Electronic Supplementary Information

Four-, and six-connected entangled frameworks based on flexible bis(imidazole) ligands and long dicarboxylate anions

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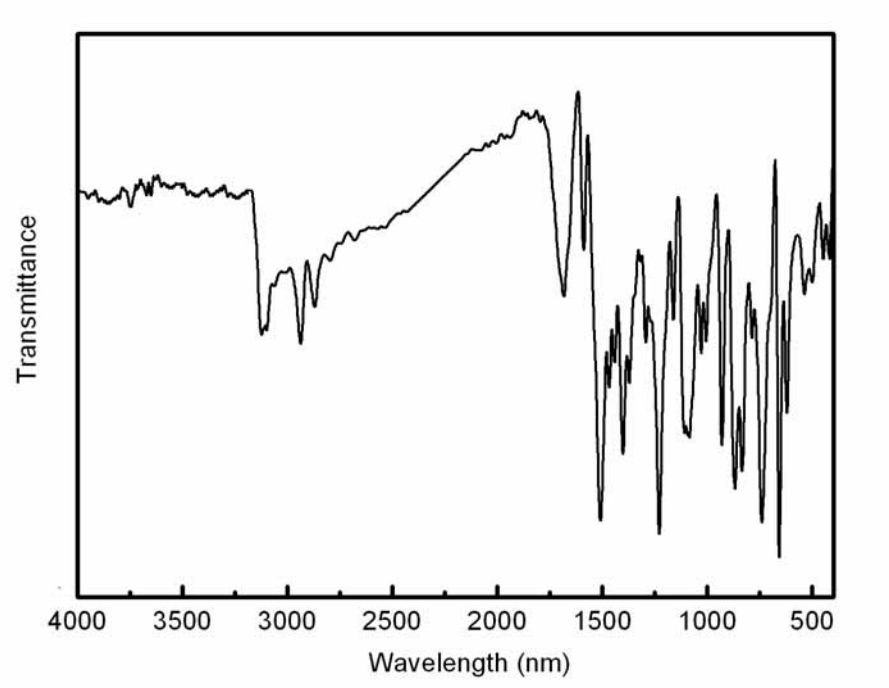

Fig. S1. IR spectrum of compound **1**.

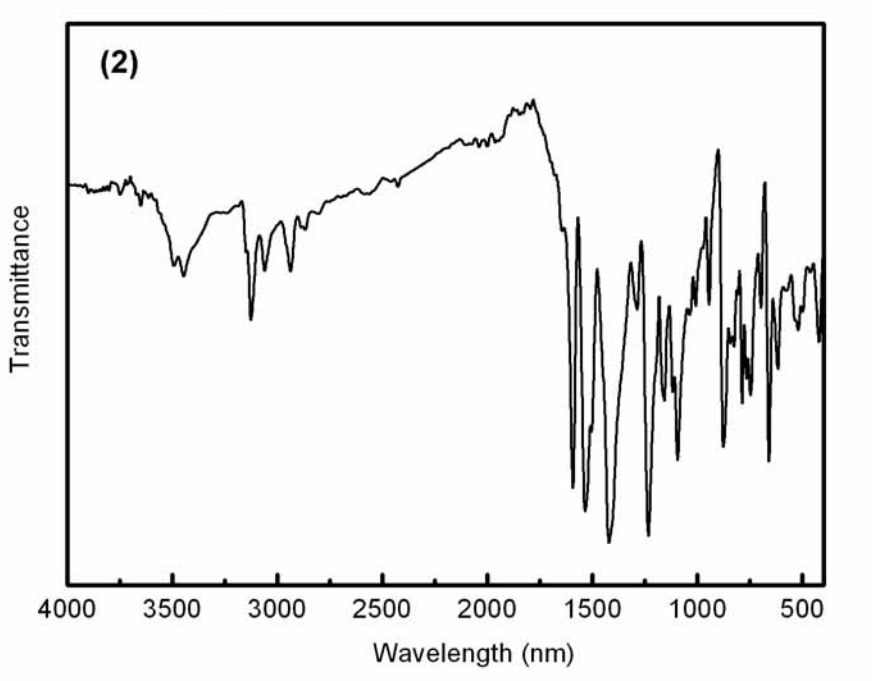

Fig. S2. IR spectrum of compound **2**.

