Electronic Supplementary Material (ESI) for Dalton Transactions

Structural Evolution and Magnetic Properties of Co^{II} Coordination Polymers Varied From 1D to 3D Constructed by 1,4-Bis(1,2,4-triazol-1-ylmethyl)-Benzene

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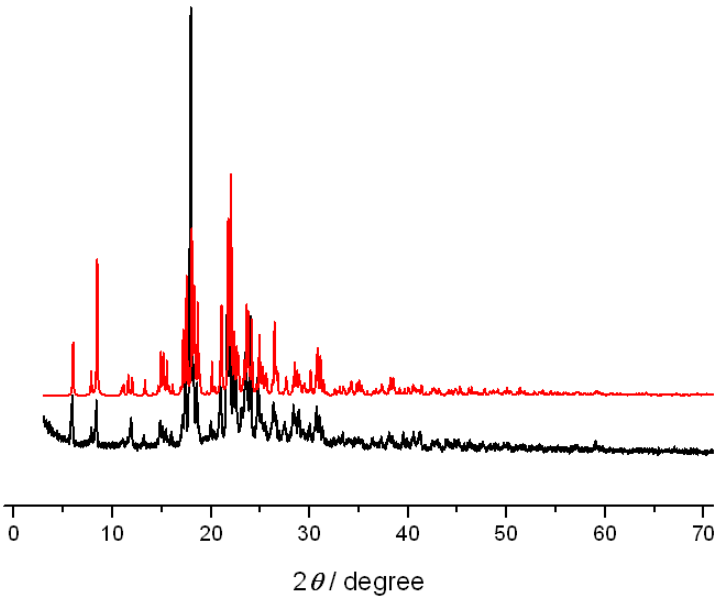
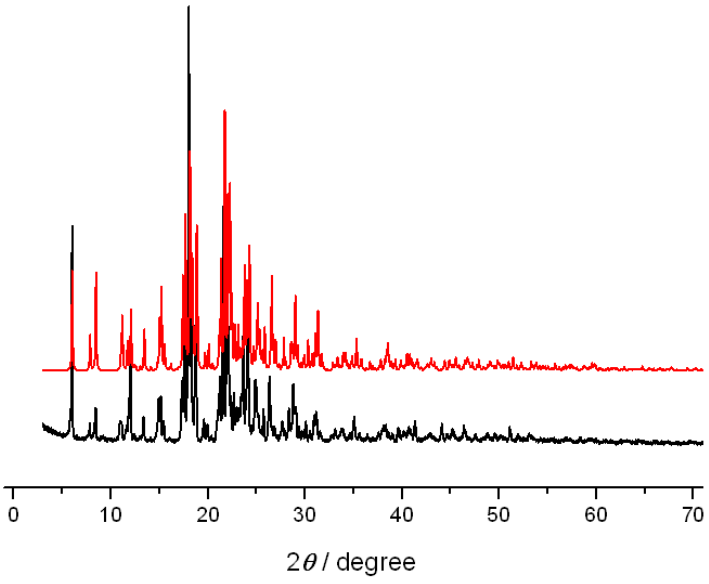


(a)



