**Supporting Information**

# Entanglement in Co(II) coordination networks: polycatenation from single net to 2-fold and 3-fold interpenetrated nets

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**Fig. S1.** The TGA curves of complexes **1** – **4** and **6**.
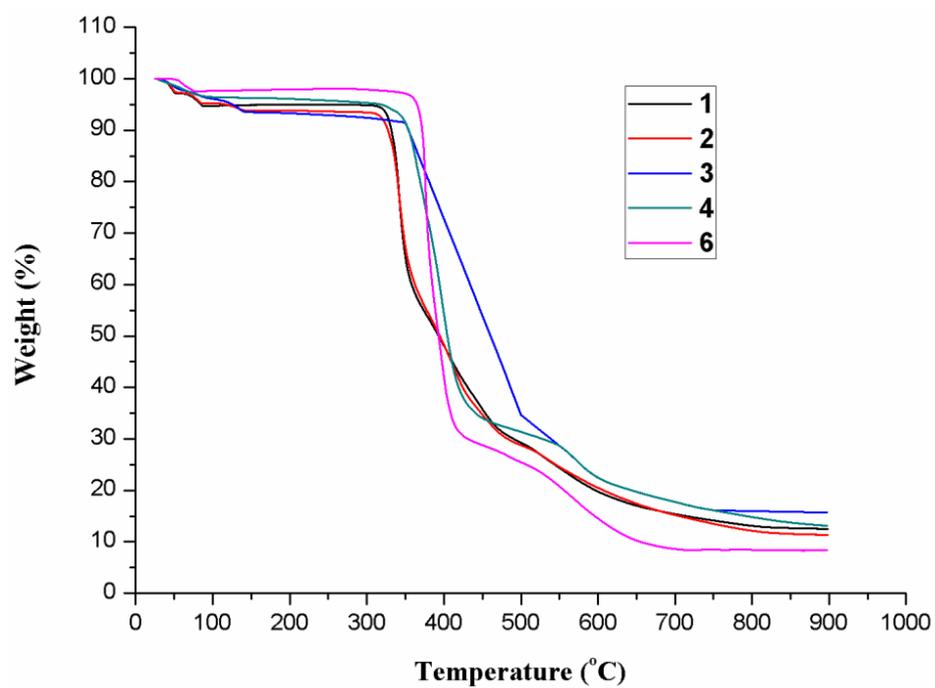
**Fig. S2.** Simulated (black) and as synthesized (red) PXRD patterns of complex **1**, and the pattern (blue) of the compound heated at 150 °C for 3hr.
