Supporting Information

Structural diversity of Mn(II), Zn(II) and Pb(II) coordination polymers constructed from isomeric pyridylbenzoate *N*-oxide ligands: structures and electrochemical properties

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Table S1. Selected Bond Distances (Å) and Angles (°) for compounds **1-6**

compound **1**			
Mn(1)-O(6)	2.104(4)	O(2)-Mn(1)-O(2W)	84.87(14)
Mn(1)-O(2)	2.142(4)	O(1W)-Mn(1)-O(2W)	175.02(14)
Mn(1)-O(1W)	2.170(4)	O(6)-Mn(1)-O(4)	88.53(14)
Mn(1)-O(2W)	2.186(4)	O(2)-Mn(1)-O(4)	94.11(15)
Mn(1)-O(4)	2.205(4)	O(1W)-Mn(1)-O(4)	93.34(15)
Mn(1)-O(1)	2.236(4)	O(2W)-Mn(1)-O(4)	88.87(14)
O(6)-Mn(1)-O(2)	177.30(15)	O(6)-Mn(1)-O(1)	87.11(14)
O(6)-Mn(1)-O(1W)	89.92(14)	O(2)-Mn(1)-O(1)	90.22(14)
O(2)-Mn(1)-O(1W)	90.52(14)	O(1W)-Mn(1)-O(1)	90.38(15)
O(6)-Mn(1)-O(2W)	94.60(14)	O(2W)-Mn(1)-O(1)	87.77(14)
		O(4)-Mn(1)-O(1)	174.26(14)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+1,-z+1; #2 -x,y+1/2,-z+1/2; #3 -x,y-1/2,-z+1/2

compound **2**			
Zn(1)-O(4)#1	1.882(5)	O(4)#1-Zn(1)-O(4)#2	168.51(9)
Zn(1)-O(4)#2	1.890(5)	O(4)#1-Zn(1)-O(2)#1	93.0(2)
Zn(1)-O(2)#1	1.972(5)	O(4)#2-Zn(1)-O(2)#1	83.3(2)
Zn(1)-O(3)#2	1.996(5)	O(4)#1-Zn(1)-O(3)#2	86.2(2)
Zn(1)-O(1)	2.381(5)	O(4)#2-Zn(1)-O(3)#2	96.0(2)
O(2)-Zn(1)#1	1.972(5)	O(2)#1-Zn(1)-O(3)#2	172.1(2)
O(3)-Zn(1)#3	1.996(5)	O(4)#1-Zn(1)-O(1)	93.4(2)
O(4)-Zn(1)#1	1.882(5)	O(4)#2-Zn(1)-O(1)	97.6(2)
O(4)-Zn(1)#3	1.890(5)	O(2)#1-Zn(1)-O(1)	92.1(2)
		O(3)#2-Zn(1)-O(1)	95.8(2)

Symmetry transformations used to generate equivalent atoms: #1 -x,-y+2,-z; #2 x+1,-y+3/2, z+1/2; #3 x-1, -y+3/2, z-1/2

compound **3**			
Pb(1)-O(2)	2.386(10)	O(2)-Pb(1)-O(1W)	74.3(3)
Pb(1)-O(1W)	2.394(9)	O(2)-Pb(1)-O(1)#	185.4(3)
Pb(1)-O(1)#1	2.490(8)	O(1W)-Pb(1)-O(1)#1	79.4(3)
Pb(1)-O(1)	2.537(8)	O(2)-Pb(1)-O(1)	75.6(3)
O(1)-Pb(1)#3	2.490(8)	O(1W)-Pb(1)-O(1)	78.8(3)
		O(1)#1-Pb(1)-O(1)	154.3(3)

Symmetry transformations used to generate equivalent atoms: #1 x,-y+1/2, z+1/2; #2 -x,-y+1,-z; #3 x, -y+1/2, z-1/2