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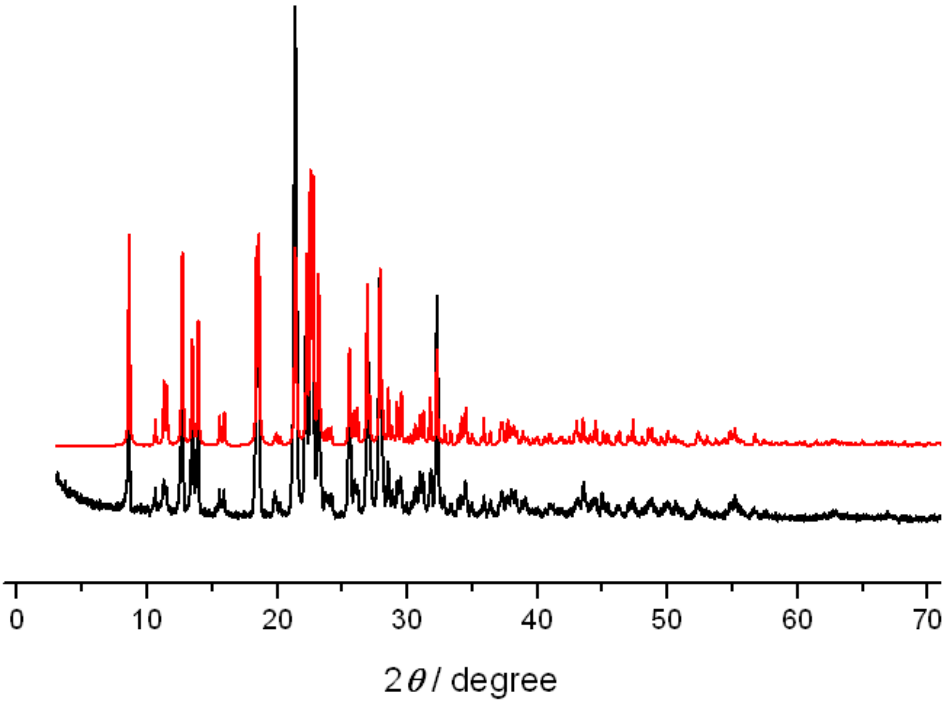

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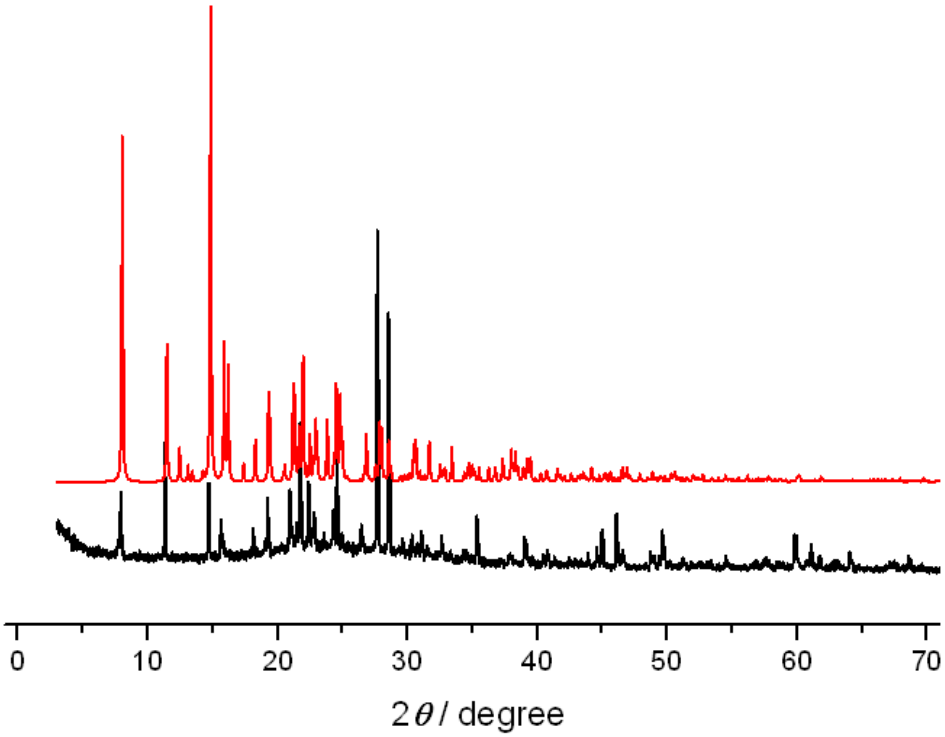

