Electronic Supplementary Material (ESI) for Dalton Transactions.

Synthesis, Characterization and Magnetism of Metal-Organic Compounds: Role of Positions of the Coordinating Groups of a Meso-flexible Ligand in Placing Anisotropy to Exhibit Spin-Canting Behaviour

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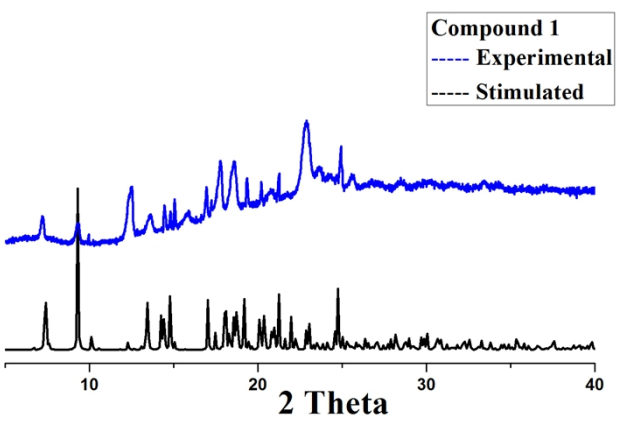
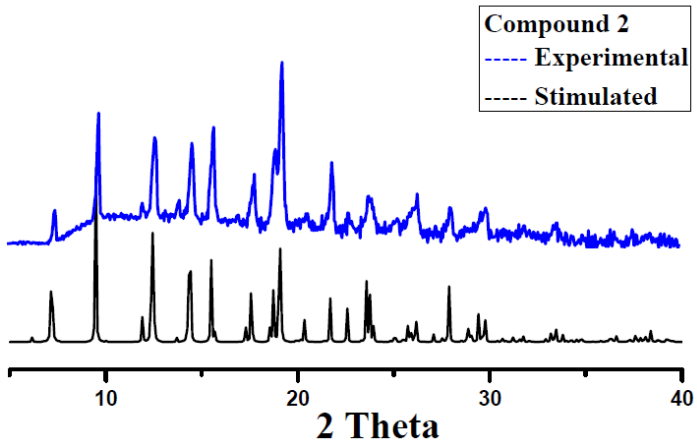
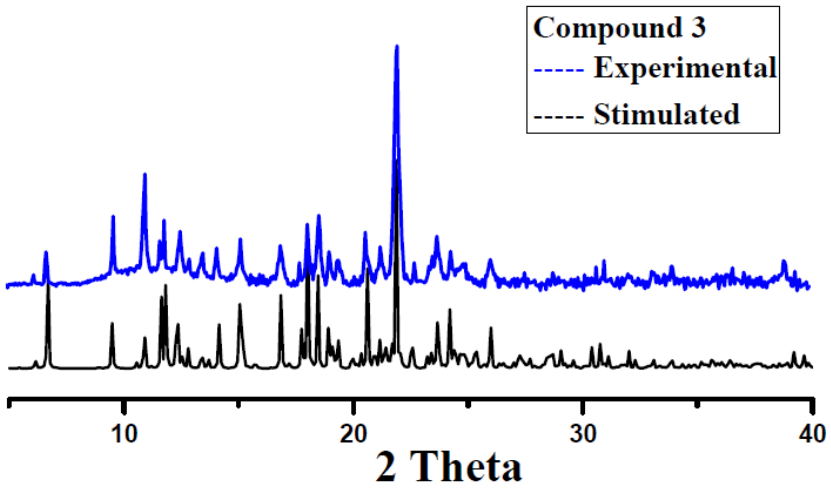
Section-1

Powder X-ray patterns of the compounds 1-3.







Section-2.

(a) Magnetic data plots of compound 1

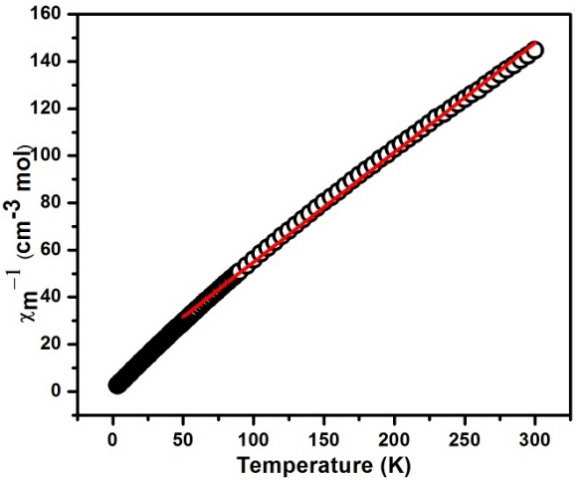


Figure S1. Fitted1/χ_M *vs T* plots of the compounds **1**.

