

A series of coordination polymers based on varied polycarboxylates and different imidazole-containing ligands: Syntheses, crystal structures and physical properties

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Supporting Information

Table S1 Selected bond lengths (Å) and angles (°) for complexes **1-7^a**

Ni(BDC)(titmb)·3H₂O (1)			
Ni(1)-O(4)#1	2.004(3)	Ni(1)-N(1)#3	2.069(4)
Ni(1)-N(3)#2	2.043(4)	Ni(1)-O(1)	2.189(3)
Ni(1)-N(5)	2.045(4)	Ni(1)-O(2)	2.200(3)
O(4)#1-Ni(1)-N(3)#2	106.15(16)	N(5)-Ni(1)-O(1)	89.56(15)
O(4)#1-Ni(1)-N(5)	92.28(16)	N(1)#3-Ni(1)-O(1)	89.27(15)
N(3)#2-Ni(1)-N(5)	91.17(16)	O(4)#1-Ni(1)-O(2)	96.44(13)
O(4)#1-Ni(1)-N(1)#3	88.87(16)	N(3)#2-Ni(1)-O(2)	157.39(14)
N(3)#2-Ni(1)-N(1)#3	88.79(15)	N(5)-Ni(1)-O(2)	88.70(14)
N(5)-Ni(1)-N(1)#3	178.81(18)	N(1)#3-Ni(1)-O(2)	90.89(15)
O(4)#1-Ni(1)-O(1)	155.69(13)	O(1)-Ni(1)-O(2)	59.35(12)
N(3)#2-Ni(1)-O(1)	98.04(14)		
Ni₂(BDC)₂(bimb)₂(H₂O)₂·3H₂O (2)			
Ni(1)-O(4)#1	2.0273(17)	Ni(1)-O(1W)	2.086(2)
Ni(1)-N(1)	2.063(2)	Ni(1)-O(1)	2.1259(19)
Ni(1)-N(4)#2	2.071(2)	Ni(1)-O(2)	2.1369(17)
O(4)#1-Ni(1)-N(1)	90.92(8)	N(4)#2-Ni(1)-O(1)	87.88(8)

O(4)#1-Ni(1)-N(4)#2	90.14(8)	O(1W)-Ni(1)-O(1)	162.08(7)
N(1)-Ni(1)-N(4)#2	178.79(8)	O(4)#1-Ni(1)-O(2)	161.10(8)
O(4)#1-Ni(1)-O(1W)	97.73(8)	N(1)-Ni(1)-O(2)	91.52(8)
N(1)-Ni(1)-O(1W)	91.88(8)	N(4)#2-Ni(1)-O(2)	87.67(7)
N(4)#2-Ni(1)-O(1W)	87.40(8)	O(1W)-Ni(1)-O(2)	100.92(8)
O(4)#1-Ni(1)-O(1)	99.56(7)	O(1)-Ni(1)-O(2)	61.61(7)
N(1)-Ni(1)-O(1)	92.52(8)		
NiZn(BTC)(titmb)Br (3)			
Ni(1)-N(1)#2	2.079(4)	Ni(1)-N(1)#1	2.079(4)
Ni(1)-O(1)#1	2.111(3)	Zn(1)-O(2)#1	1.939(3)
Ni(1)-O(1)#2	2.111(3)	Zn(1)-O(2)	1.940(3)
Ni(1)-O(1)	2.111(3)	Zn(1)-O(2)#2	1.940(3)
Ni(1)-N(1)	2.079(4)	Zn(1)-Br(1)	2.3595(17)
O(2)#1-Zn(1)-O(2)	111.91(10)	N(1)#2-Ni(1)-O(1)#1	88.46(14)
O(2)#1-Zn(1)-O(2)#2	111.91(10)	N(1)-Ni(1)-O(1)#2	88.46(14)
O(2)-Zn(1)-O(2)#2	111.91(10)	N(1)#1-Ni(1)-O(1)#2	86.17(16)
O(2)#1-Zn(1)-Br(1)	106.91(11)	N(1)#2-Ni(1)-O(1)#2	177.72(15)
O(2)-Zn(1)-Br(1)	106.91(11)	O(1)#1-Ni(1)-O(1)#2	91.55(14)
O(2)#2-Zn(1)-Br(1)	106.91(11)	N(1)-Ni(1)-O(1)	177.72(15)
N(1)-Ni(1)-N(1)#1	93.81(17)	N(1)#1-Ni(1)-O(1)	88.46(14)
N(1)-Ni(1)-N(1)#2	93.81(17)	N(1)#2-Ni(1)-O(1)	86.16(16)
N(1)#1-Ni(1)-N(1)#2	93.81(17)	O(1)#1-Ni(1)-O(1)	91.55(14)
N(1)-Ni(1)-O(1)#1	86.17(16)	O(1)#2-Ni(1)-O(1)	91.55(14)
N(1)#1-Ni(1)-O(1)#1	177.72(15)		
Ni(TBDC)(titmb)(H₂O) (4)			
Ni(1)-O(3)#1	2.040(2)	Ni(1)-N(1)	2.106(3)
Ni(1)-N(6)#2	2.071(3)	Ni(1)-O(1)	2.109(2)
Ni(1)-N(4)#3	2.081(3)	Ni(1)-O(1W)	2.144(3)
O(3)#1-Ni(1)-N(6)#2	99.19(10)	N(4)#3-Ni(1)-O(1)	90.72(10)
O(3)#1-Ni(1)-N(4)#3	91.77(10)	N(1)-Ni(1)-O(1)	91.95(10)