compound **4**			
Mn(1)-O(3)#1	2.140(6)	O(3)#2-Mn(1)-O(1W)	93.6(3)
Mn(1)-O(3)#2	2.140(6)	O(1)-Mn(1)-O(1W)	89.5(3)
Mn(1)-O(1)	2.218(6)	O(1)#3-Mn(1)-O(1W)	90.5(3)
Mn(1)-O(1)#3	2.218(6)	O(3)#1-Mn(1)-O(1W)#3	93.6(3)
Mn(1)-O(1W)	2.199(7)	O(3)#2-Mn(1)-O(1W)#3	86.4(3)
Mn(1)-O(1W)#3	2.199(7)	O(1)-Mn(1)-O(1W)#3	90.5(3)
Mn(2)-O(5)#4	2.115(6)	O(1)#3-Mn(1)-O(1W)#3	89.5(3)
Mn(2)-O(7)	2.147(9)	O(1W)-Mn(1)-O(1W)#3	180.0
Mn(2)-O(2)#2	2.128(6)	O(5)#4-Mn(2)-O(7)	91.6(3)
Mn(2)-O(4)	2.235(6)	O(5)#4-Mn(2)-O(2)#2	175.9(3)
Mn(2)-O(1)	2.241(6)	O(7)-Mn(2)-O(2)#	284.9(3)
Mn(2)-O(2W)	2.267(7)	O(5)#4-Mn(2)-O(4)	89.1(2)
O(2)-Mn(2)#4	2.128(6)	O(7)-Mn(2)-O(4)	93.7(3)
O(3)-Mn(1)#4	2.140(6)	O(2)#2-Mn(2)-O(4)	88.9(2)
O(5)-Mn(2)#2	2.115(6)	O(5)#4-Mn(2)-O(1)	90.6(2)
O(3)#1-Mn(1)-O(3)#2	180.0(5)	O(7)-Mn(2)-O(1)	92.1(3)
O(3)#1-Mn(1)-O(1)	89.6(2)	O(2)#2-Mn(2)-O(1)	91.7(2)
O(3)#2-Mn(1)-O(1)	90.4(2)	O(4)-Mn(2)-O(1)	174.2(3)
O(3)#1-Mn(1)-O(1)#3	90.4(2)	O(5)#4-Mn(2)-O(2W)	89.7(3)
O(3)#2-Mn(1)-O(1)#3	89.6(2)	O(7)-Mn(2)-O(2W)	176.4(3)
O(1)-Mn(1)-O(1)#3	180.0	O(2)#2-Mn(2)-O(2W)	94.0(3)
O(3)#1-Mn(1)-O(1W)	86.4(3)	O(4)-Mn(2)-O(2W)	89.7(3)
		O(1)-Mn(2)-O(2W)	84.5(3)

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

compound **5**			
Zn(1)-O(2W)	1.89(2)	O(2W)-Zn(1)-O(1W)	180.00(2)
Zn(1)-O(2)	1.931(9)	O(2)-Zn(1)-O(1W)	90.6(4)
Zn(1)-O(2)#1	1.931(9)	O(2)#1-Zn(1)-O(1W)	90.6(4)
Zn(1)-O(1W)	1.95(3)	O(6)#2-Zn(2)-O(6)	176.7(10)
Zn(2)-O(6)#2	1.923(9)	O(6)#2-Zn(2)-O(4W)#2	94.8(7)
Zn(2)-O(6)	1.923(9)	O(6)-Zn(2)-O(4W)#2	82.0(7)
Zn(2)-O(4W)#2	1.93(2)	O(6)#2-Zn(2)-O(4W)	82.0(7)
Zn(2)-O(4W)	1.93(2)	O(6)-Zn(2)-O(4W)	94.8(7)
Zn(2)-O(3W)	2.00(3)	O(4W)#2-Zn(2)-O(4W)	26.3(9)
O(2W)-Zn(1)-O(2)	89.4(4)	O(6)#2-Zn(2)-O(3W)	91.6(5)
O(2W)-Zn(1)-O(2)#1	89.4(4)	O(6)-Zn(2)-O(3W)	91.6(5)
O(2)-Zn(1)-O(2)#1	178.9(8)	O(4W)#2-Zn(2)-O(3W)	166.9(5)
		O(4W)-Zn(2)-O(3W)	166.9(5)

Symmetry transformations used to generate equivalent atoms: #1 -x+2, y, -z+2; #2 -x+2, y, -z+1.

compound **6**			
Pb(1)-O(3)	2.450(6)	O(4)-Pb(1)-O(6)#	171.9(2)
Pb(1)-O(4)	2.464(6)	O(3)-Pb(1)-O(5)	86.4(2)
Pb(1)-O(6)#1	2.541(6)	O(4)-Pb(1)-O(5)	51.2(2)
Pb(1)-O(5)	2.638(7)	O(6)#1-Pb(1)-O(5)	122.6(2)
Pb(1)-O(2)	2.653(6)	O(3)-Pb(1)-O(2)	51.22(19)
O(6)-Pb(1)#2	2.541(6)	O(4)-Pb(1)-O(2)	111.1(2)
O(3)-Pb(1)-O(4)	80.8(2)	O(6)#1-Pb(1)-O(2)	124.55(19)
O(3)-Pb(1)-O(6)#	176.6(2)	O(5)-Pb(1)-O(2)	76.4(2)

Symmetry transformations used to generate equivalent atoms: #1 -x, y-1/2, -z+1/2; #2 -x, y+1/2, -z+1/2.