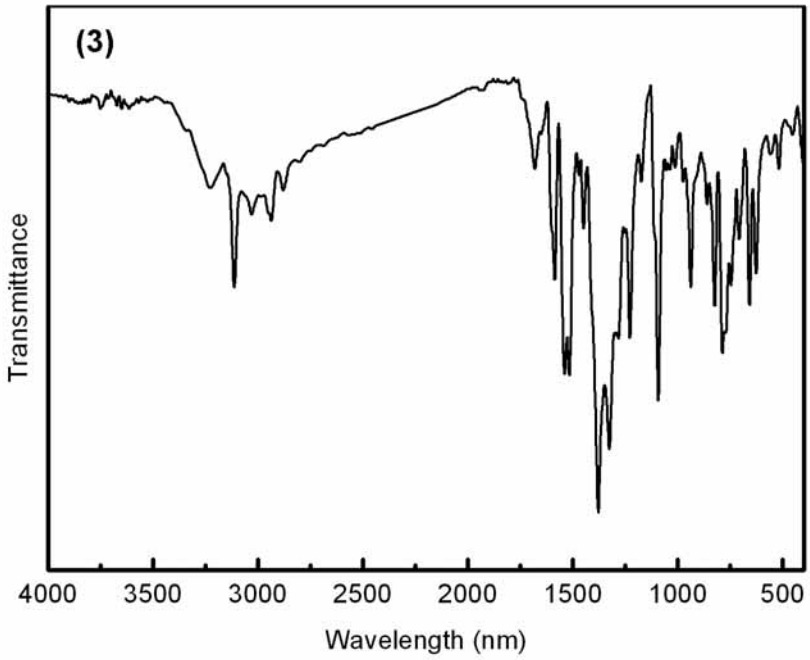

Fig. S3. IR spectrum of compound **3**.

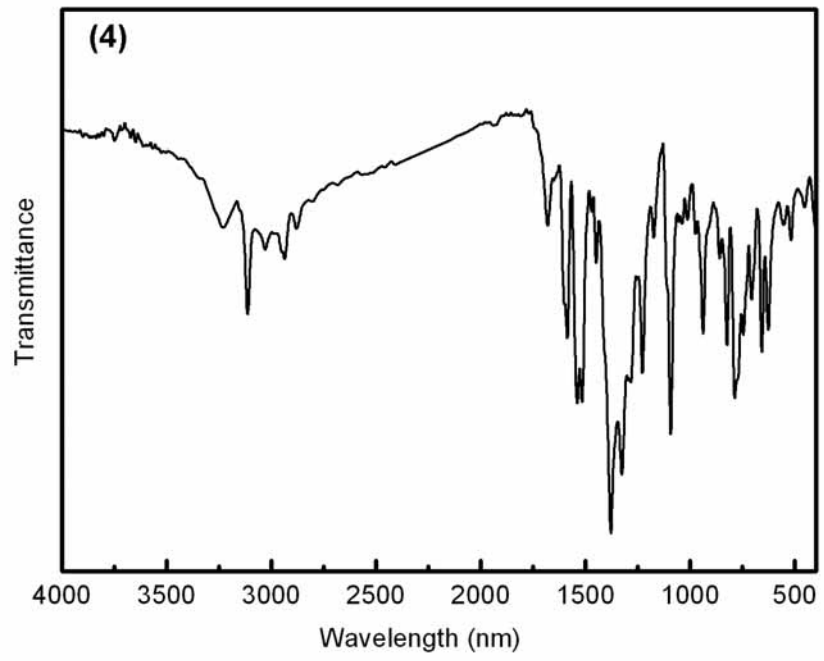

Fig. S4. IR spectrum of compound **4**.

