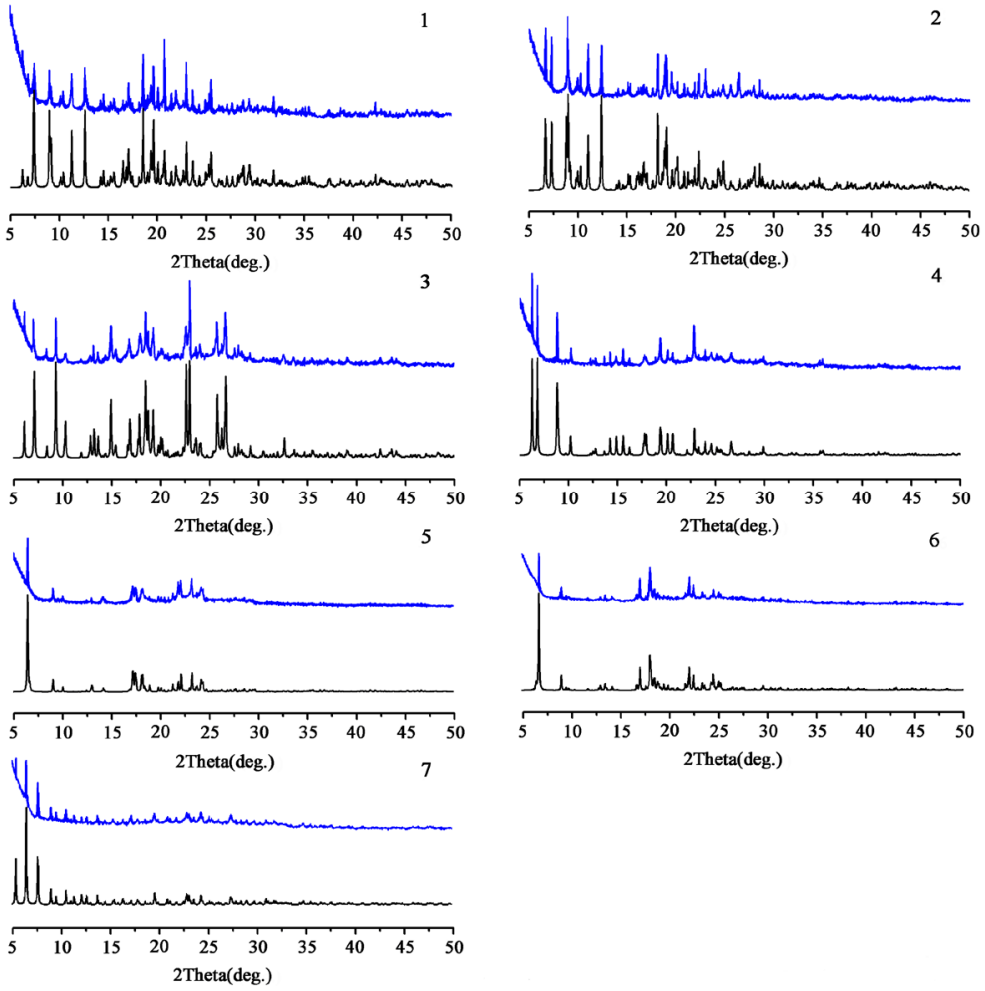

Fig. S2 The simulated (black) and experimental (blue) PXRD patterns for compounds **1**-**7**.