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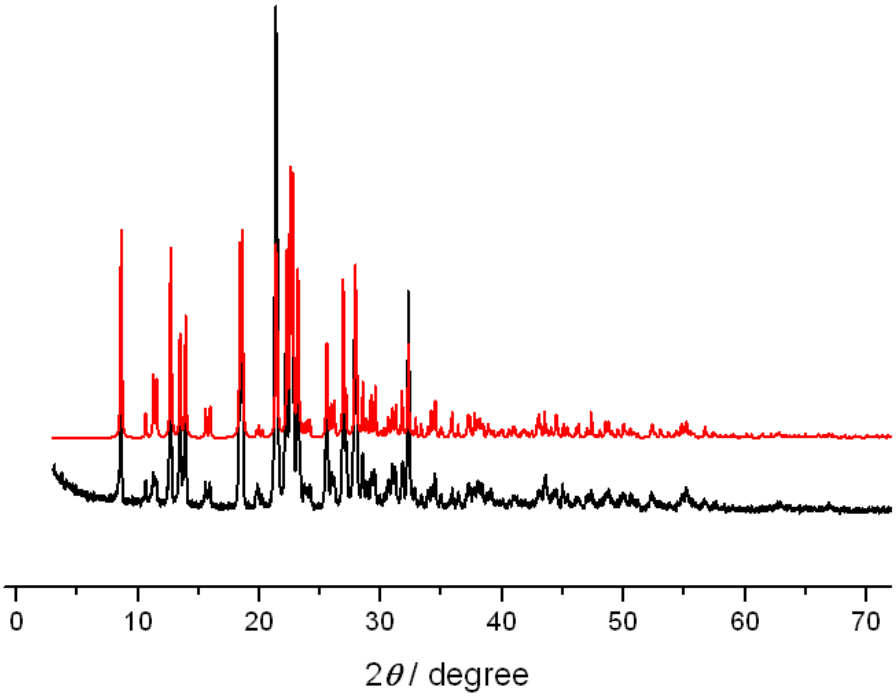

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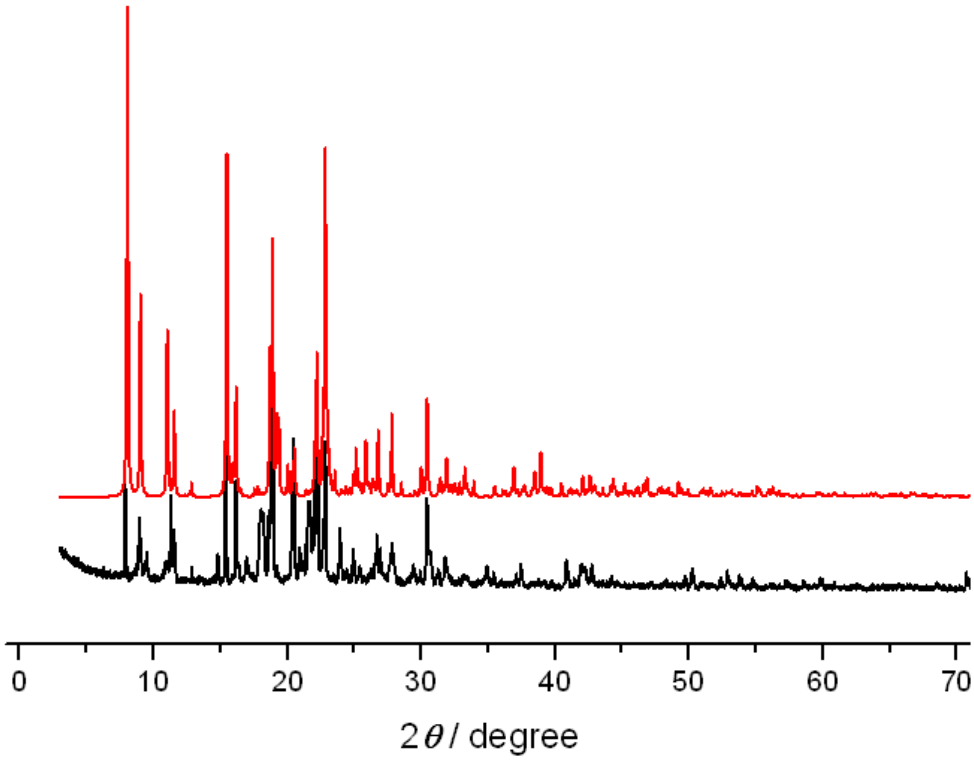