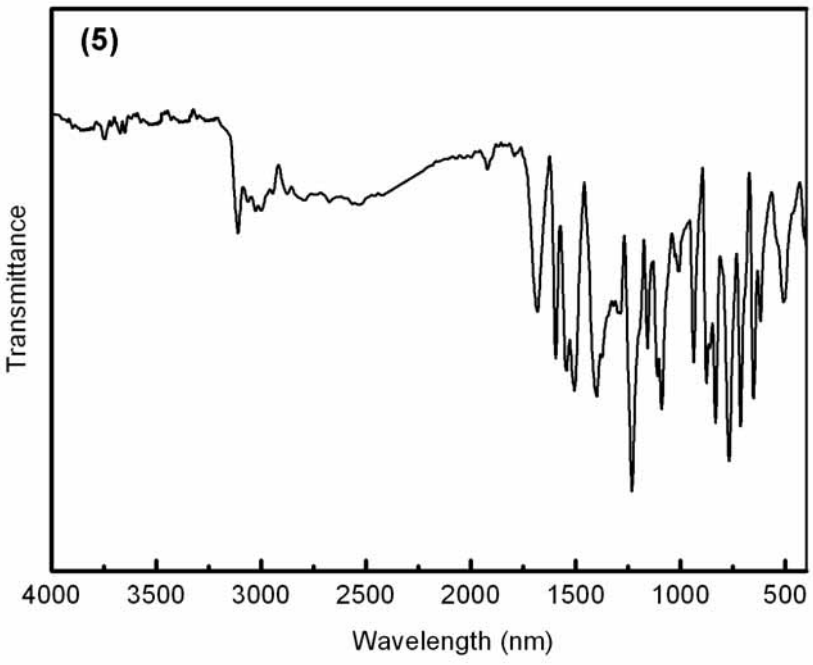

Fig. S5. IR spectrum of compound **5**.

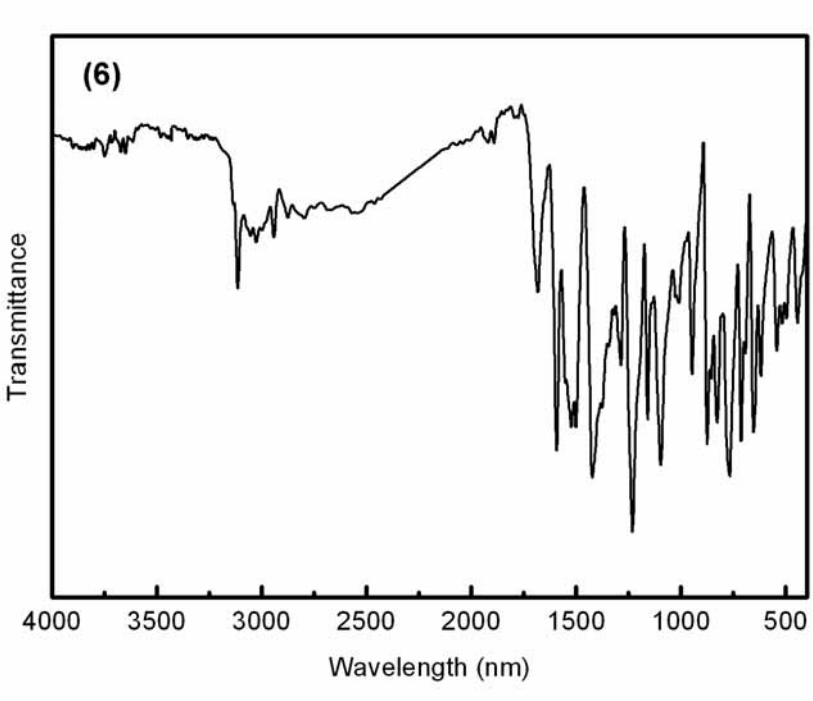

Fig. S6. IR spectrum of compound **6**.

