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Tetra- and poly-nuclear Cd(II) complexes of an N_3O_4 Schiff base ligand: Crystal structures, electrical conductivity and photoswitching property

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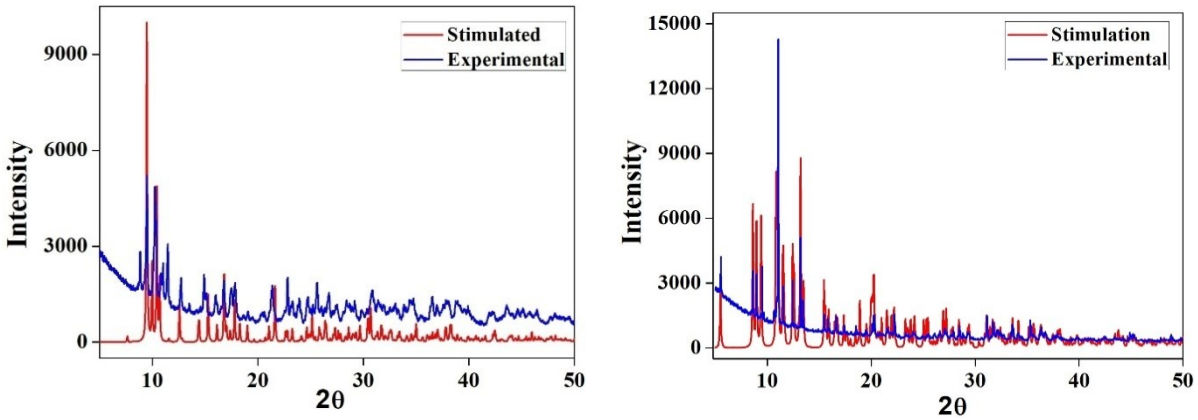

Fig. S1 PXRD of complex **1**(left) and complex **2** (right) with simulated data from single crystal.

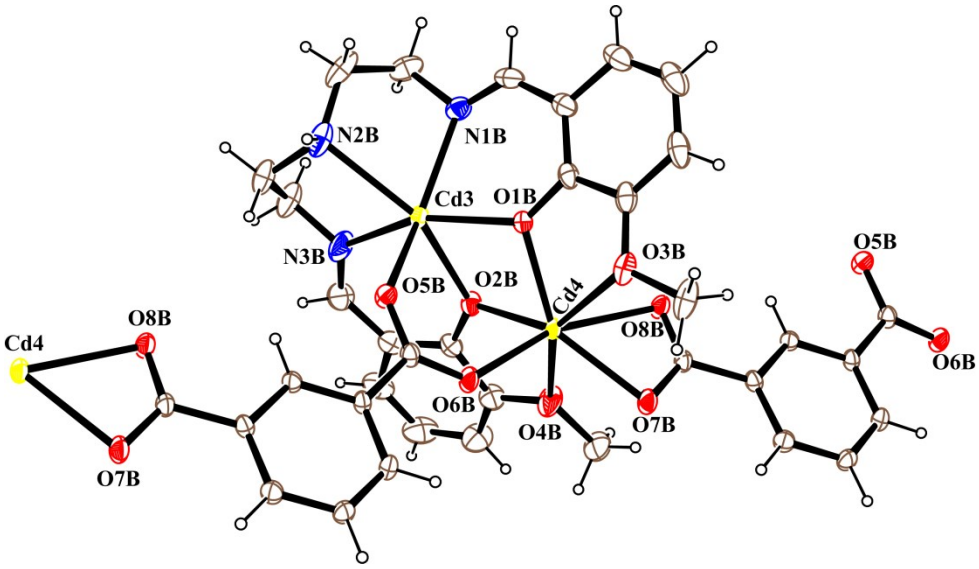

Fig. S2 ORTEP diagram of complex **2B** with 20% ellipsoid probability.