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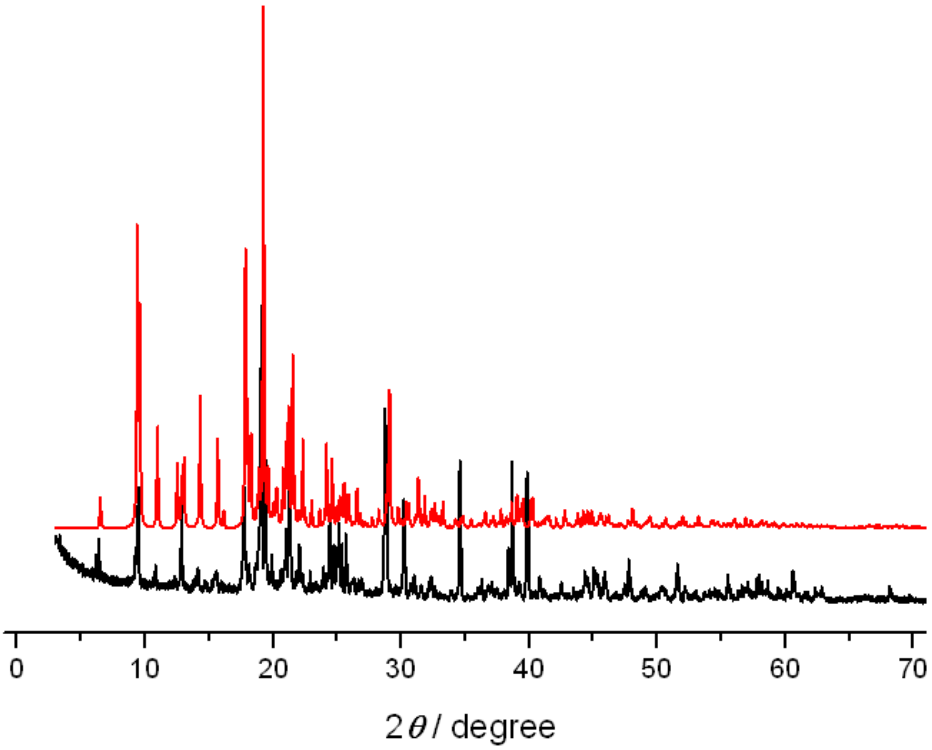
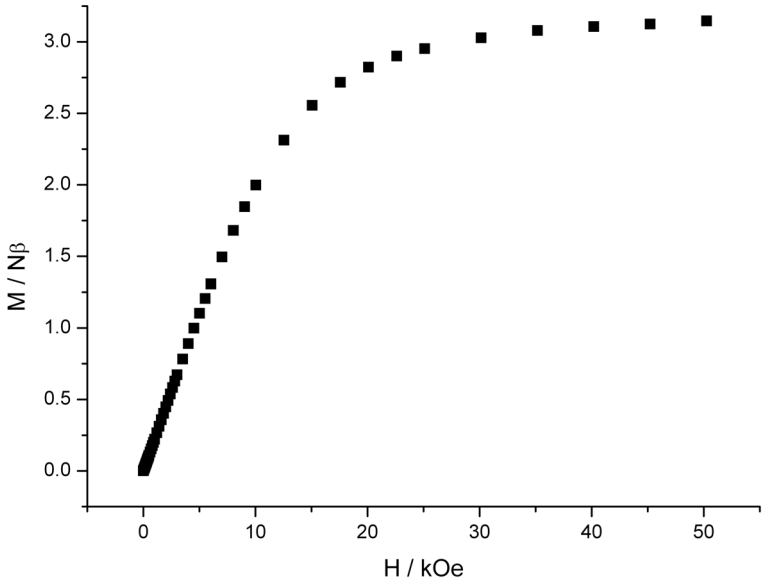
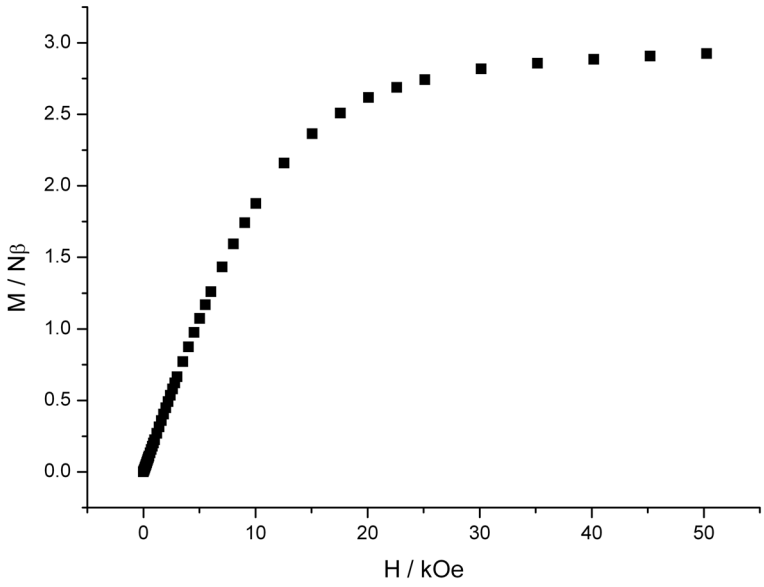