(b) Fitting equation for magnetic data of compound 2

The magnetic data of compound **2** were fitted assuming the carboxylate bridges of the two Co(II) ions form a isolated spin dimer. By introducing inter-dimer magnetic coupling constant zJ' the magnetic susceptibility data was fitted from the following equation which was deduced from the spin Hamiltonian.[25]

$$H = -2JS_1 \bullet S$$

(where S_1 and S_2 are the spin operators with $S_1=S_2=3/2$)

$$E(S_T) = -JS_T(S_T+1)$$

$$S_T = 0, 1, 2, 3.$$

$$E(S_T) = 0, -J, -3J, -6J$$

$$\chi_M = \chi_M'/\{1-\chi_M'(2zJ'/Ng^2\beta^2)\}$$

$$\chi_M' = (2Ng^2\beta^2/k_BT)[A/B]$$

Where $A=[\exp(2J/k_BT) +5\exp(6J/k_BT) +14\exp(12J/k_BT)]$ and

$$B=[1+ 3\exp(2J/k_BT) +5\exp(6J/k_BT) +7\exp(12J/k_BT)]$$

The parameters ***N***, β and k_B have their normal meanings. The best fit of the theoretical equation to the experimental data leads to the g= 2.35 (4) J= –47.23 (3) cm^{-1} and zJ'= –2.46 (6).