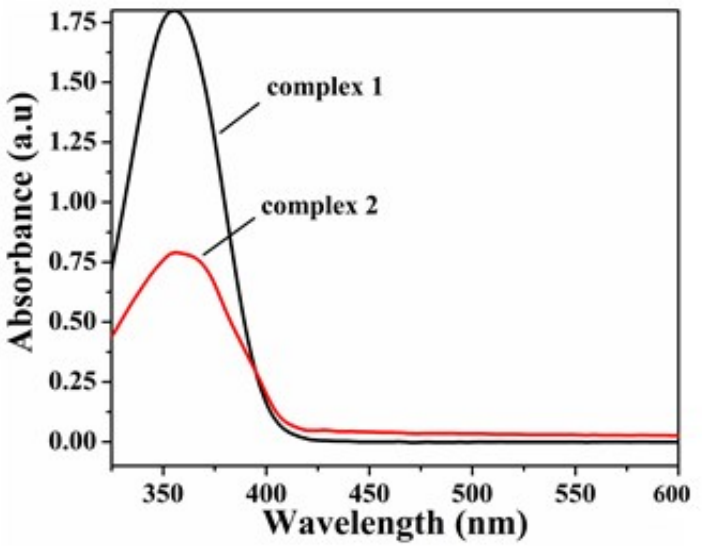

Fig. S3 UV-Vis spectra of complexes **1** and **2** in methanol solution.

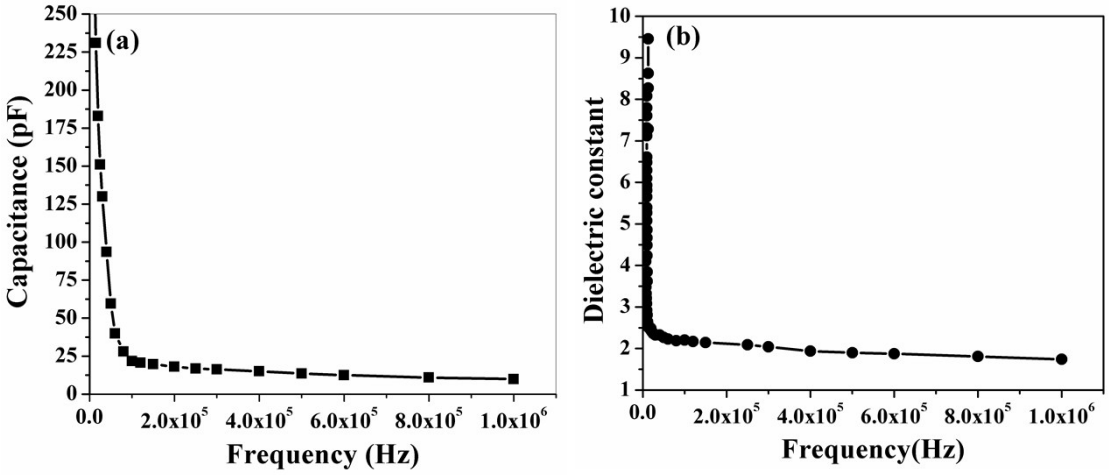

Fig. S4 (a) Capacitance *vs*. Frequency plot (b) Dielectric *vs*. Frequency plot for complex