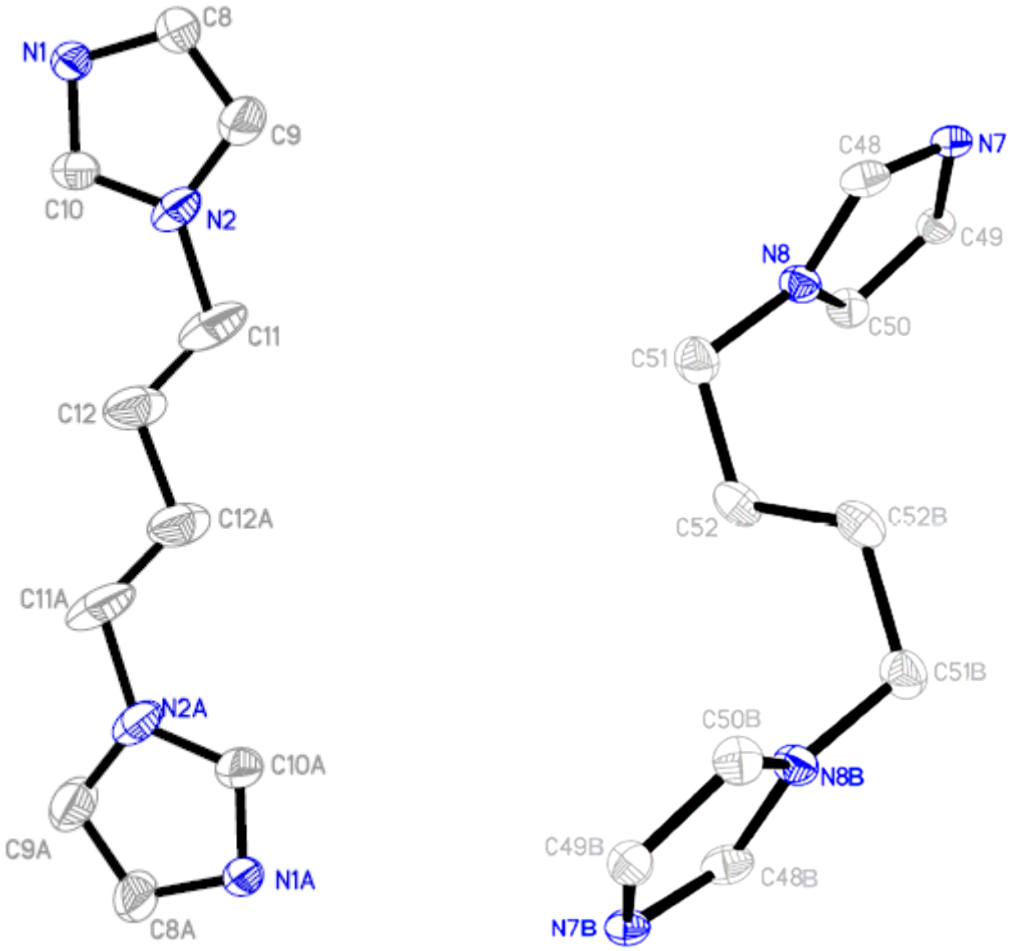

Fig. S7. The TTT (left) and TGT (right) conformations of bbi ligands. (The TTT and TGT conformations are present in compounds **3** and **4**, respectively). Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (A) -x, 2-y, 2-z; (B) -2-x, 2-y, 3-z.]