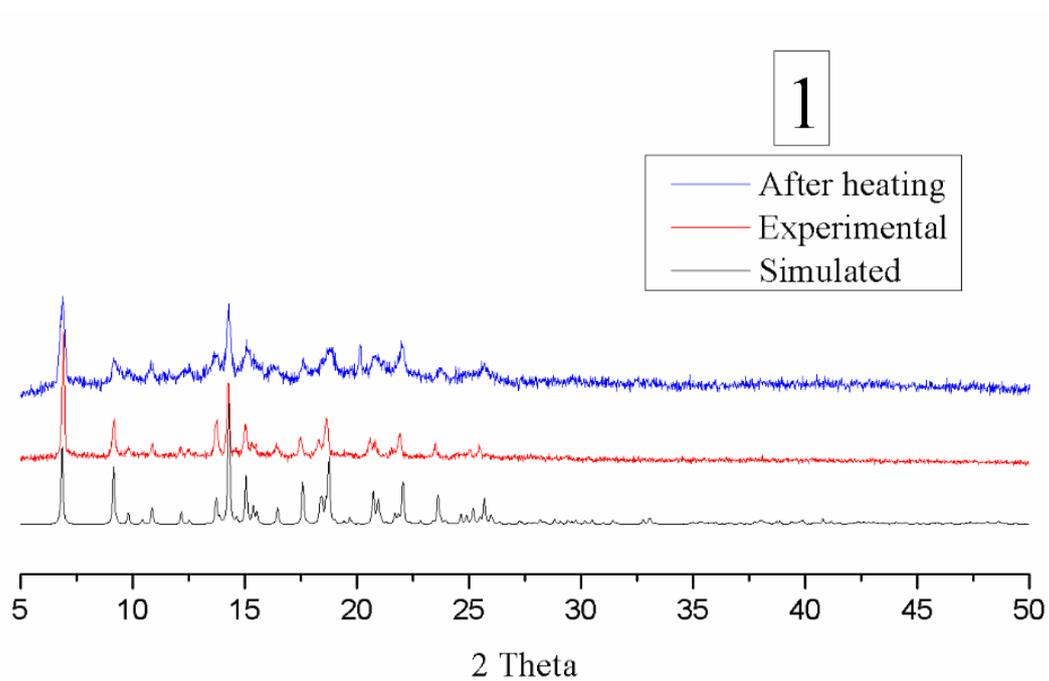
**Fig. S3.** Simulated (black) and as synthesized (red) PXRD patterns of complex **2**, and the pattern (blue) of the compound heated at 150 $^o$C for 3hr.
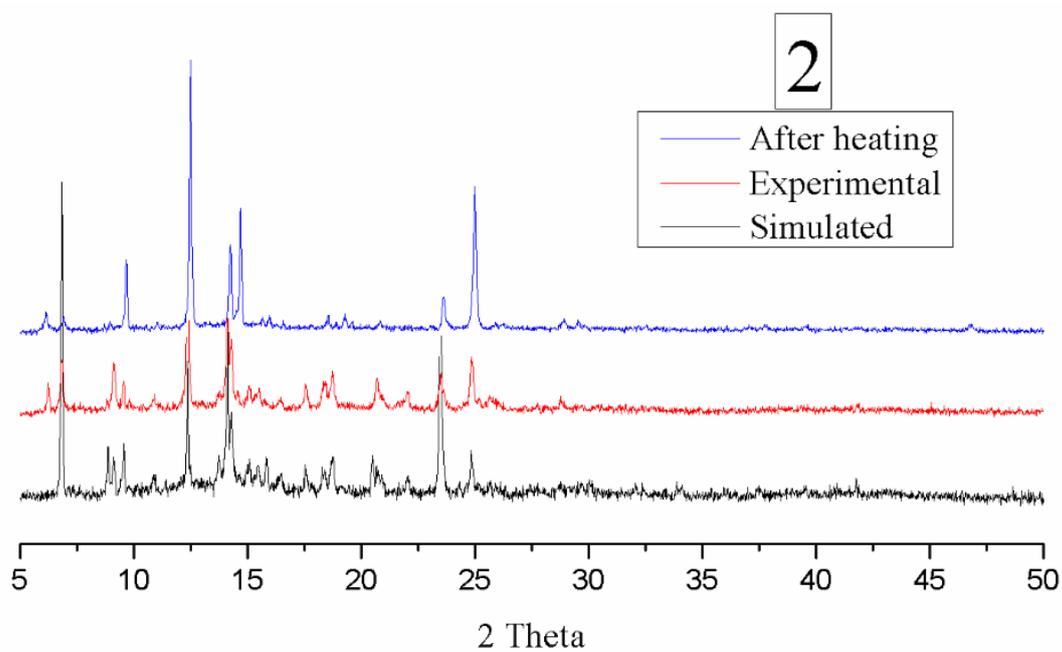
**Fig. S4.** Simulated (black) and as synthesized (red) PXRD patterns of complex **3**, and the pattern (blue) of the compound heated at 150 $^{o}$C for 3hr.