Table S1. Selected bond lengths (Å) and angles (°) of Complex **1.**

Bond lengths (Å)			
Cd(1)–O(1)	2.266(2)	Cd(2)–O(1)	2.305(3)
Cd(1)–O(2)	2.284(2)	Cd(2)–O(2)	2.302(2)
Cd(1)–O(5)	2.386(3)	Cd(2)–O(3)	2.518(3)
Cd(1)–N(1)	2.265(3)	Cd(2)–O(4)	2.459(3)
Cd(1)–N(2)	2.508(3)	Cd(2)–O(6)	2.767(7)
Cd(1)–N(3)	2.289(3)	Cd(2)–O(7)	2.419(5)
		Cd(2)–N(5)	2.401(3)
		Cd(2)–N(5*)	2.283(3)
Bond angles (°)			
O(1)–Cd(1)–O(5)	85.16(11)	O(1)–Cd(2)–O(3)	64.99(9)
O(1)–Cd(1)–N(1)	79.92(11)	O(1)–Cd(2)–O(4)	139.11(9)
O(1)–Cd(1)–N(2)	137.26(9)	O(1)–Cd(2)–O(6)	115.91(16)
O(1)–Cd(1)–N(3)	148.69(10)	O(1)–Cd(2)–O(7)	78.23(14)
O(2)–Cd(1)–O(5)	84.07(10)	O(1)–Cd(2)–N(5)	84.38(10)
O(2)–Cd(1)–N(1)	141.89(10)	O(1)–Cd(2)–N(5*)	134.42(11)
O(2)–Cd(1)–N(2)	143.20(9)	O(2)–Cd(2)–O(3)	136.77(9)
O(2)–Cd(1)–N(3)	79.71(10)	O(2)–Cd(2)–O(4)	66.41(8)
O(5)–Cd(1)–N(1)	121.74(11)	O(2)–Cd(2)–O(6)	113.64(15)
O(5)–Cd(1)–N(2)	81.95(11)	O(2)–Cd(2)–O(7)	79.71(13)
O(5)–Cd(1)–N(3)	109.86(12)	O(2)–Cd(2)–N(5)	84.33(11)
N(1)–Cd(1)–N(2)	72.93(11)	O(2)–Cd(2)–N(5*)	139.30(11)
N(1)–Cd(1)–N(3)	111.67(13)	O(3)–Cd(2)–O(4)	149.27(9)
N(2)–Cd(1)–N(3)	73.45(10)	O(3)–Cd(2)–O(6)	76.20(15)
		O(3)–Cd(2)–O(7)	80.45(14)
		O(3)–Cd(2)–N(5)	102.68(11)
		O(3)–Cd(2)–N(5*)	81.98(11)
		O(4)–Cd(2)–O(6)	74.90(15)
		O(4)–Cd(2)–O(7)	86.69(14)
		O(4)–Cd(2)–N(5)	99.25(11)
		O(4)–Cd(2)–N(5*)	84.29(11)
		O(6)–Cd(2)–O(7)	45.46(19)
		O(6)–Cd(2)–N(5)	155.45(16)
		O(6)–Cd(2)–N(5*)	82.89(16)
		O(7)–Cd(2)–N(5)	159.09(15)
		O(7)–Cd(2)–N(5*)	128.03(15)
		N(5)–Cd(2)–N(5*)	72.74(12)