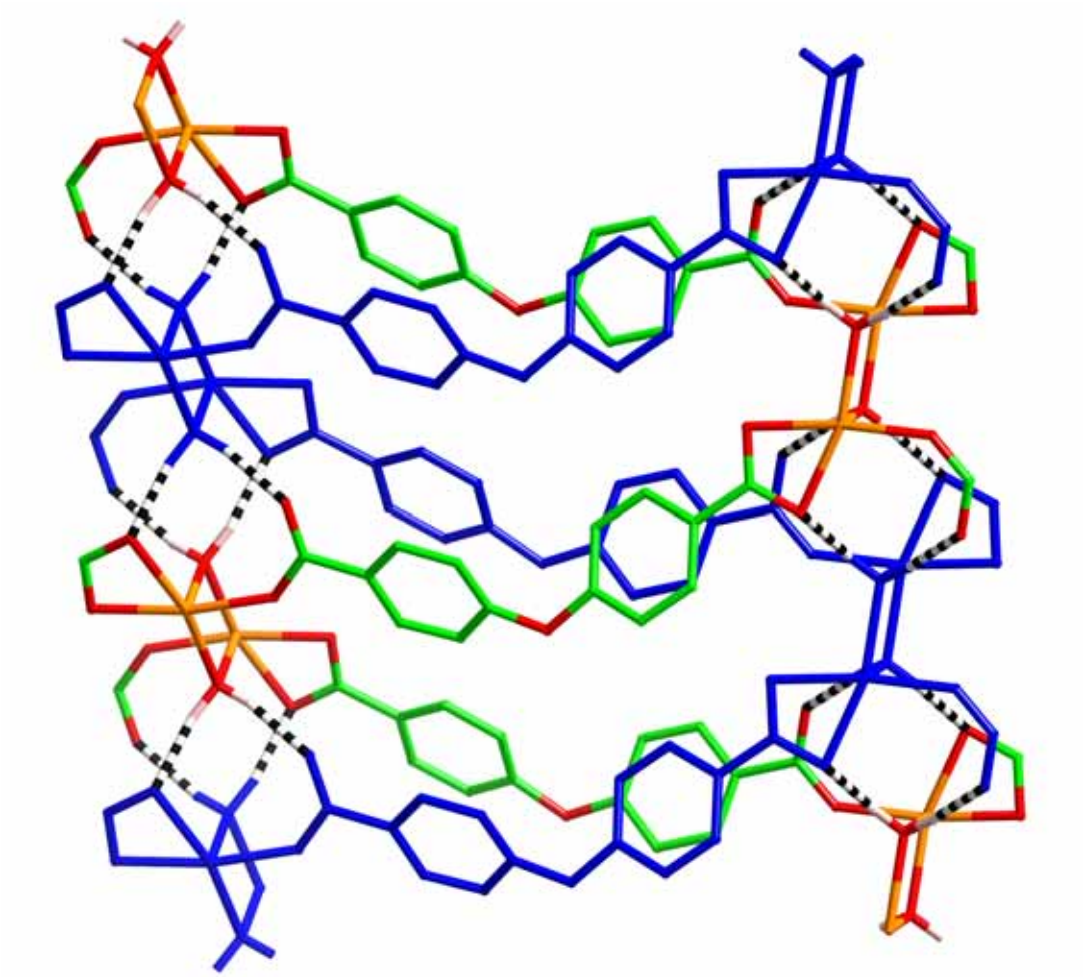

Fig. S8. A double helix motif in the $[Ni_2(oba)_2]$ layers, showing the crosslinking of the two strands by hydrogen bonds (striped bonds).

Table S1. Selected Bond Lengths [Å] and Angles [deg] for **1**.

