Electronic Supplementary Material (ESI) for RSC Advances.

Non-hydrothermal synthesis, structural characterization and thermochemistry of water soluble and neutral coordination polymers of Zn(II) and Cd(II): precursors for the submicron-sized crystalline ZnO/CdO

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Electronic Supplementary Information

Table S1. Selected bond distances and angles for **1**, **2** and **3**.

Bond distances (Å)

1		**2**		**3**	
Zn1-N1	2.122(5)	Zn1-N1	2.0934(18)	Zn1-N1	2.028(3)
Zn1-N2	2.206(5)	Zn1-N2	2.241(2)	Zn1-N2	2.440(3)
Zn1-N3	2.100(5)	Zn1-N3	2.1249(19)	Zn1-N3	2.055(3)
Zn1-O2	2.013(4)	Zn1-O1	2.0317(16)	Zn1-O1	1.986(3)
Zn1-O5	1.974(4)	Zn1-O3	1.9834(16)	Zn1-O4	2.083(3)
C18-C18$^{\#2}$	1.177(11)	C16-C16$^{\#1}$	1.187(5)	C2-C3	1.187(5)
C22-C22$^{\#1}$	1.175(11)	C18-C18$^{\#2}$	1.192(4)		
#1	-x+1, -y+1, -z+1	#1	-x, -y, -z+1		
#2	-x+2, -y, -z+1	#2	-x+1, -y+1, -z+1		

Bond angles (°)

1		**2**		**3**	
O5-Zn1-O2	108.22(19)	O3-Zn1-O1	108.46(8)	O1-Zn1-N1	134.12(13)
O2-Zn1-N3	97.34(18)	O1-Zn1-N1	96.57(7)	N1-Zn1-N3	116.96(13)
O2-Zn1-N1	96.9(2)	O1-Zn1-N3	96.10(7)	N1-Zn1-O4	96.52(11)
O5-Zn1-N2	109.2(2)	O3-Zn1-N2	114.33(7)	O1-Zn1-N2	101.71(11)
N3-Zn1-N2	77.2(2)	N1-Zn1-N2	78.13(7)	N3-Zn1-N2	76.15(12)
O5-Zn1-N3	108.3(2)	O3-Zn1-N1	108.91(7)	O1-Zn1-N3	106.88(13)
O5-Zn1-N1	89.4(2)	O3-Zn1-N3	88.89(7)	O1-Zn1-O4	90.77(11)
N3-Zn1-N1	152.4(2)	N1-Zn1-N3	153.48(8)	N3-Zn1-O4	96.99(12)
O2-Zn1-N2	142.0(2)	O1-Zn1-N2	136.29(7)	N1-Zn1-N2	77.39(12)
N1-Zn1-N2	77.0(2)	N3-Zn1-N2	76.60(7)	O4-Zn1-N2	167.03(10)

Table S2. Selected bond distances and angles for **6**.

Bond distances (Å)

Cd1-O1	2.462(5)	Cd2-O3$^{\#1}$	2.602(8)	Cd3-O10	2.241(4)	Cd4-O11$^{\#2}$	2.427(5)
Cd1-O2	2.392(4)	Cd2-O4$^{\#1}$	2.308(6)	Cd3-O13	2.212(4)	Cd4-O12$^{\#2}$	2.405(4)
Cd1-O5	2.267(4)	Cd2-O7	2.542(5)	Cd3-N7	2.325(4)	Cd4-O15	2.315(5)
Cd1-O6	2.615(4)	Cd2-O8	2.255(6)	Cd3-N8	2.383(5)	Cd4-O16	2.477(5)
Cd1-N1	2.414(5)	Cd2-N4	2.332(6)	Cd3-N9	2.298(4)	Cd4-N10	2.296(4)
Cd1-N2	2.337(5)	Cd2-N5	2.425(5)	C56-C57	1.196(8)	Cd4-N11	2.465(5)
Cd1-N3	2.323(4)	Cd2-N6	2.290(5)			Cd4-N12	2.333(5)
C20-C21	1.178(8)						

Bond angles (°)

