Electronic Supplementary Material (ESI) for Dalton Transactions

Syntheses, crystal structures and thermal properties of six coordination polymers based on 2-(p-methylphenyl)-imidazole dicarboxylate

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Supporting Information

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

		1	
Pb(1) -N(11)	2.470(4)	Pb(1)-O(7)	2.565(4)
Pb(1)-O(2)	2.614(3)	Pb(1)-N(4)	2.627(4)
Pb(1)-O(5)#2	2.636(3)	Pb(1)-N(5)	2.672(4)
N(11)-Pb(1)-O(7)	66.76(13)	N(11)-Pb(1)-O(2)	95.36(12)
O(7)-Pb(1)-O(2)	74.45(14)	N(11)-Pb(1)-N(4)	79.40(13)
O(7)-Pb(1)-N(4)	128.99(14)	O(2)-Pb(1)-N(4)	71.93(12)
N(11)-Pb(1)-O(5)#2	72.44(13)	O(7)-Pb(1)-O(5)#2	81.68(14)
O(2)-Pb(1)-O(5)#2	155.99(12)	N(4)-Pb(1)-O(5)#2	123.74(12)
N(11)-Pb(1)-N(5)	100.81(13)	O(7)-Pb(1)-N(5)	157.46(15)
N(4)-Pb(1)-N(5)	62.18(13)	O(5)#2-Pb(1)-N(5)	76.50(13)
		2	
N(1)-Pb(1)	2.695(3)	O(2)-Pb(1)	2.476(3)
O(3)-Pb(1)#1	2.645(2)	Pb(1)-O(2)#2	2.476(3)
Pb(1)-O(3)#3	2.645(3)	Pb(1)-O(3)#4	2.645(3)
Pb(1)-N(1)#2	2.695(3)	O(2)-Pb(1)-O(2)#2	101.14(15)
O(2)-Pb(1)-O(3)#3	152.87(8)	O(2)#2-Pb(1)-O(3)#3	85.10(9)
O(2)#2-Pb(1)-O(3)#4	152.87(8)	O(3)#3-Pb(1)-O(3)#4	101.41(12)
O(2)-Pb(1)-N(1)#2	80.99(8)	O(2)#2-Pb(1)-N(1)#2	64.85(8)
O(3)#3-Pb(1)-N(1)#2	124.77(8)	O(3)#4-Pb(1)-N(1)#2	90.55(9)
O(3)#4-Pb(1)-N(1)	124.77(8)	N(1)#2-Pb(1)-N(1)	125.51(12)
		3	
Cd(1)-N(1)	2.253(4)	Cd(1)-N(1)#1	2.253(4)