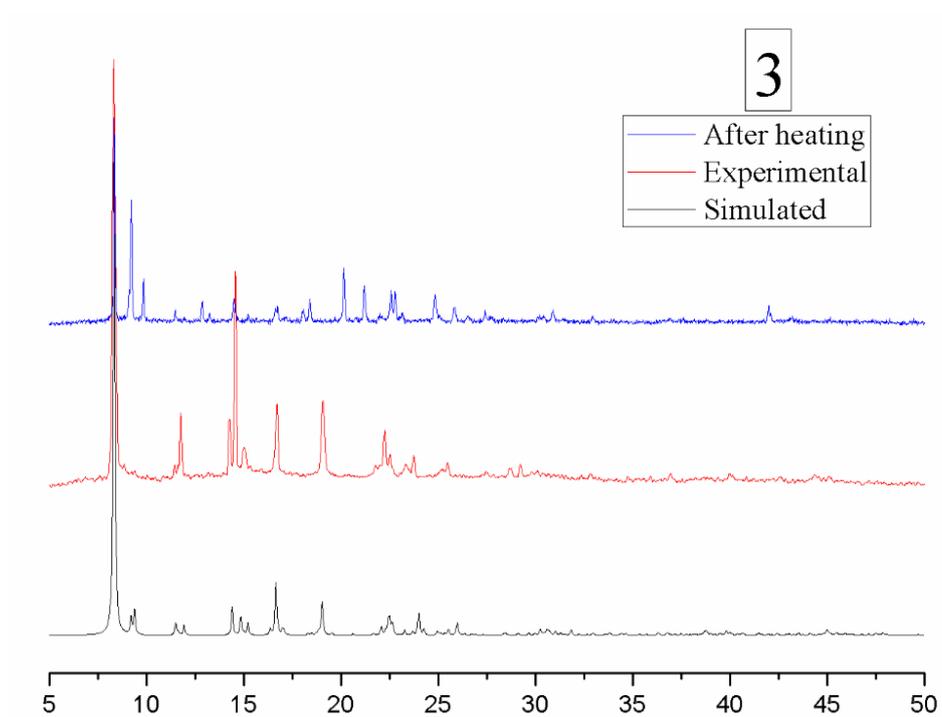
**Fig. S5.** Simulated (black) and as synthesized (red) PXRD patterns of complex **4**, and the pattern (blue) of the compound heated at 150 °C for 3hr.
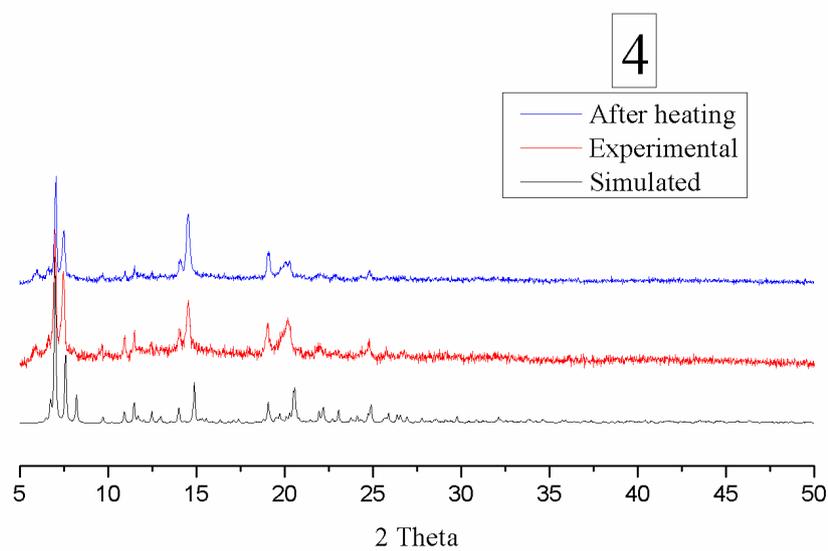
**Fig. S6.** Simulated (black) and as synthesized (red) PXRD patterns of complex **5**, and the pattern (blue) of the compound heated at 150 ºC for 3hr.
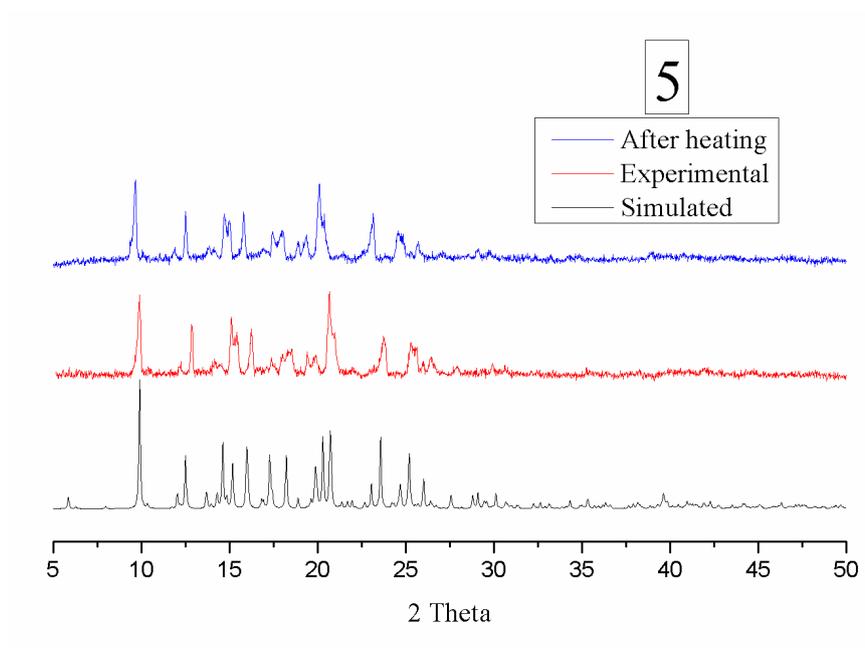