(g)

Figure S1 Powder X-ray diffraction spectra comparison of complexes **1**-**7**, corresponding to (a)-(g). Black lines response to the experimental data and red lines response to the simulated data.



(a)



(b)

Figure S2 The magnetization curves of **6** (a) and **7** (b) measured at 2 K.

Table S1 The Coordination Environment of the Cobalt Atom in Compounds **1**-**7**. Selected Interatomic Distances (Å) and Angles (deg)

complex **1**					
Co(1)-O(1)	2.067(2)	O(1)-Co(1)-N(1)	89.94(11)	N(1)-Co(1)-N(7)	88.93(10)
Co(1)-O(1)#1	2.067(2)	O(1)#1-Co(1)-N(1)	90.06(11)	N(1)#1-Co(1)-N(7)	91.07(10)
Co(1)-N(1)	2.154(3)	O(1)-Co(1)-N(1)#1	90.06(11)	O(1)-Co(1)-N(7)#1	90.69(10)
Co(1)-N(1)#1	2.154(3)	O(1)#1-Co(1)-N(1)#1	89.94(11)	O(1)#1-Co(1)-N(7)#1	89.31(10)
Co(1)-N(7)	2.171(3)	N(1)-Co(1)-N(1)#1	180.000(1)	N(1)-Co(1)-N(7)#1	91.07(10)
Co(1)-N(7)#1	2.171(3)	O(1)-Co(1)-N(7)	89.31(10)	N(1)#1-Co(1)-N(7)#1	88.93(10)
O(1)-Co(1)-O(1)#1	180.00(6)	O(1)#1-Co(1)-N(7)	90.69(10)	N(7)-Co(1)-N(7)#1	180.00(13)
complex **2**					
Co(1)-O(1)	2.082(2)	O(1)-Co(1)-N(7)	90.71(11)	N(7)-Co(1)-N(1)	91.09(12)
Co(1)-O(1)#1	2.082(2)	O(1)#1-Co(1)-N(7)	89.29(11)	N(7)#1-Co(1)-N(1)	88.91(12)
Co(1)-N(7)	2.142(3)	O(1)-Co(1)-N(7)#1	89.29(11)	O(1)-Co(1)-N(1)#1	89.86(11)
Co(1)-N(7)#1	2.142(3)	O(1)#1-Co(1)-N(7)#1	90.71(11)	O(1)#1-Co(1)-N(1)#1	90.14(11)
Co(1)-N(1)	2.150(3)	N(7)-Co(1)-N(7)#1	180.00(16)	N(7)-Co(1)-N(1)#1	88.91(12)
Co(1)-N(1)#1	2.150(3)	O(1)-Co(1)-N(1)	90.14(11)	N(7)#1-Co(1)-N(1)#1	91.09(12)
O(1)-Co(1)-O(1)#1	180.00(18)	O(1)#1-Co(1)-N(1)	89.86(11)	N(1)-Co(1)-N(1)#1	180
complex **3**					
Co(1)-O(1)#1	2.098(2)	O(1)#1-Co(1)-N(3)	92.15(11)	N(3)-Co(1)-N(2)	93.11(11)
Co(1)-O(1)	2.098(2)	O(1)-Co(1)-N(3)	87.85(11)	N(3)#1-Co(1)-N(2)	86.89(11)
Co(1)-N(3)	2.159(3)	O(1)#1-Co(1)-N(3)#1	87.85(11)	O(1)#1-Co(1)-N(2)#1	87.74(10)
Co(1)-N(3)#1	2.159(3)	O(1)-Co(1)-N(3)#1	92.15(11)	O(1)-Co(1)-N(2)#1	92.26(10)
Co(1)-N(2)	2.169(3)	N(3)-Co(1)-N(3)#1	180.0(2)	N(3)-Co(1)-N(2)#1	86.89(11)
Co(1)-N(2)#1	2.169(3)	O(1)#1-Co(1)-N(2)	92.26(10)	N(3)#1-Co(1)-N(2)#1	93.11(11)
O(1)#1-Co(1)-O(1)	180.00(14)	O(1)-Co(1)-N(2)	87.74(10)	N(2)-Co(1)-N(2)#1	180.00(13)