Cd(1)-O(7)	2.399(4)	Cd(1)-O(7)#1	2.399(4)
Cd(1)-O(5)	2.405(4)	Cd(1)-O(5)#1	2.405(4)
Cd(2)-N(2)	2.236(4)	Cd(2)-O(6)#2	2.282(4)
Cd(2)-O(2)#3	2.284(4)	Cd(2)-O(9)	2.313(4)
Cd(2)-N(3)#2	2.326(4)	Cd(2)-O(2)	2.488(4)
N(1)-Cd(1)-N(1)#1	180.00(14)	N(1)-Cd(1)-O(7)	72.78(14)
N(1)#1-Cd(1)-O(7)	107.22(14)	N(1)-Cd(1)-O(5)	88.07(15)
N(1)#1-Cd(1)-O(5)	91.93(15)	O(7)-Cd(1)-O(5)	76.26(14)
O(7)#1-Cd(1)-O(5)	103.74(14)	N(2)-Cd(2)-O(6)#2	109.43(15)
N(2)-Cd(2)-O(2)#3	142.35(15)	O(6)#2-Cd(2)-O(2)#3	81.94(14)
N(2)-Cd(2)-O(9)	99.15(15)	O(6)#2-Cd(2)-O(9)	151.41(14)
O(2)#3-Cd(2)-N(3)#2	112.38(15)	N(2)-Cd(2)-O(2)	70.24(14)
O(9)-Cd(2)-O(2)	78.37(14)	N(3)#2-Cd(2)-O(2)	174.72(14)
		4	
Cd(1)-N(2)#1	2.185(10)	Cd(1)-O(4)#1	2.517(11)
Cd(1)-N(1)	2.240(11)	Cd(1)-O(5)	2.28(2)
Cd(1)-O(1)#2	2.285(9)	Cd(1)-O(1)	2.395(9)
N(2)#1-Cd(1)-N(1)	113.9(4)	N(2)#1-Cd(1)-O(5)	118.5(7)
N(1)-Cd(1)-O(5)	93.7(6)	N(2)#1-Cd(1)-O(1)#2	96.6(3)
N(1)-Cd(1)-O(1)#2	142.3(4)	O(5)-Cd(1)-O(1)#2	90.3(7)
N(2)#1-Cd(1)-O(1)	144.8(4)	N(1)-Cd(1)-O(1)	70.9(4)
O(1)-Cd(1)-O(4)#1	74.7(4)	O(5)-Cd(1)-O(4)#1	168.9(8)
N(1)-Cd(1)-O(4)#1	87.0(4)	O(1)#2-Cd(1)-O(4)#1	82.5(4)
		5	
Cd(1)-N(2)	2.2349(18)	Cd(1)-N(3)#1	2.2777(19)
Cd(1)-O(1)	2.2949(16)	Cd(1)-N(1)	2.338(2)
Cd(1)-O(1)#2	2.4347(18)	Cd(1)-O(4)	2.4776(19)
N(2)-Cd(1)-N(3)#1	113.21(7)	N(2)-Cd(1)-O(1)	100.15(6)
N(3)#1-Cd(1)-O(1)	139.31(6)	N(2)-Cd(1)-N(1)	116.31(8)
N(2)-Cd(1)-O(1)#2	146.14(6)	N(3)#1-Cd(1)-O(1)#2	71.42(6)
O(1)-Cd(1)-O(1)#2	67.91(7)	N(1)-Cd(1)-O(1)#2	96.65(7)
N(3)#1-Cd(1)-O(4)	81.17(7)	O(1)-Cd(1)-O(4)	88.20(7)
N(1)-Cd(1)-O(4)	170.61(7)	O(1)#2-Cd(1)-O(4)	76.15(6)
		6	
Mn(1)-O(7)#4	2.120(2)	Mn(1)-N(6)#5	2.223(3)
Mn(1)-N(6)#6	2.223(3)	Mn(1)-O(9)#4	2.235(3)

Mn(1)-O(9)	2.235(3)	Mn(2)-O(8)#5	2.125(2)
Mn(2)-O(3)	2.131(2)	Mn(2)-O(1)	2.164(3)
Mn(2)-O(4)	2.203(2)	Mn(2)-N(1)	2.261(3)
Mn(2)-N(2)	2.277(3)	O(7)#4-Mn(1)-O(7)	180.00(17)
O(7)#4-Mn(1)-N(6)#5	91.42(10)	O(7)-Mn(1)-N(6)#5	88.58(10)
O(7)#4-Mn(1)-O(9)#4	91.96(10)	O(7)-Mn(1)-O(9)#4	88.04(10)
N(6)#5-Mn(1)-O(9)#4	75.45(10)	N(6)#6-Mn(1)-O(9)#4	104.55(10)
N(6)#5-Mn(1)-O(9)	104.55(10)	N(6)#6-Mn(1)-O(9)	75.45(10)
O(8)#5-Mn(2)-O(3)	87.54(10)	O(8)#5-Mn(2)-O(1)	91.28(10)
O(3)-Mn(2)-O(1)	178.28(10)	O(8)#5-Mn(2)-O(4)	84.29(9)
O(8)#5-Mn(2)-N(1)	95.24(11)	O(4)-Mn(2)-N(1)	179.53(11)
O(8)#5-Mn(2)-N(2)	157.32(10)	O(3)-Mn(2)-N(2)	92.84(11)
O(4)-Mn(2)-N(2)	73.03(10)	N(1)-Mn(2)-N(2)	107.45(11)

Symmetry transformations used to generate equivalent atoms for **1**: #1: -x+2,y,-z+1/2. #2: x,-y+1,z+1/2. #3: x,-y+1,z-1/2. For **2**: #1: -y+1/4,x+3/4,z-1/4. #2: -x+0,-y+1/2,z+0. #3: -y+3/4,x+1/4,z+1/4. #4: y-3/4,-x+1/4,z+1/4. For **3**: #1: -x+2,-y,-z+2. #2 -x+2,-y+1,-z+2. #3 -x+3,-y+1,-z+2. For **4**: #1: y-1/4,-x+7/4,z-1/4. #2: -x+3/2,-y+3/2,-z+3/2. #3: -y+7/4,x+1/4,z+1/4. For **5**: #1: y+1/4,-x+5/4,z+1/4 #2: -x+2,-y+1,-z+2. For **6:** #1: -x,-y+2,-z+1. #2: -x+1/2,y-1/2,-z+1/2. #3: x+1/2,-y+1/2,z+1/2. #4 -x,-y+1,-z. #5 -x+1/2,y+1/2,-z+1/2.