Table S2 The twisting angles between benzene and pyridine ring of 4,3-opybz and 4,4-opybz ligands.

Complex	**1**	**2**	**3**	**4**	**5**	**6**
Twisting angles	23.56	6.86	39.97	5.52	29.11	13.75
	38.59			16.43	29.13	25.18

Text report

No.	Name	Weight [mg]	C [%]	H [%]	N [%]	C/N ratio	C/H ratio	Date	Time
110	1-Mn	1.8830	55.53	3.86	5.38	10.3216	14.3860	13.06.2016	21:41
111	2-Zn	1.8210	48.57	3.04	4.75	10.2253	15.9769	13.06.2016	21:49
112	3-Pb	1.9390	28.76	2.05	5.54	5.1913	14.0293	13.06.2016	21:56
113	4-Mn	1.8537	46.51	4.19	4.33	10.7413	11.1002	13.06.2016	22:04
114	5-Zn	1.8932	54.39	3.81	5.30	10.2623	14.2756	13.06.2016	22:12
115	6-Pb	1.9156	40.41	5.27	7.13	5.6676	7.6679	13.06.2016	22:19

Fig. S1 C, H, N contents of the obtained compounds.

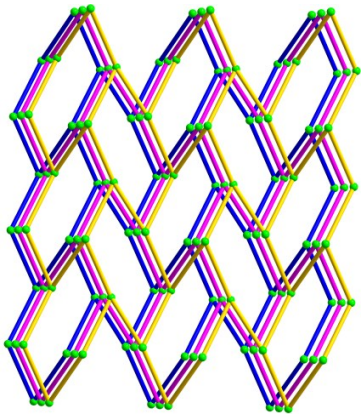

Fig. S2 Schematic view of parallel packing of the 2D layers in **1**.

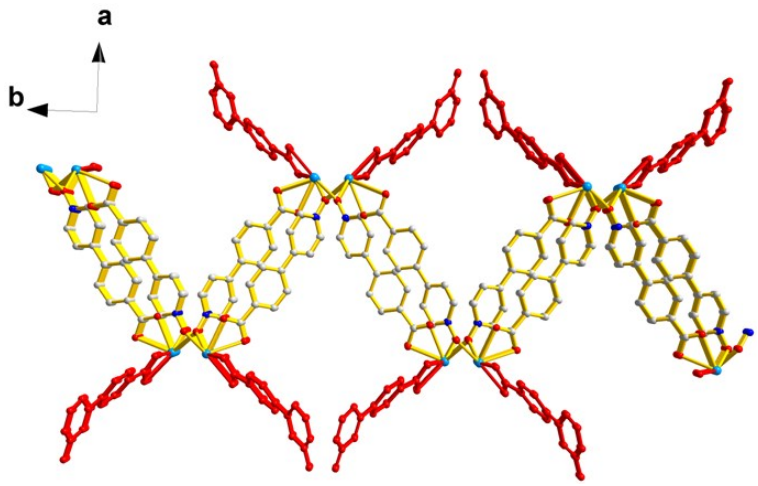

Fig. S3 The 2-D framework of **6** showing the terminal 4,3-opybz ligand as viewed along the *c* axis (the 4,3-opybz ligand are highlighted using red color).