(c) Magnetic data plots of compound 2

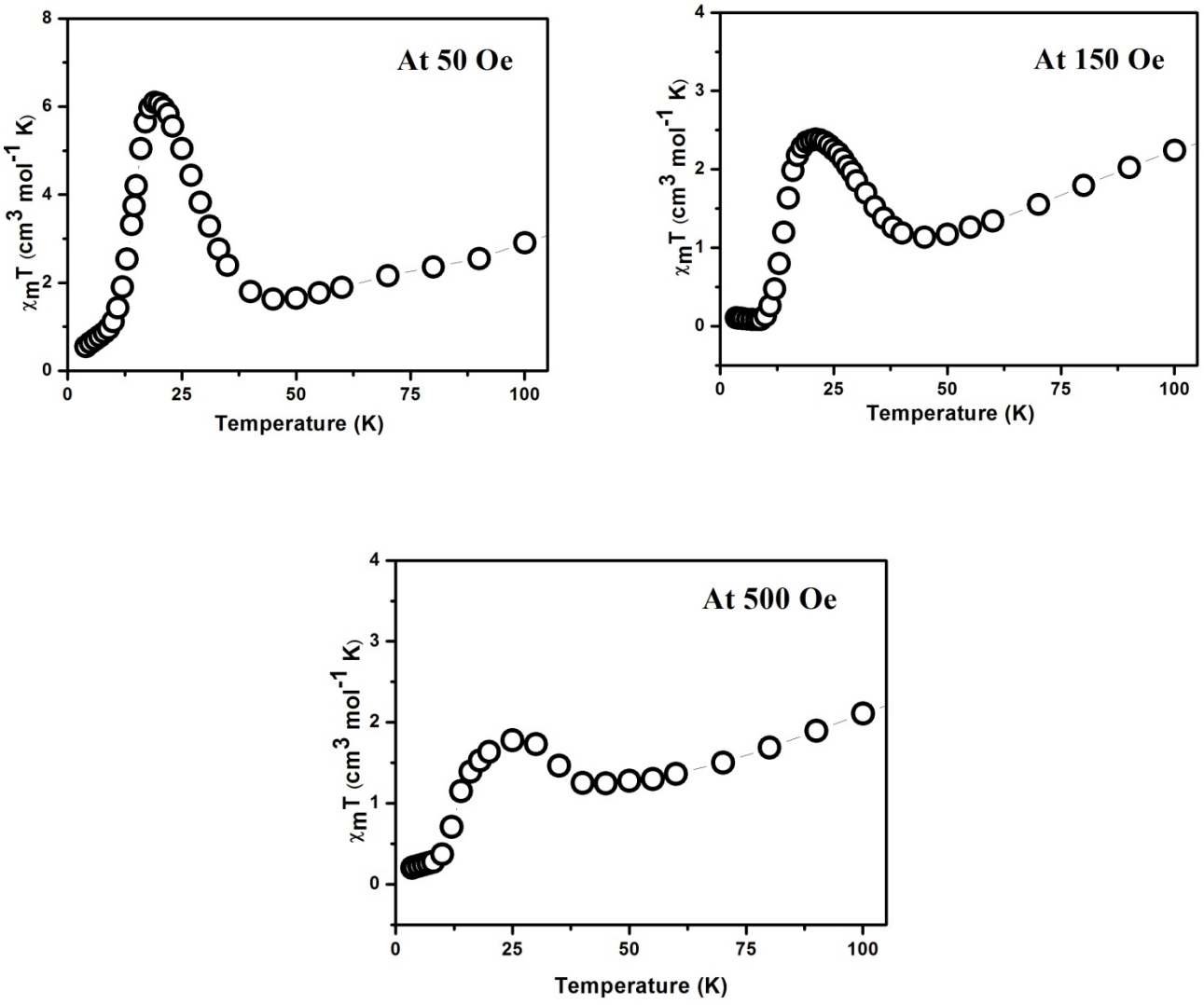


Figure S2. Plots of $\chi_M T$ *vs* T upto 100K at different fields for compound **2**.

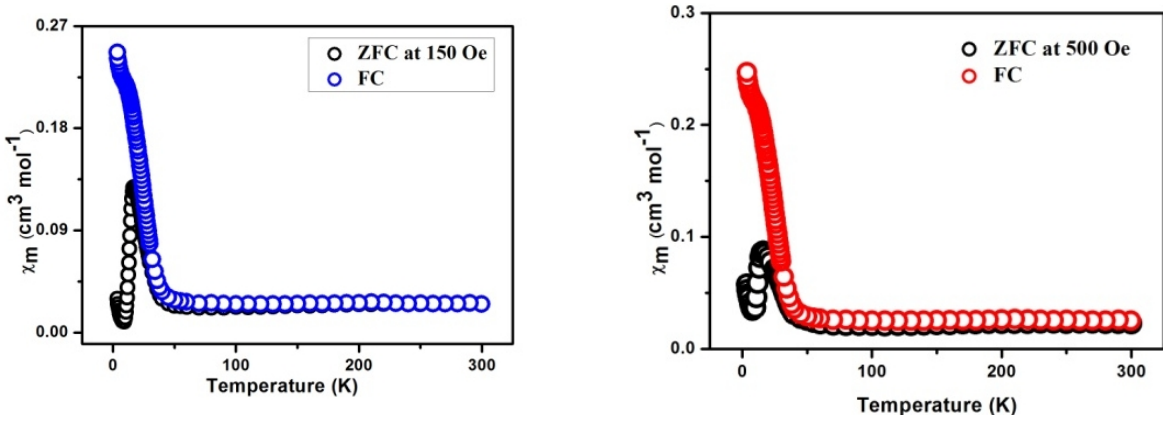


Figure S3. The zero-field-cooled (ZFC) and field-cooled (FC) magnetization at the field 150 Oe and 500 oe for compound **3**.