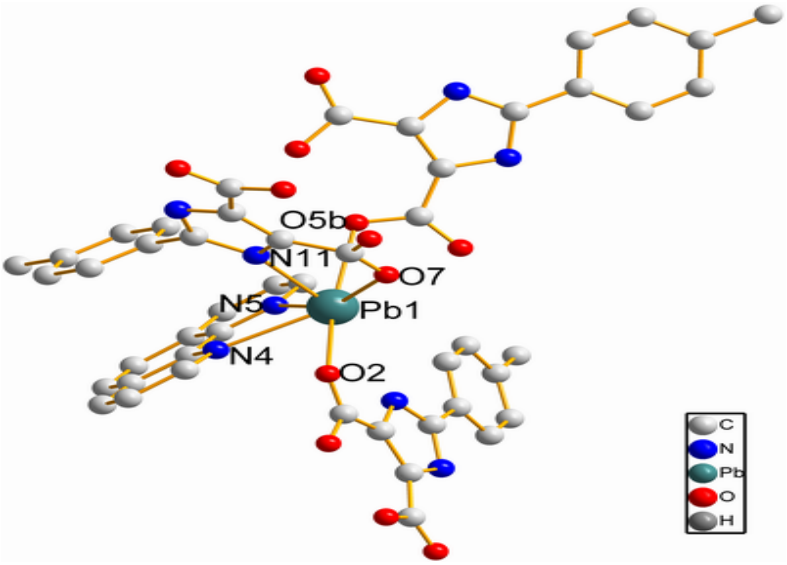

Figure S1. Local coordination environment of Pb(II) ion in **1** (symmetry code: b: x, -y+1, z+1/2. hydrogen atoms omitted for clarity).

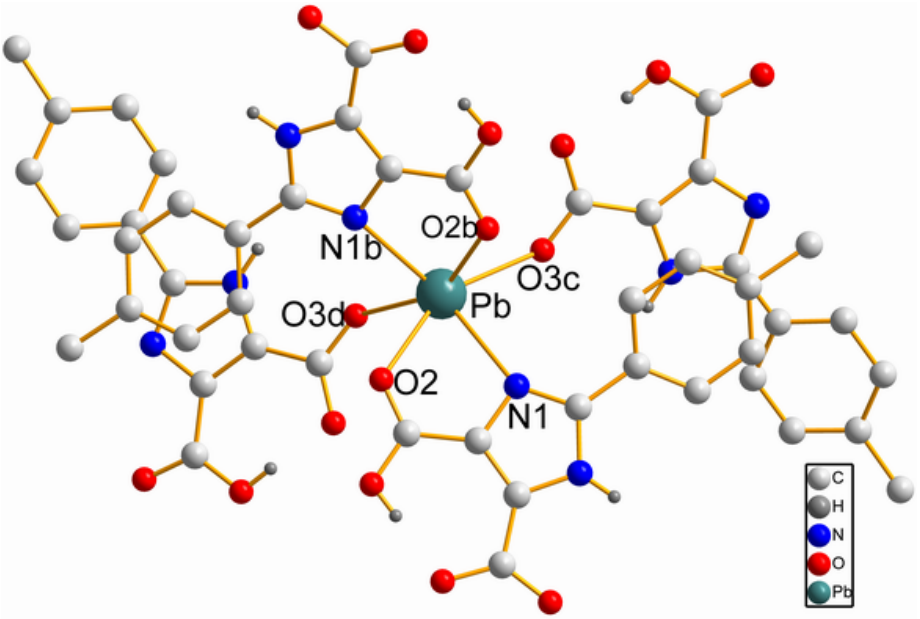

Figure S2. Coordination arrangement of the Pb(II) atom in complex **2** (symmetry code: a: -y+1/4, x+3/4, z-1/4. b: -x+0, -y+1/2, z+0. c: -y+3/4, x+1/4, z+1/4. Partial hydrogen atoms omitted for clarity).