N(6)#2-Ni(1)-N(4)#3	94.07(11)	O(3)#1-Ni(1)-O(1W)	86.87(10)
O(3)#1-Ni(1)-N(1)	85.22(10)	N(6)#2-Ni(1)-O(1W)	173.76(11)
N(6)#2-Ni(1)-N(1)	90.03(12)	N(4)#3-Ni(1)-O(1W)	87.20(12)
N(4)#3-Ni(1)-N(1)	175.26(11)	N(1)-Ni(1)-O(1W)	88.98(12)
O(3)#1-Ni(1)-O(1)	174.24(9)	O(1)-Ni(1)-O(1W)	88.07(9)
N(6)#2-Ni(1)-O(1)	85.81(10)		
Ni(TBDC)(bix)·H ₂ O (5)			
Ni(1)-O(1)#1	2.016(2)	Ni(1)-N(5)	2.092(3)
Ni(1)-N(1)	2.048(3)	Ni(1)-O(4)	2.115(2)
Ni(1)-N(3)	2.076(3)	Ni(1)-O(3)	2.234(2)
O(1)#1-Ni(1)-N(1)	109.44(10)	N(3)-Ni(1)-O(4)	92.53(10)
O(1)#1-Ni(1)-N(3)	86.48(10)	N(5)-Ni(1)-O(4)	88.07(10)
N(1)-Ni(1)-N(3)	92.05(11)	O(1)#1-Ni(1)-O(3)	96.73(9)
O(1)#1-Ni(1)-N(5)	92.35(10)	N(1)-Ni(1)-O(3)	153.84(10)
N(1)-Ni(1)-N(5)	89.52(10)	N(3)-Ni(1)-O(3)	89.33(10)
N(3)-Ni(1)-N(5)	178.28(12)	N(5)-Ni(1)-O(3)	89.56(9)
O(1)#1-Ni(1)-O(4)	157.30(9)	O(4)-Ni(1)-O(3)	60.57(8)
N(1)-Ni(1)-O(4)	93.26(10)		
Ni(TBDC)(mbix)(H ₂ O)·H ₂ O (6)			
Ni(1)-O(4)#1	2.0395(18)	Ni(1)-O(1W)	2.0778(19)
Ni(1)-N(3)	2.066(2)	Ni(1)-O(1)	2.1374(19)
Ni(1)-N(1)#2	2.068(2)	Ni(1)-O(2)	2.1784(17)
O(4)#1-Ni(1)-N(3)	89.61(8)	N(1)#2-Ni(1)-O(1)	91.12(9)
O(4)#1-Ni(1)-N(1)#2	88.94(9)	O(1W)-Ni(1)-O(1)	162.08(8)
N(3)-Ni(1)-N(1)#2	177.86(8)	O(4)#1-Ni(1)-O(2)	162.64(8)
O(4)#1-Ni(1)-O(1W)	96.36(8)	N(3)-Ni(1)-O(2)	89.48(8)
N(3)-Ni(1)-O(1W)	93.54(9)	N(1)#2-Ni(1)-O(2)	91.43(8)
N(1)#2-Ni(1)-O(1W)	88.19(9)	O(1W)-Ni(1)-O(2)	101.00(7)
O(4)#1-Ni(1)-O(1)	101.52(7)	O(1)-Ni(1)-O(2)	61.12(7)
N(3)-Ni(1)-O(1)	87.63(9)		

Ni(TBDC)(obix)(H₂O) (7)

Ni(1)-O(4)#1	2.0227(18)	Ni(1)-N(1)	2.086(2)
Ni(1)-N(4)#2	2.071(2)	Ni(1)-O(1)	2.1548(18)
Ni(1)-O(1W)	2.072(2)	Ni(1)-O(2)	2.1634(18)
O(4)#1-Ni(1)-N(4)#2	88.07(8)	O(1W)-Ni(1)-O(1)	160.32(8)
O(4)#1-Ni(1)-O(1W)	96.57(8)	N(1)-Ni(1)-O(1)	90.73(8)
N(4)#2-Ni(1)-O(1W)	93.61(9)	O(4)#1-Ni(1)-O(2)	164.28(7)
O(4)#1-Ni(1)-N(1)	89.27(9)	N(4)#2-Ni(1)-O(2)	92.27(8)
N(4)#2-Ni(1)-N(1)	176.82(9)	O(1W)-Ni(1)-O(2)	99.09(7)
O(1W)-Ni(1)-N(1)	88.43(9)	N(1)-Ni(1)-O(2)	89.82(8)
O(4)#1-Ni(1)-O(1)	103.08(7)	O(1)-Ni(1)-O(2)	61.24(7)
N(4)#2-Ni(1)-O(1)	88.18(8)		

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