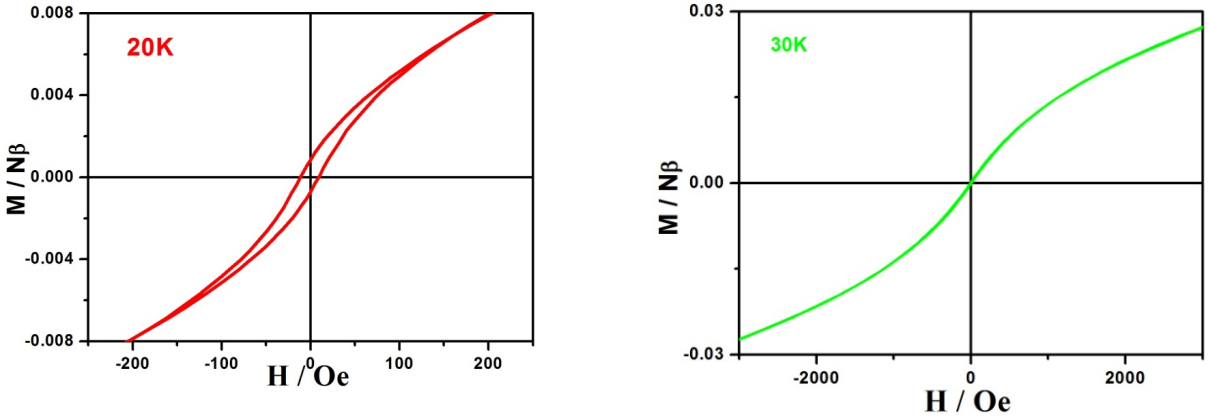


Figure S4. M(H) plots at temperatures 20K & 30K for compound **2.**

(d) Magnetic data plots of compound 3

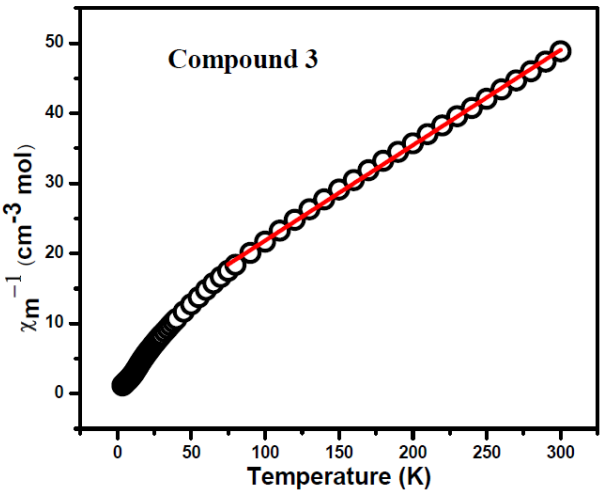


Figure S5. Fitted1/χ_M *vs T* plots of the compounds **3** in the temperature range 80 – 300 K.

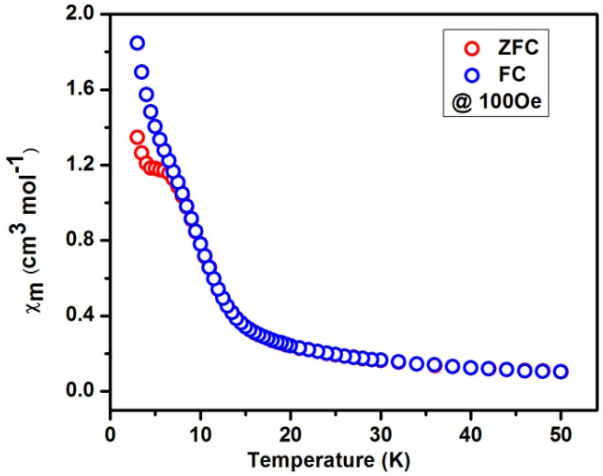


Figure S6. The zero-field-cooled (ZFC) and field-cooled (FC) magnetization at the field 100 Oe for compound **3**.