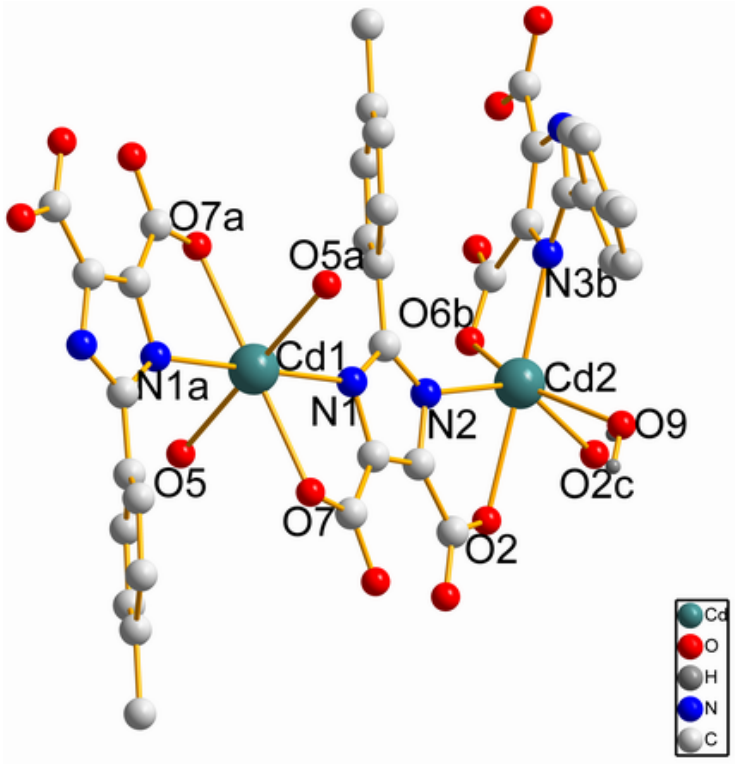

Figure S3. Coordination environments of the Cd(II) atoms with atomic labels in **3** (symmetry code: a: -x+2, -y, -z+2. b: -x+2, -y+1, -z+2. c: -x+3, -y+1, -z+2. hydrogen atoms omitted for clarity).

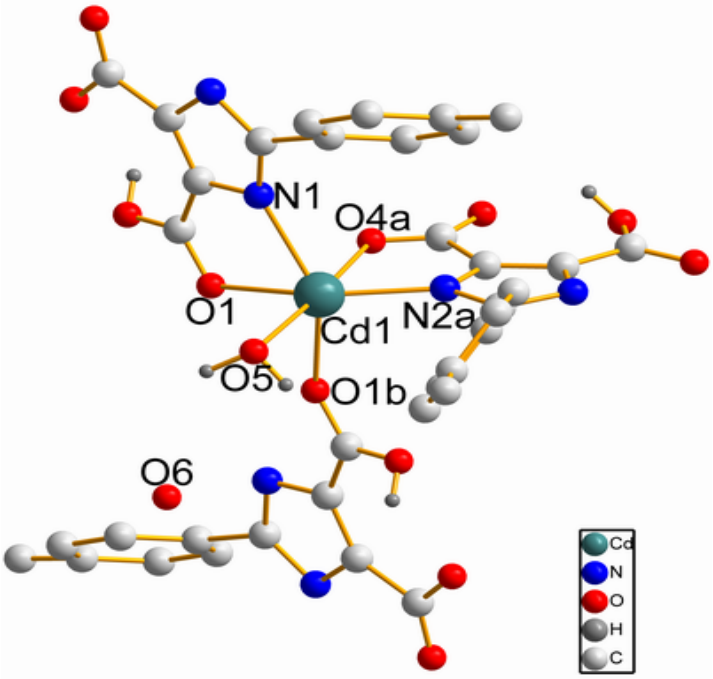

Figure S4. Coordination environment of the Cd(II) atom with atomic labels in **4** (symmetry code: a: y-1/4, -x+7/4, z-1/4. b: -x+3/2, -y+3/2, -z+3/2. hydrogen atoms omitted for clarity).