**Fig. S7.** Simulated (black) and as synthesized (red) PXRD patterns of complex **6**, and the pattern (blue) of the compound heated at 150 ᵒC for 3hr.
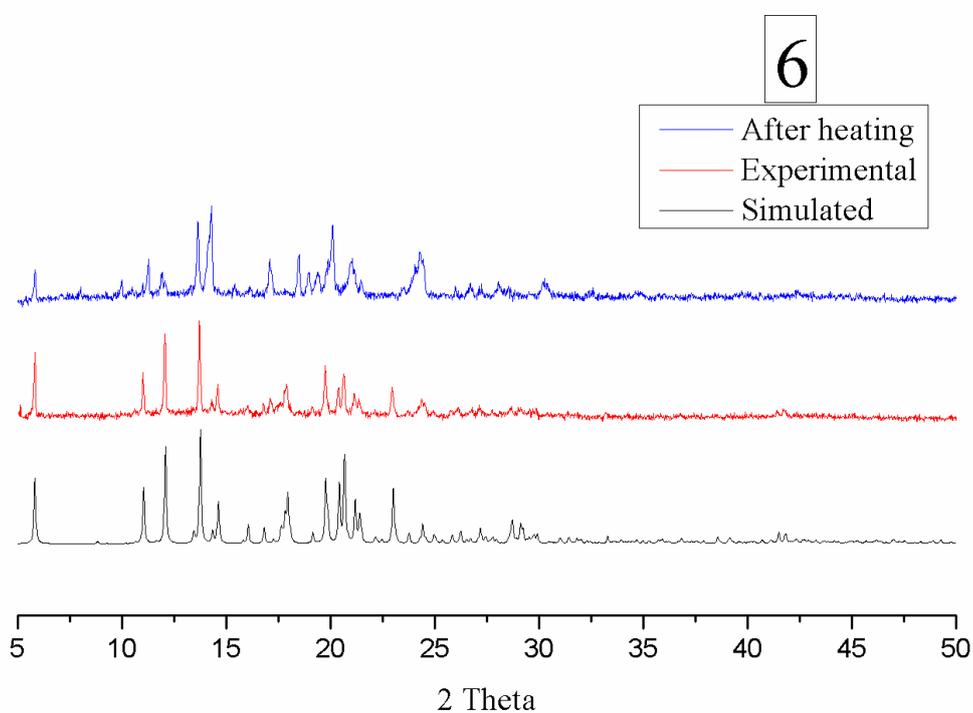
**Fig. S8.** (a) The adsorption isotherms for complex **4'**. (b) Isosteric heat of adsorption of **4'** at different $CO_2$ uptake amounts.
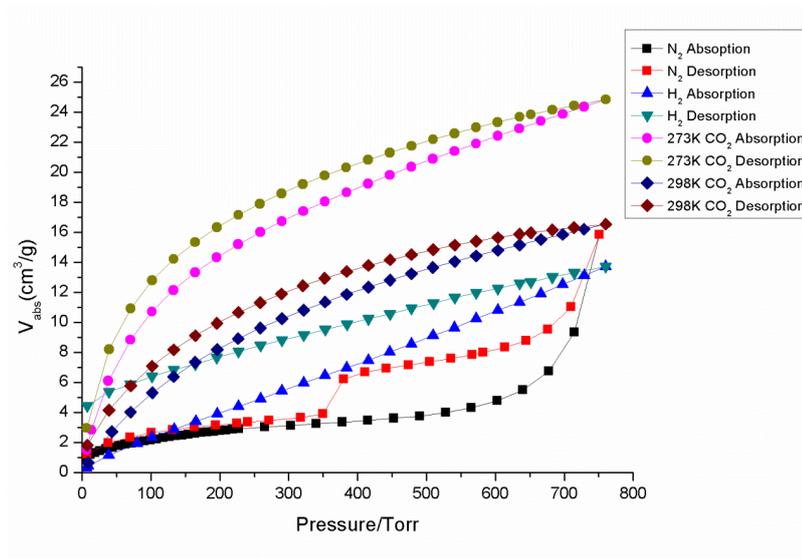