Cd(1)-N(1)	2.286(7)	Cd(1)-N(3)$^{\#2}$	2.240(6)
Cd(1)-O(1)	2.404(5)	Cd(1)-O(2)	2.309(4)
Cd(1)-O(3)$^{\#1}$	2.432(4)	Cd(1) -O(4)$^{\#1}$	2.298(5)
N(3)$^{\#3}$-Cd(1)-N(1)	96.0(2)	N(3)$^{\#3}$-Cd(1)-O(4)$^{\#4}$	146.3(2)
N(1)-Cd(1)-O(4)$^{\#4}$	86.3(2)	N(3)$^{\#3}$-Cd(1)-O(2)	104.78(19)
N(1)-Cd(1)-O(2)	99.5(2)	O(4)$^{\#4}$-Cd(1)-O(2)	108.04(18)
N(3)$^{\#3}$-Cd(1)-O(1)	99.23(19)	N(1)-Cd(1)-O(1)	153.75(18)
O(4)$^{\#4}$-Cd(1)-O(1)	92.69(19)	O(2)-Cd(1)-O(1)	55.96(19)
N(3)$^{\#3}$-Cd(1)-O(3)$^{\#4}$	92.2(2)	N(1)-Cd(1)-O(3)$^{\#4}$	100.46(19)
O(4)$^{\#4}$-Cd(1)-O(3)$^{\#4}$	54.50(18)	O(2)-Cd(1)-O(3)$^{\#4}$	152.21(18)
O(1)-Cd(1)-O(3)$^{\#4}$	100.20(17)		

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ -x+1/4, y+1/4, z+1/4; $^{\#2}$ x-1/2, y, z-1/2; $^{\#3}$ x+1/2, y, z+1/2; $^{\#4}$ -x+1/4, y-1/4, z-1/4.

Table S2. Selected Bond Lengths [Å] and Angles [deg] for **2**.

Ni(1)-N(1)	2.040(6)	Ni(1)-N(4)$^{\#3}$	2.023(6)
Ni(2)-N(5)	2.057(6)	Ni(2)-N(7)$^{\#3}$	2.032(6)
Ni(1)-O(1)	2.102(5)	Ni(1)-O(2)	2.145(5)
Ni(1)-O(3)$^{\#1}$	2.137(5)	Ni(1)-O(4)$^{\#1}$	2.113(5)
Ni(2)-O(5)	2.114(5)	Ni(2)-O(8)$^{\#2}$	2.210(5)
Ni(2)-O(7)$^{\#2}$	2.066(5)	Ni(2)-O(6)	2.117(5)
N(4)$^{\#4}$-Ni(1)-N(1)	93.6(2)	N(4)$^{\#4}$-Ni(1)-O(1)	99.5(2)
N(1)-Ni(1)-O(1)	99.2(2)	N(4)$^{\#4}$-Ni(1)-O(4)$^{\#5}$	95.7(2)
N(1)-Ni(1)-O(4)$^{\#5}$	96.3(2)	O(1)-Ni(1)-O(4)$^{\#5}$	157.5(2)
N(4)$^{\#4}$-Ni(1)-O(3)$^{\#5}$	157.7(2)	N(1)-Ni(1)-O(3)$^{\#5}$	87.4(2)
O(1)-Ni(1)-O(3)$^{\#5}$	102.30(19)	O(4)$^{\#5}$-Ni(1)-O(3)$^{\#5}$	62.13(18)
N(4)$^{\#4}$-Ni(1)-O(2)	97.5(2)	N(1)-Ni(1)-O(2)	159.74(19)
O(1)-Ni(1)-O(2)	62.25(19)	O(4$^{)\#5}$-Ni(1)-O(2)	99.39(19)
O(3)$^{\#5}$-Ni(1)-O(2)	88.68(18)	O(6)-Ni(2)-O(8)$^{\#6}$	87.94(18)
N(7)$^{\#4}$-Ni(2)-N(5)	95.8(2)	N(7)$^{\#4}$-Ni(2)-O(7)$^{\#6}$	97.9(2)
N(5)-Ni(2)-O(7)$^{\#6}$	97.9(2)	N(7)$^{\#4}$-Ni(2)-O(5)	98.1(2)
N(5)-Ni(2)-O(5)	99.3(2)	O(7)$^{\#6}$-Ni(2)-O(5)	155.5(2)
N(7)$^{\#4}$-Ni(2)-O(6)	160.3(2)	N(5)-Ni(2)-O(6)	88.4(2)
O(7)$^{\#6}$-Ni(2)-O(6)	100.9(2)	O(5)-Ni(2)-O(6)	62.46(18)
N(7)$^{\#4}$-Ni(2)-O(8)$^{\#6}$	94.9(2)	N(5)-Ni(2)-O(8)$^{\#6}$	158.31(19)
O(7)$^{\#6}$-Ni(2)-O(8)$^{\#6}$	61.9(2)	O(5)-Ni(2)-O(8)$^{\#6}$	97.86(19)