complex **4**					
N(4)-Co(1)#1	2.1236(19)	N(4)#2-Co(1)-N(4)#3	180.00(5)	N(4)#3-Co(1)-Cl(1)	89.18(5)
Co(1)-N(4)#2	2.1236(19)	N(4)#2-Co(1)-N(1)	91.95(7)	N(1)-Co(1)-Cl(1)	89.04(6)
Co(1)-N(4)#3	2.1236(19)	N(4)#3-Co(1)-N(1)	88.05(7)	N(1)#4-Co(1)-Cl(1)	90.96(6)
Co(1)-N(1)	2.1589(19)	N(4)#2-Co(1)-N(1)#4	88.05(7)	N(4)#2-Co(1)-Cl(1)#4	89.18(5)
Co(1)-N(1)#4	2.1589(19)	N(4)#3-Co(1)-N(1)#4	91.95(7)	N(4)#3-Co(1)-Cl(1)#4	90.82(5)
Co(1)-Cl(1)	2.5189(10)	N(1)-Co(1)-N(1)#4	180.000(1)	N(1)-Co(1)-Cl(1)#4	90.96(6)
Co(1)-Cl(1)#4	2.5189(10)	N(4)#2-Co(1)-Cl(1)	90.82(5)	N(1)#4-Co(1)-Cl(1)#4	89.04(6)
				Cl(1)-Co(1)-Cl(1)#4	180
complex **5**					
Co(1)-O(2)#3	2.030(2)	O(2)#3-Co(1)-O(3)#4	97.08(8)	O(3)#4-Co(1)-N(1)	87.44(10)
Co(1)-O(1)	2.036(2)	O(1)-Co(1)-O(3)#4	153.60(9)	N(4)-Co(1)-N(1)	173.40(10)
Co(1)-O(3)#4	2.136(2)	O(2)#3-Co(1)-N(4)	86.35(10)	O(2)#3-Co(1)-O(4)#4	156.78(8)
Co(1)-N(4)	2.143(3)	O(1)-Co(1)-N(4)	89.29(9)	O(1)-Co(1)-O(4)#4	94.53(8)
Co(1)-N(1)	2.155(3)	O(3)#4-Co(1)-N(4)	86.56(10)	O(3)#4-Co(1)-O(4)#4	59.74(8)
Co(1)-O(4)#4	2.257(2)	O(2)#3-Co(1)-N(1)	91.68(10)	N(4)-Co(1)-O(4)#4	93.12(9)
O(2)#3-Co(1)-O(1)	108.67(9)	O(1)-Co(1)-N(1)	97.30(10)	N(1)-Co(1)-O(4)#4	86.20(10)
complex **6**					
Co(1)-O(4)#1	2.017(3)	O(1)-Co(1)-O(6)#2	104.78(10)	O(7)#3-Co(2)-O(2)	92.94(11)
Co(1)-O(1)	2.057(3)	O(4)#1-Co(1)-N(2)	89.27(12)	O(7)-Co(2)-O(2)	87.06(11)
Co(1)-O(6)#2	2.126(3)	O(1)-Co(1)-N(2)	87.54(12)	O(7)#3-Co(2)-O(2)#3	87.06(11)
Co(1)-N(2)	2.130(3)	O(6)#2-Co(1)-N(2)	89.65(12)	O(7)-Co(2)-O(2)#3	92.94(11)
Co(1)-N(1)	2.147(4)	O(4)#1-Co(1)-N(1)	96.14(12)	O(2)-Co(2)-O(2)#3	180.000(1)
Co(1)-O(5)#2	2.176(3)	O(1)-Co(1)-N(1)	87.41(13)	O(7)#3-Co(2)-N(5)#3	85.96(14)
Co(2)-O(7)#3	2.083(3)	O(6)#2-Co(1)-N(1)	87.19(12)	O(7)-Co(2)-N(5)#3	94.04(14)