Symmetry element *= 1-x,1-y,1-z

Table S2. Selected bond lengths (Å) and angles (°) of Complex **2.**

Bond lengths (Å)			
Cd(1)−O(1A)	2.281(4)	Cd(3)−O(1B)	2.260(3)
Cd(1)−O(2A)	2.256(4)	Cd(3)−O(2B)	2.280(3)
Cd(1)−O(5A)	2.279(3)	Cd(3)−O(5B)	2.309(3)
Cd(1)−N(1A)	2.285(5)	Cd(3)−N(1B)	2.298(6)
Cd(1)−N(2A)	2.520(6)	Cd(3)−N(2B)	2.467(6)
Cd(1)−N(3A)	2.303(5)	Cd(3)−N(3B)	2.315(7)
Cd(2)−O(1A)	2.238(4)	Cd(4)−O(1B)	2.227(3)
Cd(2)−O(2A)	2.261(3)	Cd(4)−O(2B)	2.306(3)
Cd(2)−O(3A)	2.700(4)	Cd(4)−O(3B)	2.689(5)
Cd(2)−O(4A)	2.569(3)	Cd(4)−O(4B)	2.605(5)
Cd(2)−O(6A)	2.210(4)	Cd(4)−O(6B)	2.226(4)
Cd(2)−O(7A^a)	2.290(3)	Cd(2)−O(7B^a)	2.321(4)
Cd(2)−O(8A^a)	2.372(4)	Cd(2)−O(8B^a)	2.345(4)
Bond angles (°)			
O(1A)−Cd(1)−O(2A)	77.42(12)	O(1B)−Cd(3)−O(2B)	76.96(12)
O(1A)−Cd(1)−O(5A)	86.50(13)	O(1B)−Cd(3)−O(5B)	83.76(12)
O(1A)−Cd(1)−N(1A)	77.56(16)	O(1B)−Cd(3)−N(1B)	77.47(16)
O(1A)−Cd(1)−N(2A)	133.02(15)	O(1B)−Cd(3)−N(2B)	132.14(18)
O(1A)−Cd(1)−N(3A)	151.38(16)	O(1B)−Cd(3)−N(3B)	155.56(19)
O(2A)−Cd(1)−O(5A)	86.12(12)	O(2B)−Cd(3)−O(5B)	88.12(12)
O(2A)−Cd(1)−N(1A)	129.71(17)	O(2B)−Cd(3)−N(1B)	119.88(16)
O(2A)−Cd(1)−N(2A)	149.09(15)	O(2B)−Cd(3)−N(2B)	150.81(18)
O(2A)−Cd(1)−N(3A)	79.30(15)	O(2B)−Cd(3)−N(3B)	78.74(19)
O(5A)−Cd(1)−N(1A)	134.57(16)	O(5B)−Cd(3)−N(1B)	140.80(15)
O(5A)−Cd(1)−N(2A)	90.20(16)	O(5B)−Cd(3)−N(2B)	96.52(17)
O(5A)−Cd(1)−N(3A)	108.34(15)	O(5B)−Cd(3)−N(3B)	98.11(19)
N(1A)−Cd(1)−N(2A)	71.9(2)	N(1B)−Cd(3)−N(2B)	72.7(2)
N(1A)−Cd(1)−N(3A)	105.55(18)	N(1B)−Cd(3)−N(3B)	113.1(2)
N(2A)−Cd(1)−N(3A)	72.79(17)	N(2B)−Cd(3)−N(3B)	72.1(2)
O(1A)−Cd(2)−O(2A)	78.19(12)	O(1B)−Cd(4)−O(2B)	77.09(12)
O(1A)−Cd(2)−O(3A)	63.07(12)	O(1B)−Cd(4)−O(3B)	62.71(14)
O(1A)−Cd(2)−O(4A)	144.04(12)	O(1B)−Cd(4)−O(4B)	136.73(14)
O(1A)−Cd(2)−O(6A)	91.27(14)	O(1B)−Cd(4)−O(6B)	93.94(13)
O(1A)−Cd(2)−O(7A^a)	136.54(13)	O(1B)−Cd(4)−O(7B^a)	137.55(15)
O(1A)−Cd(2)−O(8A^a)	102.29(14)	O(1B)−Cd(4)−O(8B^a)	99.15(12)
O(2A)−Cd(2)−O(3A)	140.19(11)	O(2B)−Cd(4)−O(3B)	139.74(13)
O(2A)−Cd(2)−O(4A)	65.89(12)	O(2B)−Cd(4)−O(4B)	63.78(14)
O(2A)−Cd(2)−O(6A)	93.31(15)	O(2B)−Cd(4)−O(6B)	86.66(14)
O(2A)−Cd(2)−O(7A^a)	137.83(12)	O(2B)−Cd(4)−O(7B^a)	140.72(15)
O(2A)−Cd(2)−O(8A^a)	100.13(12	O(2B)−Cd(4)−O(8B^a)	110.66(12)
O(3A)−Cd(2)−O(4A)	151.44(12)	O(3B)−Cd(4)−O(4B)	150.99(15)
O(3A)−Cd(2)−O(6A)	96.21(15)	O(3B)−Cd(4)−O(6B)	97.66(16)
O(3A)−Cd(2)−O(7A^a)	75.44(12)	O(3B)−Cd(4)−O(7B^a)	76.97(16)
O(3A)−Cd(2)−O(8A^a)	80.57(12)	O(3B)−Cd(4)−O(8B^a)	75.61(13)
O(4A)−Cd(2)−O(6A)	92.42(14)	O(4B)−Cd(4)−O(6B)	101.15(19)
O(4A)−Cd(2)−O(7A^a)	76.01(12)	O(4B)−Cd(4)−O(7B^a)	77.06(16)
O(4A)−Cd(2)−O(8A^a)	83.08(13)	O(4B)−Cd(4)−O(8B^a)	79.29(13)
O(6A)−Cd(2)−O(7A^a)	106.07(14)	O(6B)−Cd(4)−O(7B^a)	104.48(12)
O(6A)−Cd(2)−O(8A^a)	162.54(13)	O(6B)−Cd(4)−O(8B^a)	160.20(12)
O(7A^a)−Cd(2)−O(8A^a)	56.48(12)	O(7B^a)−Cd(4)−O(8B^a)	56.07(12)

Symmetry element [a]= 1+x,y,z

Table S3. Geometrical features of hydrogen bonding interactions (distances (Å) and angles (°)) of Complexes **1-2**. [a]

Complex	**D−H···A**	**D–H**	**H···A**	**D···A**	**∠D−H···A**	**Symmetry Element**
1	O(5)−H(5A) ···O(7)	0.87	2.14	2.768(6)	129	
2	N(2B)−H(2AA) ···O(9)	0.98	2.29	3.144(8)	145	-1+x,y,z
	O(9)−H(3AA) ···O(5B)	0.82	1.99	2.770(6)	160	1+x,y,z

[a](D, donor; H, hydrogen; A, acceptor)