(a)
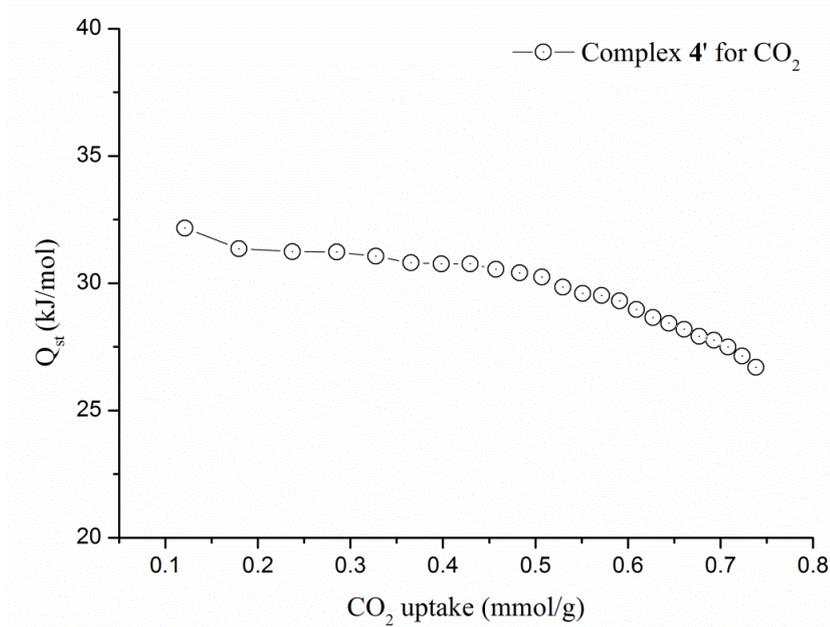


(b)