Co(2)-O(7)	2.083(3)	N(2)-Co(1)-N(1)	173.17(13)	O(2)-Co(2)-N(5)#3	86.61(13)
Co(2)-O(2)	2.107(3)	O(4)#1-Co(1)-O(5)#2	94.72(11)	O(2)#3-Co(2)-N(5)#3	93.39(13)
Co(2)-O(2)#3	2.107(3)	O(1)-Co(1)-O(5)#2	165.14(10)	O(7)#3-Co(2)-N(5)	94.04(14)
Co(2)-N(5)#3	2.117(4)	O(6)#2-Co(1)-O(5)#2	60.39(10)	O(7)-Co(2)-N(5)	85.96(14)
Co(2)-N(5)	2.117(4)	N(2)-Co(1)-O(5)#2	92.99(12)	O(2)-Co(2)-N(5)	93.39(13)
O(4)#1-Co(1)-O(1)	100.14(11)	N(1)-Co(1)-O(5)#2	90.72(13)	O(2)#3-Co(2)-N(5)	86.61(13)
O(4)#1-Co(1)-O(6)#2	155.00(11)	O(7)#3-Co(2)-O(7)	180.00(16)	N(5)#3-Co(2)-N(5)	180.00(11)
complex **7**					
Co(1)-O(2)#1	2.105(2)	O(2)#1-Co(1)-O(1)	93.59(9)	O(1)-Co(1)-N(1)	94.30(11)
Co(1)-O(2)	2.105(2)	O(2)-Co(1)-O(1)	86.41(9)	O(1)#1-Co(1)-N(1)	85.70(11)
Co(1)-O(1)	2.115(2)	O(2)#1-Co(1)-O(1)#1	86.41(9)	O(2)#1-Co(1)-N(1)#1	90.95(10)
Co(1)-O(1)#1	2.115(2)	O(2)-Co(1)-O(1)#1	93.59(9)	O(2)-Co(1)-N(1)#1	89.05(10)
Co(1)-N(1)	2.126(3)	O(1)-Co(1)-O(1)#1	180.00(13)	O(1)-Co(1)-N(1)#1	85.70(11)
Co(1)-N(1)#1	2.126(3)	O(2)#1-Co(1)-N(1)	89.05(10)	O(1)#1-Co(1)-N(1)#1	94.30(11)
O(2)#1-Co(1)-O(2)	180.00(13)	O(2)-Co(1)-N(1)	90.95(10)	N(1)-Co(1)-N(1)#1	180.0(2)

Symmetry transformations used to generate equivalent atoms: (1) #1 -x,-y+2,-z+1; #2 -x-1,-y+1,-z+1; #3 -x,-y+1,-z. (2) #1 -x+1,-y+1,-z; #2 -x,-y,-z; #3 -x+1,-y,-z+1. (3) #1 -x+2,-y,-z; #2 -x+1,-y,-z+1. (4) #1 -x+1,y-1/2,-z+3/2; #2 x-1,-y+1/2,z+1/2; #3 -x+1,y+1/2,-z+3/2; #4 -x,-y+1,-z+2. (5) #1 -x+1,-y+1,-z; #2 -x+2,-y+1,-z. (6) #1 -x,-y+3,-z+2; #2 -x+2,-y+2,-z; #3 -x,-y+2,-z+1; #4 x,y+1,z; #5 x,y-1,z. (7) #1 x,y+1,z; #2 -x,y+1/2,-z+3/2; #3 -x+1,-y,-z+2; #4 -x,y-1/2,-z+3/2; #5 x,y-1,z; #6 x-1,y-1,z; #7 x+1,y+1,z; #8 -x+2,-y+1,-z+2.