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ x+1/2, -y+3/2, z+1/2; $^{\#2}$ x, -y+2, z+1/2; $^{\#3}$ x-1/2, y+1/2, z; $^{\#4}$ x+1/2, y-1/2, z; $^{\#5}$ x-1/2, -y+3/2, z-1/2; $^{\#6}$ x, -y+2, z-1/2.

Table S3. Selected Bond Lengths [Å] and Angles [deg] for **3**.

Co(1)-N(1)	2.028(5)	Co(1)-N(1)$^{\#1}$	2.028(5)
Co(1)-O(1)$^{\#1}$	2.212(8)	Co(1)-O(2)	2.235(10)
Co(1)-O(1)	2.212(8)	Co(1)-O(2)$^{\#1}$	2.235(10)
N(1)-Co(1)-N(1)$^{\#1}$	107.2(3)	N(1)-Co(1)-O(1)	94.3(3)
N(1)$^{\#1}$-Co(1)-O(1)	92.6(2)	N(1)-Co(1)-O(1)$^{\#1}$	92.6(2)
N(1)$^{\#1}$-Co(1)-O(1)$^{\#1}$	94.3(3)	O(1)-Co(1)-O(1)$^{\#1}$	168.3(5)
N(1)-Co(1)-O(2)	96.3(3)	N(1)$^{\#1}$-Co(1)-O(2)	141.8(3)
O(1)-Co(1)-O(2)	55.1(3)	O(1)$^{\#1}$-Co(1)-O(2)	114.7(3)
N(1)-Co(1)-O(2)$^{\#1}$	141.8(3)	N(1)$^{\#1}$-Co(1)-O(2)$^{\#1}$	96.3(3)
O(1)-Co(1)-O(2)$^{\#1}$	114.7(3)	O(1)$^{\#1}$-Co(1)-O(2)$^{\#1}$	55.1(3)
O(2)-Co(1)-O(2)$^{\#1}$	82.1(5)		

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ -x, y, -z+3/2.

Table S4. Selected Bond Lengths [Å] and Angles [deg] for **4**.

Co(1)-O(3)	1.972(3)	Co(1)-O(1)	1.998(3)
Co(1)-N(5)	2.014(3)	Co(1)-N(1)	2.035(3)
Co(2)-O(8)$^{\#1}$	1.960(3)	Co(2)-O(6)	1.976(3)
Co(2)-N(7)	2.025(3)	Co(2)-N(4)$^{\#2}$	2.044(4)
O(3)-Co(1)-O(1)	110.48(13)	O(3)-Co(1)-N(5)	119.11(13)
O(1)-Co(1)-N(5)	114.30(13)	O(3)-Co(1)-N(1)	106.36(13)
O(1)-Co(1)-N(1)	98.38(13)	N(5)-Co(1)-N(1)	105.57(14)
O(8)$^{\#1}$-Co(2)-O(6)	102.00(13)	O(8)$^{\#1}$-Co(2)-N(7)	130.50(14)
O(6)-Co(2)-N(7)	116.12(13)	O(8)$^{\#1}$-Co(2)-N(4)$^{\#2}$	104.40(13)
O(6)-Co(2)-N(4)$^{\#2}$	101.69(13)	N(7)-Co(2)-N(4)$^{\#2}$	97.76(14)

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ x, y+1, z+1; $^{\#2}$ x-2, y, z+1.