O5-Cd1-N3	111.14(18)	O5-Cd1-N2	91.32(18)
N3-Cd1-N2	144.37(17)	O5-Cd1-O2	85.36(16)
N3-Cd1-O2	82.69(17)	N2-Cd1-O2	127.95(17)
O5-Cd1-N1	136.06(16)	N3-Cd1-N1	72.99(17)
N2-Cd1-N1	71.70(17)	O2-Cd1-N1	137.16(17)
O5-Cd1-O1	116.89(19)	N3-Cd1-O1	107.64(18)
N2-Cd1-O1	84.24(17)	O2-Cd1-O1	52.74(16)
N1-Cd1-O1	101.76(18)	O5-Cd1-O6	52.76(14)
N3-Cd1-O6	87.91(15)	N2-Cd1-O6	84.25(15)
O2-Cd1-O6	129.80(15)	N1-Cd1-O6	84.71(15)
O1-Cd1-O6	164.27(18)	O5-Cd1-C15	102.09(16)
N3-Cd1-C15	95.64(17)	N2-Cd1-C15	106.61(18)
O2-Cd1-C15	26.50(16)	N1-Cd1-C15	121.40(17)
O1-Cd1-C15	26.24(16)	O6-Cd1-C15	153.57(15)
O8-Cd2-N6	106.9(3)	O8-Cd2-O4$^{\#1}$	118.4(3)
N6-Cd2-O4$^{\#1}$	105.0(3)	O8-Cd2-N4	97.3(3)
N6-Cd2-N4	144.96(19)	O4$^{\#1}$-Cd2-N4	84.2(2)
O8-Cd2-N5	140.69(19)	N6-Cd2-N5	73.57(16)
O4$^{\#1}$-Cd2-N5	98.3(2)	N4-Cd2-N5	71.66(19)
O8-Cd2-O7	51.44(19)	N6-Cd2-O7	89.66(17)
O4$^{\#1}$-Cd2-O7	164.7(3)	N4-Cd2-O7	85.99(19)
N5-Cd2-O7	89.60(16)	O8-Cd2-O3$^{\#1}$	76.5(2)
N6-Cd2-O3$^{\#1}$	97.3(3)	O4$^{\#1}$-Cd2-O3$^{\#1}$	48.2(2)
N4-Cd2-O3$^{\#1}$	112.9(3)	N5-Cd2-O3$^{\#1}$	142.8(2)
O7-Cd2-O3$^{\#1}$	126.98(19)	O8-Cd2-C22	25.7(2)
N6-Cd2-C22	98.90(19)	O4$^{\#1}$-Cd2-C22	143.2(3)

N4-Cd2-C22	92.0(2)	N5-Cd2-C22	115.22(19)
O7-Cd2-C22	25.74(17)	O3$^{\#1}$-Cd2-C22	101.7(2)
O13-Cd3-O10	109.74(18)	O13-Cd3-N9	108.98(17)
O10-Cd3-N9	105.82(17)	O13-Cd3-N7	89.22(16)
O10-Cd3-N7	93.64(17)	N9-Cd3-N7	146.22(16)
O13-Cd3-N8	110.26(18)	O10-Cd3-N8	137.56(16)
N9-Cd3-N8	73.63(15)	N7-Cd3-N8	73.40(16)
N10-Cd4-O15	128.18(18)	N10-Cd4-N12	142.78(18)
O15-Cd4-N12	83.2(2)	N10-Cd4-O12$^{\#2}$	92.07(17)
O15-Cd4-O12$^{\#2}$	119.06(19)	N12-Cd4-O12$^{\#2}$	87.10(17)
N10-Cd4-O11$^{\#2}$	87.25(19)	O15-Cd4-O11$^{\#2}$	81.40(19)
N12-Cd4-O11$^{\#2}$	120.7(2)	O12$^{\#2}$-Cd4-O11$^{\#2}$	53.70(17)
N10-Cd4-N11	72.50(16)	O15-Cd4-N11	136.97(19)
N12-Cd4-N11	70.42(17)	O12$^{\#2}$-Cd4-N11	93.52(17)
O11$^{\#2}$-Cd4-N11	141.29(15)	N10-Cd4-O16	84.95(17)
O15-Cd4-O16	52.54(17)	N12-Cd4-O16	105.8(2)
O12$^{\#2}$-Cd4-O16	162.3(2)	O11$^{\#2}$-Cd4-O16	108.6(2)
N11-Cd4-O16	102.17(18)		

#1 x, y, z+1, #2 x, y-1, z

Table S3. Selected bond distances and angles for **7**.