**Table S1.** Selected bond lengths (Å) and angles (°) for complex **1**.

| | |
|---|---|
| Co-O(5B) | 2.026(7) |
| Co-N(4A) | 2.071(8) |
| Co-N(1) | 2.079(8) |
| Co-O(4) | 2.133(7) |
| Co-O(3) | 2.186(7) |
| Co-O(6B) | 2.332(7) |
| | |
| O(5B)-Co-N(4A) | 101.9(3) |
| O(5B)-Co-N(1) | 95.0(3) |
| N(4A)-Co-N(1) | 98.9(3) |
| O(5B)-Co-O(4) | 159.8(3) |
| N(4A)-Co-O(4) | 92.8(3) |
| N(1)-Co-O(4) | 96.3(3) |
| O(5B)-Co-O(3) | 101.9(3) |
| N(4A)-Co-O(3) | 150.7(3) |
| N(1)-Co-O(3) | 95.7(3) |
| O(4)-Co-O(3) | 60.3(3) |
| O(5B)-Co-O(6B) | 59.4(2) |
| N(4A)-Co-O(6B) | 88.6(3) |
| N(1)-Co-O(6B) | 154.4(3) |
| O(4)-Co-O(6B) | 107.8(3) |
| O(3)-Co-O(6B) | 89.1(3) |

Symmetry transformations used to generate equivalent atoms:
(A) -x, y + 1/2, -z + 3/2   (B) x, y + 1, z.

**Table S2.** Selected bond lengths (Å) and angles (º) for complex **2**.

| | |
|---|---|
| Co-O(3A) | 2.0071(18) |
| Co-O(2) | 2.0278(17) |
| Co-O(5D) | 2.0362(18) |
| Co-N(1) | 2.0543(17) |
| Co-O(4C) | 2.0741(18) |
| | |
| O(3A)-Co-O(2) | 165.43(6) |
| O(3A)-Co-O(5D) | 91.47(8) |
| O(2)-Co-O(5D) | 88.45(7) |
| O(3A)-Co-N(1) | 98.56(7) |
| O(2)-Co-N(1) | 95.57(7) |
| O(5D)-Co-N(1) | 104.29(7) |
| O(3A)-Co-O(4C) | 87.05(8) |
| O(2)-Co-O(4C) | 89.26(7) |
| O(5D)-Co-O(4C) | 164.97(6) |
| N(1)-Co-O(4C) | 90.72(7) |

Symmetry transformations used to generate equivalent atoms:
(A) -x + 1, -y + 1, -z + 1 (B) -x + 2, -y + 1, -z + 3 (C) x + 1, y, z
(D)-x, -y + 1, -z + 1 (E) x - 1, y, z - 2.

**Table S3.** Selected bond lengths (Å) and angles (°) for complex **3.**

| | |
|---|---|
| Co-O(3A) | 2.001(2) |
| Co-O(2) | 2.002(2) |
| Co-N(1) | 2.059(2) |
| Co-O(4D) | 2.066(2) |
| Co-O(5B) | 2.1889(19) |
| | |
| O(3A) -Co-O(2) | 163.26(8) |
| O(3A)-Co-N(1) | 97.75(10) |
| O(2)-Co-N(1) | 96.11(9) |
| O(3A) -Co-O(4D) | 90.79(9) |
| O(2)-Co-O(4D) | 93.81(9) |
| N(1)-Co-O(4D) | 108.00(9) |
| O(3A)-Co-O(5A) | 86.01(8) |
| O(2)-Co-O(5E) | 84.90(8) |
| N(1)-Co-O(5E) | 88.94(9) |
| O(4D)-Co-O(5E) | 163.04(7) |

Symmetry transformations used to generate equivalent atoms:
(A) -x + 1 , -y + 1 , -z + 1 (B) -x + 3/2 , -y + 3/2 , -z
(C) x - 1/2 , y + 1/2 , z (D) -x + 1/2 , -y + 3/2 , -z + 1
(E) x + 1/2 , y - 1/2 , z