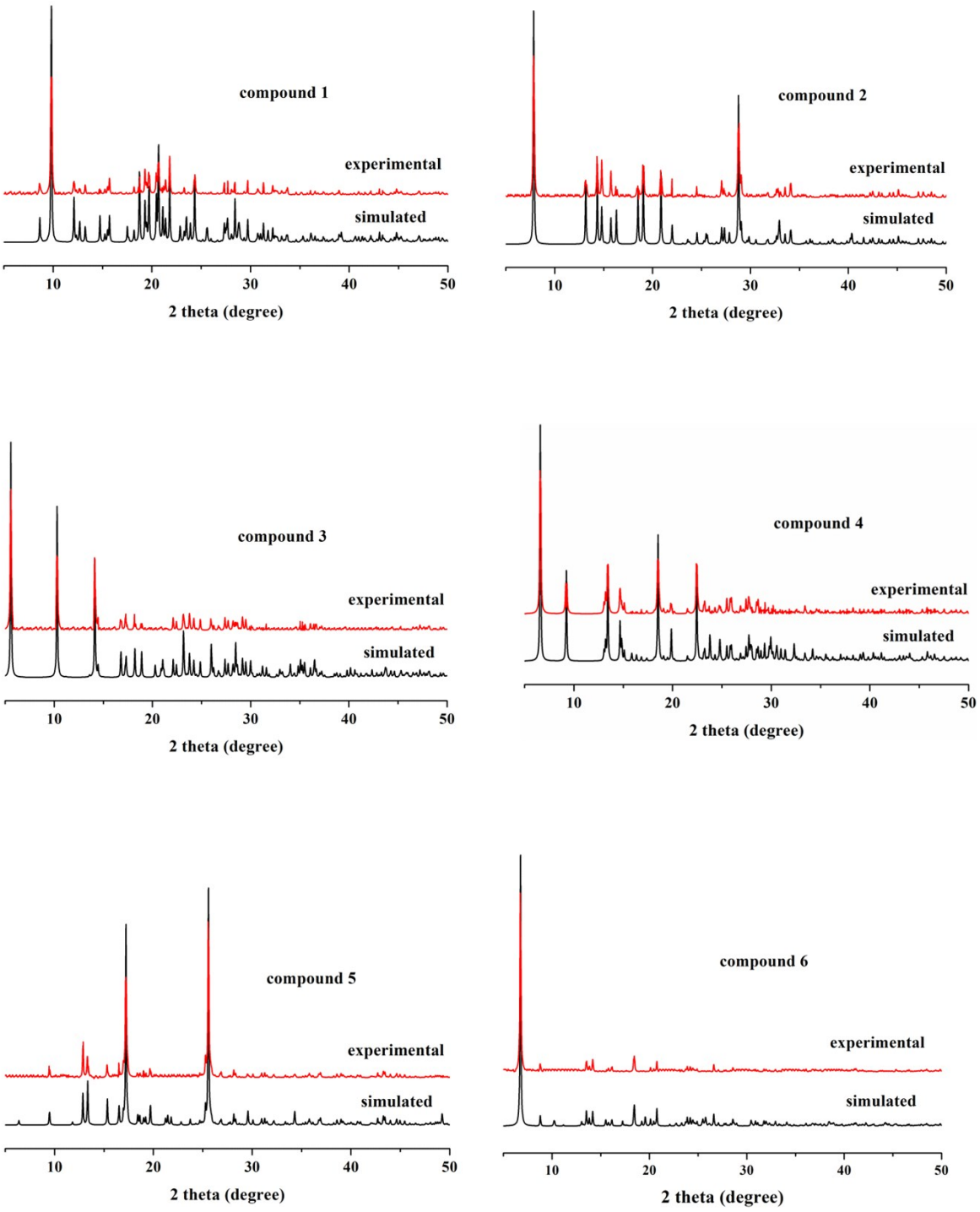

Fig. S4 The PXRD patterns of compounds **1–6** at room temperature.

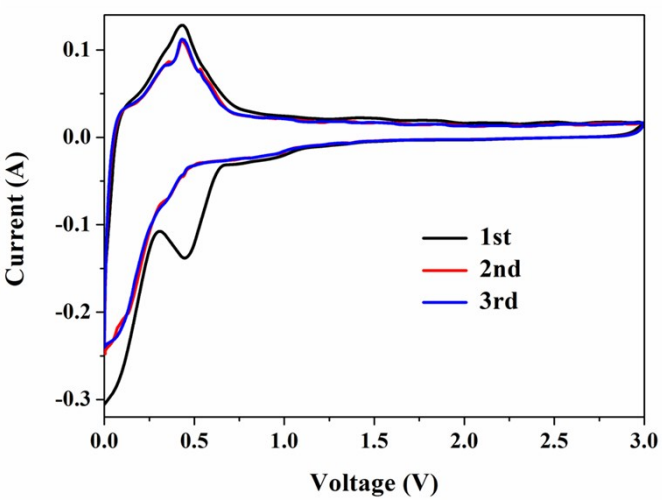

Fig. S5 Cyclic voltammetry curve at 0.1 mV s^{-1} scan rate.