Table S5. Selected Bond Lengths [Å] and Angles [deg] for **5**.

Cd(1)-O(2)	2.2102(17)	Cd(1)-N(1)	2.2387(15)
Cd(1)-N(1)$^{\#1}$	2.2387(15)	Cd(1)-O(4)$^{\#2}$	2.4191(14)
Cd(1)-O(4)$^{\#3}$	2.4191(14)	Cd(1)-O(1)	2.5313(18)
O(2)-Cd(1)-N(1)	119.53(4)	O(2)-Cd(1)-N(1)$^{\#1}$	119.53(4)
N(1)-Cd(1)-N(1)$^{\#1}$	104.21(8)	O(2)-Cd(1)-O(4)$^{\#2}$	97.93(5)
N(1)-Cd(1)-O(4)$^{\#2}$	127.92(5)	N(1)$^{\#1}$-Cd(1)-O(4)$^{\#2}$	83.88(5)
O(2)-Cd(1)-O(4)$^{\#3}$	97.93(5)	N(1)-Cd(1)-O(4)$^{\#3}$	83.88(5)
N(1)$^{\#1}$-Cd(1)-O(4)$^{\#3}$	127.92(5)	O(4)$^{\#2}$-Cd(1)-O(4)$^{\#3}$	54.38(7)
O(2)-Cd(1)-O(1)	55.24(6)	N(1)-Cd(1)-O(1)	88.85(4)
N(1)$^{\#1}$-Cd(1)-O(1)	88.85(4)	O(4)$^{\#2}$-Cd(1)-O(1)	143.19(4)
O(4)$^{\#3}$-Cd(1)-O(1)	143.19(4)		

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ x, -y+1/2, z; $^{\#2}$ x+1, y, z; $^{\#3}$ x+1, -y+1/2, z.

Table S6. Selected Bond Lengths [Å] and Angles [deg] for **6**.

Ni(1)-O(1)	1.9816(19)	Ni(1)-N(1)	2.047(2)
Ni(1)-O(4)$^{\#1}$	2.1046(18)	Ni(1)-O(1W)$^{\#2}$	2.109(2)
Ni(1)-O(5)$^{\#1}$	2.1194(19)	Ni(1)-O(1W)	2.124(2)
O(1)-Ni(1)-N(1)	91.07(9)	O(1)-Ni(1)-O(4)$^{\#1}$	170.45(8)
N(1)-Ni(1)-O(4)$^{\#1}$	94.25(8)	O(1)-Ni(1)-O(1W)$^{\#2}$	88.76(8)
N(1)-Ni(1)-O(1W)$^{\#2}$	171.64(9)	O(4)$^{\#1}$-Ni(1)-O(1W)$^{\#2}$	87.13(8)
O(1)-Ni(1)-O(5)$^{\#1}$	109.17(8)	N(1)-Ni(1)-O(5)$^{\#1}$	94.85(8)
O(4)$^{\#1}$-Ni(1)-O(5)$^{\#1}$	62.50(7)	O(1W)$^{\#2}$-Ni(1)-O(5)$^{\#1}$	93.09(8)
O(1)-Ni(1)-O(1W)	87.87(8)	N(1)-Ni(1)-O(1W)	91.40(9)
O(4)$^{\#1}$-Ni(1)-O(1W)	99.91(8)	O(1W)$^{\#2}$-Ni(1)-O(1W)	80.24(8)
O(5)$^{\#1}$-Ni(1)-O(1W)	161.67(8)		

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ x+1/2, -y-1/2, z+1/2; $^{\#2}$ -x+3/2, -y+1/2, -z+1; $^{\#3}$ x-1/2, -y-1/2, z-1/2.