**Table S4**. Selected bond lengths (Å) and angles (º) for complex **4**.

| | |
|---|---|
| Co(1)-O(3) | 1.933(4) |
| Co(1)-O(12C) | 1.974(4) |
| Co(1)-O(6B) | 1.989(4) |
| Co(1)-N(1) | 2.022(5) |
| Co(2)-O(11C) | 2.003(4) |
| Co(2)-O(4) | 2.063(4) |
| Co(2)-O(8) | 2.082(4) |
| Co(2)-N(4A) | 2.112(5) |
| Co(2)-O(9) | 2.184(4) |
| Co(2)-O(6B) | 2.301(4) |
| | |
| O(3)-Co(1)-O(12C) | 105.42(16) |
| O(3)-Co(1)-O(6B) | 121.87(16) |
| O(12C) -Co(1)-O(6B) | 101.60(15) |
| O(3)-Co(1)-N(1) | 110.37(17) |
| O(12C) -Co(1)-N(1) | 104.35(17) |
| O(6B)-Co(1)-N(1) | 111.19(17) |
| O(11C)-Co(2)-O(4) | 101.33(16) |
| O(11C)-Co(2)-O(8) | 154.97(15) |
| O(4)-Co(2)-O(8) | 103.20(14) |
| O(11C) -Co(2)-N(4A) | 95.48(17) |
| O(4)-Co(2)-N(4A) | 87.66(16) |
| O(8)-Co(2)-N(4A) | 90.45(16) |
| O(11C)-Co(2)-O(9) | 93.74(15) |
| O(4)-Co(2)-O(9) | 164.93(15) |
| O(8)-Co(2)-O(9) | 61.78(14) |
| N(4A) -Co(2)-O(9) | 91.04(16) |
| O(11C) -Co(2)-O(6B) | 86.70(14) |
| O(4)-Co(2)-O(6B) | 96.43(14) |
| O(8)-Co(2)-O(6B) | 85.68(14) |
| N(4S) -Co(2)-O(6B) | 174.92(16) |
| O(9)-Co(2)-O(6B) | 84.23(14) |

Symmetry transformations used to generate equivalent atoms:
(A) x - 1 , -y + 1/2 , z - 3/2    (B) -x + 1 , y + 1/2 , -z - 5/2
(C) -x , y - 1/2 , -z - 5/2

**Table S5.** Selected bond lengths (Å) and angles (°) for complex **5.**

| | |
|---|---|
| Co-N(4B) | 2.084(5) |
| Co-N(1) | 2.089(5) |
| Co-O(5A) | 2.134(4) |
| Co-O(4) | 2.143(4) |
| Co-O(3) | 2.166(4) |
| Co-O(6A) | 2.168(4) |
| | |
| N(4B) -Co-N(1) | 99.1(2) |
| N(4B) -Co-O(5A) | 95.71(18) |
| N(1)-Co-O(5A) | 92.88(18) |
| N(4B)-Co-O(4) | 93.25(18) |
| N(1)-Co-O(4) | 98.00(19) |
| O(5A) -Co-O(4) | 164.64(17) |
| N(4B)-Co-O(3) | 151.97(18) |
| N(1)-Co-O(3) | 94.46(18) |
| O(5A)-Co-O(3) | 108.04(17) |
| O(4)-Co-O(3) | 60.46(16) |
| N(4B)-Co-O(6A) | 91.36(18) |
| N(1)-Co-O(6A) | 152.88(18) |
| O(5A)-Co-O(6A) | 61.04(16) |
| O(4)-Co-O(6A) | 106.36(16) |
| O(3)-Co-O(6A) | 87.49(16) |

Symmetry transformations used to generate equivalent atoms:
(A) x , y , z + 1 (B) -x + 1/2 , y - 1/2 , -z + 1/2

**Table S6.** Selected bond lengths (Å) and angles (°) for complex **6.**

| | |
|---|---|
| Co-O(5C) | 1.960(3) |
| Co-O(3) | 1.960(3) |
| Co-N(1) | 2.023(4) |
| Co-N(3) | 2.045(4) |
| | |
| O(5C)-Co-O(3) | 99.82(16) |
| O(5C)-Co-N(1) | 117.79(16) |
| O(3)-Co-N(1) | 113.37(15) |
| O(5C)-Co-N(3) | 97.96(15) |
| O(3)-Co-N(3) | 128.49(15) |
| N(1)-Co-N(3) | 99.71(15) |

Symmetry transformations used to generate equivalent atoms:
(A) -x + 3, -y + 1 , -z + 4 (B) -x + 4 , -y + 1 , -z + 2 (C) x + 1, y , z + 1