Bond distances (Å)

Cd1-O1	2.260(3)	Cd1-N1	2.513(4)
Cd1-O3	2.308(3)	Cd1-N2	2.248(4)
Cd1-O4	2.486(3)	Cd1-N3	2.267(4)
C18-C19	1.176(6)		

Bond angles (°)

N2-Cd1-O1	97.72(14)	N2-Cd1-N3	110.74(15)
O1-Cd1-N3	94.27(14)	N2-Cd1-O3	147.73(14)
O1-Cd1-O3	86.93(12)	N3-Cd1-O3	100.66(14)
N2-Cd1-O4	93.78(14)	O1-Cd1-O4	87.46(12)
N3-Cd1-O4	154.90(14)	O3-Cd1-O4	54.37(13)
N2-Cd1-N1	74.17(14)	O1-Cd1-N1	160.70(12)
N3-Cd1-N1	73.11(14)	O3-Cd1-N1	109.40(12)
C19-C18-C17	175.2(6)	C18-C19-C20$^{\#1}$	176.7(6)
#1	-x+5/2, y-1/2, z		

Table S4. Selected bond distances and angles for **8**.

Bond distances (Å)

Cd1-N1	2.348(3)	Cd1-O2	2.250(2)
Cd1-N2	2.293(2)	Cd1-O4	2.486(2)
Cd1-N3	2.449(2)	Cd1-O5	2.292(2)
C17-C19	1.184(4)		

Bond angles (°)

O2-Cd1-O5	89.96(9)	O2-Cd1-N2	98.20(9)
O5-Cd1-N2	156.32(9)	O2-Cd1-N1	83.73(10)
O5-Cd1-N1	90.72(9)	N2-Cd1-N1	112.17(9)
O2-Cd1-N3	146.75(9)	O5-Cd1-N3	111.31(8)
N2-Cd1-N3	72.72(8)	N1-Cd1-N3	71.23(8)
O2-Cd1-O4	124.21(9)	O5-Cd1-O4	54.39(8)
N2-Cd1-O4	103.47(8)	N1-Cd1-O4	130.70(9)
N3-Cd1-O4	88.99(7)	O2-Cd1-C18	107.10(9)
C17-C19-C18	174.5(3)		