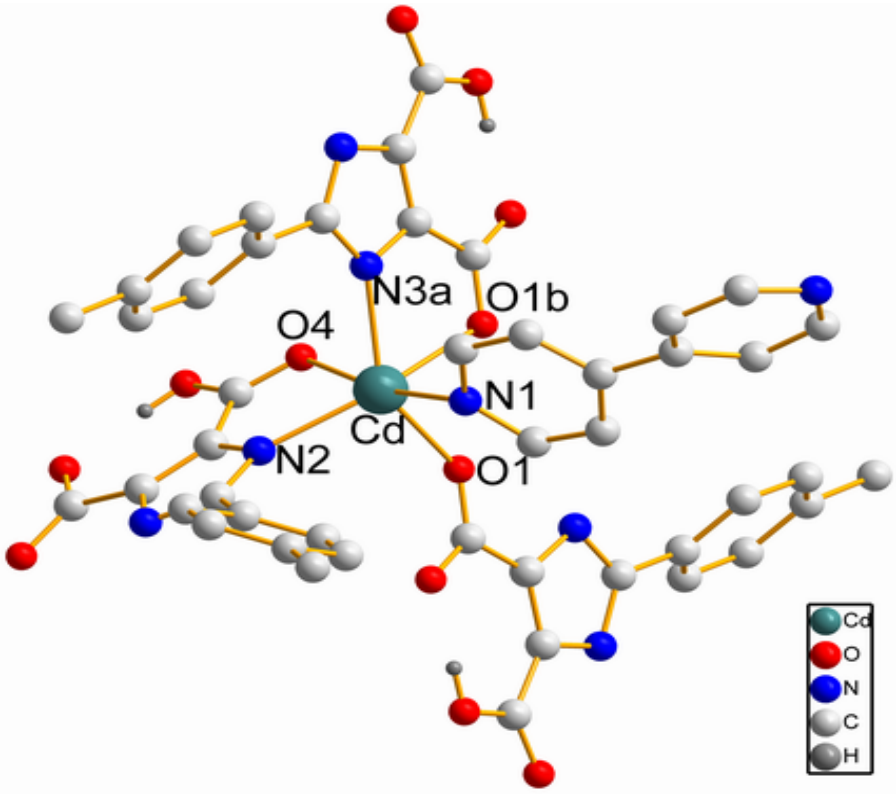

Figure S5. Coordination environment of the Cd(II) atom in **5** (symmetry code: a: y+1/4,-x+5/4,z+1/4. b: -x+2,-y+1,-z+2. Partial $MePhHIDC^{2-}$ anions omitted for clarity and hydrogen atoms omitted for clarity).

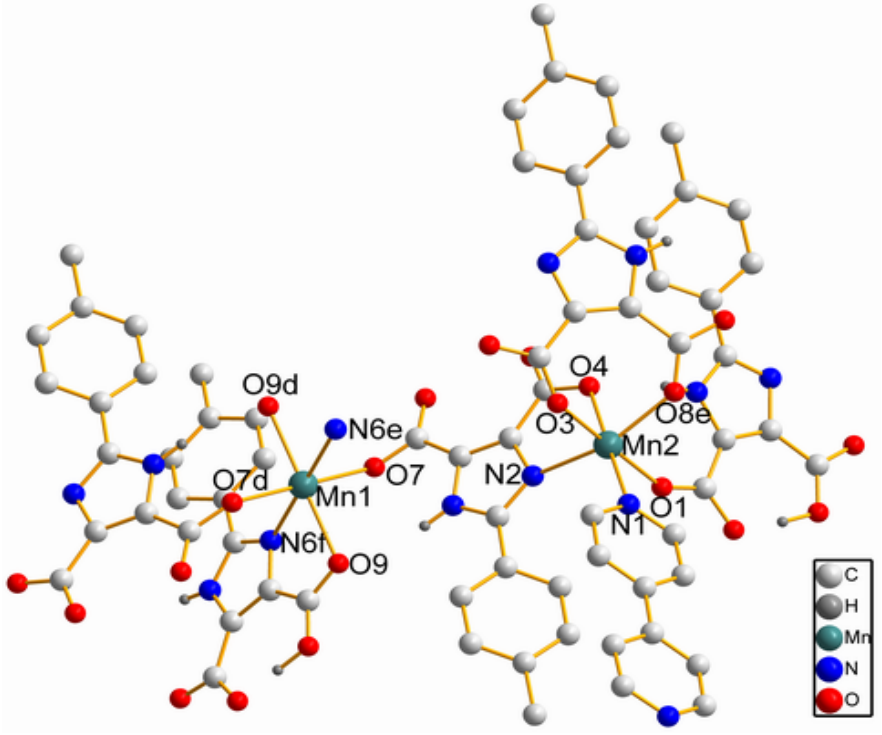

Figure S6. Coordination environments of Mn(II) atoms in polymer **6** (symmetry code: a: -x, -y+2, -z+1. b: -x+1/2, y-1/2, -z+1/2. c: x+1/2, -y+1/2, z+1/2. d: -x, -y+1, -z. e: -x+1/2, y+1/2, -z+1/2. Partial H atoms omitted for clarity).