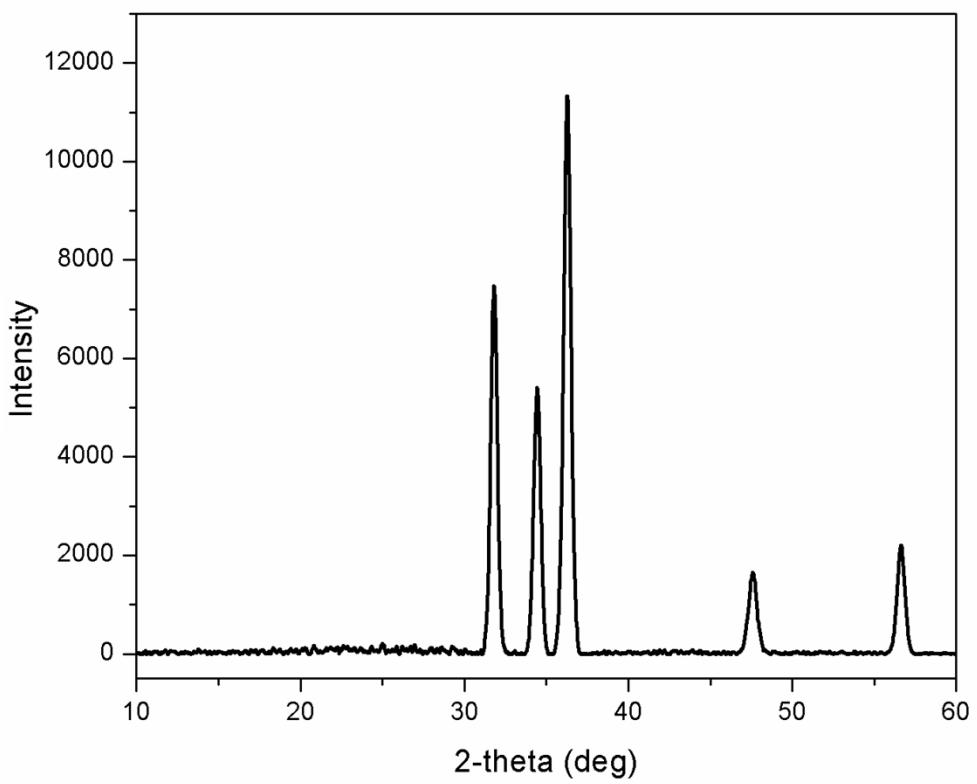


Fig S1. PXRD pattern of ZnO prepared from **3**.

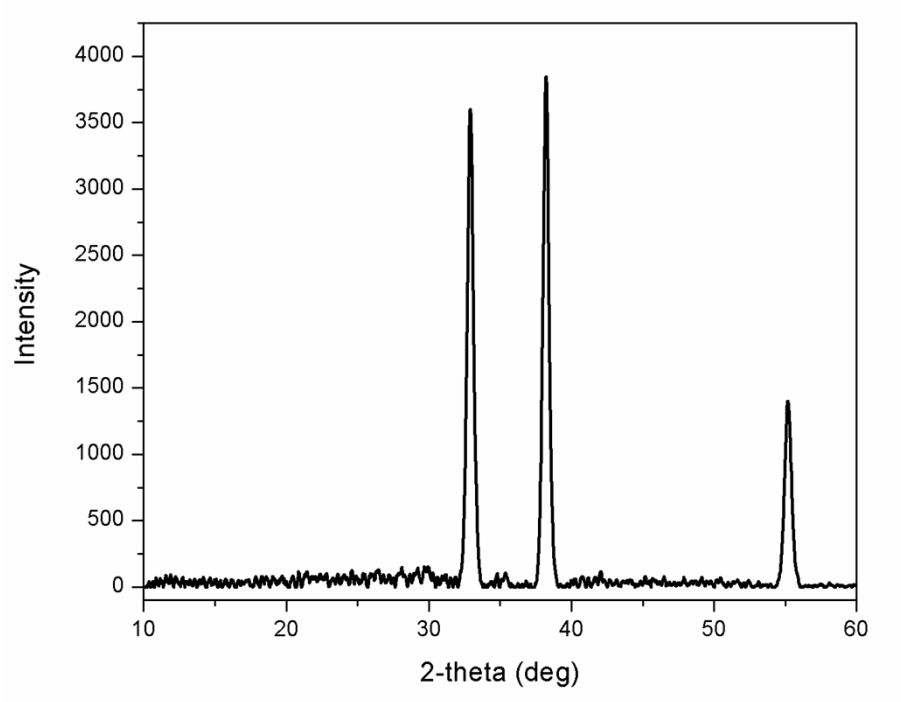
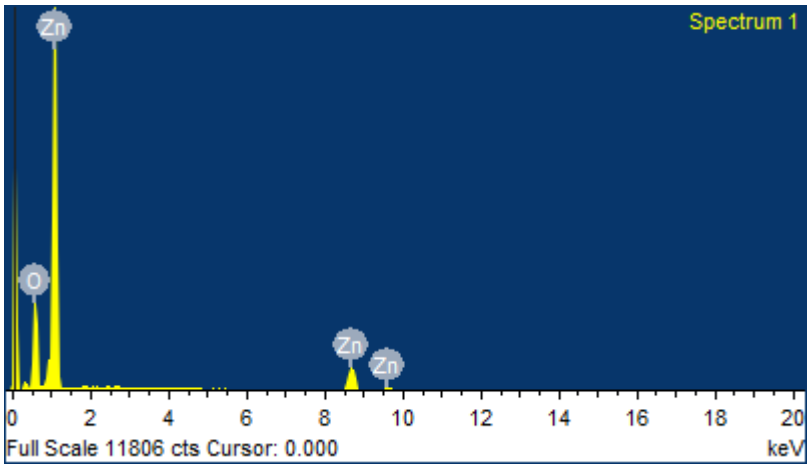


Fig S2. PXRD pattern of CdO prepared from **7**.

Element	Weight%	Atomic%
O K	22.47	54.22
Zn L	77.53	45.78
Totals	100	



Element	Weight%	Atomic%
C K	4.08	22.27
O K	6.21	25.43
Cd L	89.71	52.29
Totals	100	

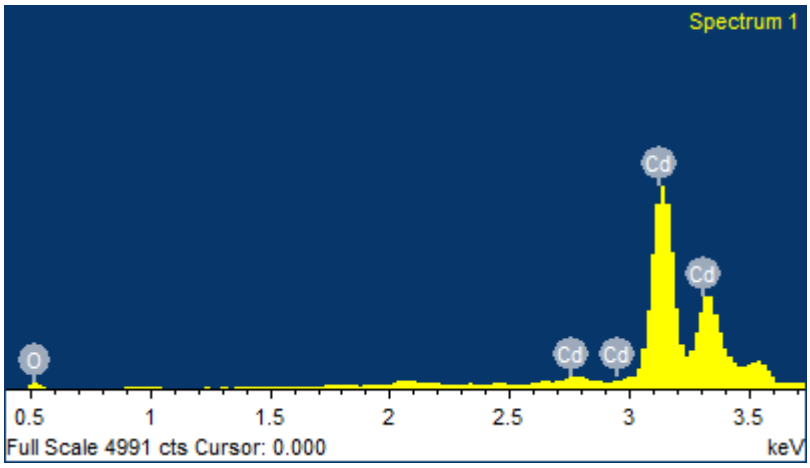


Fig S3. EDS plots for ZnO prepared from **3** (top) and CdO prepared from **7** (bottom).

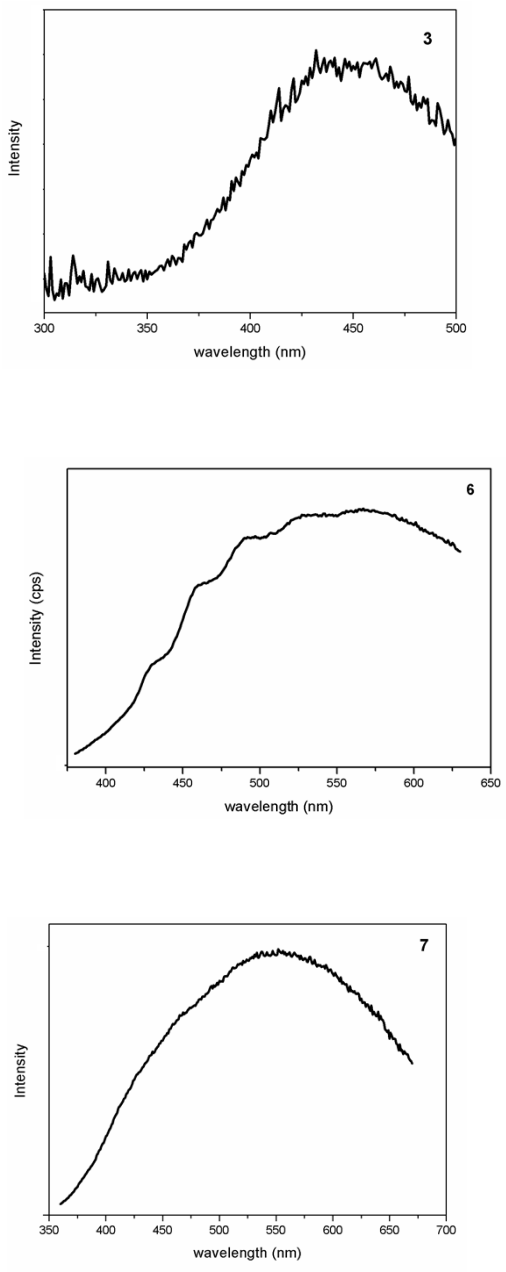


Fig S4. Emission spectra of **3, 6** and **7**.