Section-3 **Selected** Bond lengths and bond angles in the compounds **1-3**

Compound 1

Co(1)-O(3)#1	1.998(2)	N(4)-Co(1)-N(1)	91.58(10)
Co(1)-O(2)	2.042(2)	O(3)#1-Co(1)-O(1)	92.91(9)
Co(1)-N(4)	2.103(2)	O(2)-Co(1)-O(1)	60.12(8)
Co(1)-N(1)	2.108(2)	N(4)-Co(1)-O(1)	86.71(9)
Co(1)-O(1)	2.301(2)	N(1)-Co(1)-O(1)	171.49(8)
Co(1)-O(4)#1	2.410(2)	O(3)#1-Co(1)-O(4)#1	58.56(8)
O(1)-C(1)	1.249(3)	O(2)-Co(1)-O(4)#1	91.22(9)
O(2)-C(1)	1.280(3)	N(4)-Co(1)-O(4)#1	158.17(8)
O(3)-C(4)	1.277(3)	N(1)-Co(1)-O(4)#1	86.08(9)
O(3)-Co(1)#2	1.998(2)	O(1)-Co(1)-O(4)#1	98.58(9)
O(4)-C(4)	1.239(3)	C(1)-O(1)-Co(1)	84.60(17)
O(9)-C(11)	1.377(3)	C(1)-O(2)-Co(1)	95.56(16)
O(9)-C(29)	1.401(3)	C(4)-O(3)-Co(1)#2	99.04(17)
O(10)-C(12)	1.367(3)	C(11)-O(9)-C(29)	118.2(2)
O(10)-C(29)	1.401(3)	C(12)-O(10)-C(29)	118.0(2)
N(1)-C(10)	1.329(3)	C(17)-N(4)-Co(1)	121.43(18)
N(1)-C(25)	1.340(4)	C(76)-N(4)-Co(1)	120.5(2)
N(2)-C(5)	1.359(4)	O(1)-C(1)-O(2)	119.7(3)
N(2)-C(81)	1.436(4)	O(1)-C(1)-C(20)	120.7(3)
N(3)-C(23)	1.367(4)	O(2)-C(1)-C(20)	119.6(2)
N(3)-C(34)	1.446(4)	O(4)-C(4)-O(3)	120.6(3)
N(4)-C(17)	1.326(4)	O(4)-C(4)-C(3)	121.9(3)
N(4)-C(76)	1.348(4)	O(3)-C(4)-C(3)	117.4(2)
N(10)-C(59)	1.440(4)	O(10)-C(12)-C(39)	124.9(3)
N(12)-C(50)	1.323(4)	O(10)-C(12)-C(42)	115.6(3)
N(12)-C(43)	1.339(4)	O(10)-C(29)-O(9)	111.4(2)
N(10)-C(22)	1.389(4)	O(10)-C(29)-H(29A)	109.3
		O(9)-C(29)-H(29A)	109.3
O(3)#1-Co(1)-O(2)	137.34(9)	O(10)-C(29)-H(29B)	109.3
O(3)#1-Co(1)-N(4)	100.20(9)	O(9)-C(29)-H(29B)	109.3
O(2)-Co(1)-N(4)	109.58(9)		
O(3)#1-Co(1)-N(1)	95.59(9)		
O(2)-Co(1)-N(1)	112.91(9)		

Symmetry transformations used to generate equivalent atoms:

#1 x-1,y-1,z-1 #2 x+1,y+1,z+1 #3 -x+1,-y-1,-z+1 #4 -x,-y+1,-z

Compound 2

Co(1)-O(3)#2	2.0029(16)
Co(1)-O(1)	2.0214(15)
Co(1)-O(2)#3	2.0357(16)
Co(1)-N(1)	2.0488(17)
Co(1)-O(4)#4	2.0745(15)
Co(1)-Co(1)#2	2.7633(6)
O(2)-Co(1)#5	2.0357(16)
O(3)-Co(1)#2	2.0028(16)
O(4)-Co(1)#6	2.0745(15)
C(1)-O(1)	1.250(3)
C(1)-O(3)	1.250(3)
C(6)-O(13)	1.384(2)
C(8)-O(13)	1.405(2)
C(8)-O(14)	1.407(3)
C(15)-O(4)	1.253(3)
C(15)-O(2)	1.255(3)
C(44)-N(1)	1.319(3)
C(45)-N(2)	1.367(3)

O(3)#2-Co(1)-O(1)	164.45(7)
O(3)#2-Co(1)-O(2)#3	93.87(7)
O(1)-Co(1)-O(2)#3	87.48(7)
O(3)#2-Co(1)-N(1)	99.86(7)
O(1)-Co(1)-N(1)	95.27(7)
O(2)#3-Co(1)-N(1)	98.15(7)
O(3)#2-Co(1)-O(4)#4	85.18(7)
O(1)-Co(1)-O(4)#4	89.53(7)
O(2)#3-Co(1)-O(4)#4	165.04(7)
N(1)-Co(1)-O(4)#4	96.73(7)
O(3)#2-Co(1)-Co(1)#2	83.51(5)
O(1)-Co(1)-Co(1)#2	81.00(5)
O(2)#3-Co(1)-Co(1)#2	90.21(5)
N(1)-Co(1)-Co(1)#2	170.72(5)
O(4)#4-Co(1)-Co(1)#2	74.84(5)
C(44)-N(1)-Co(1)	121.46(14)
C(48)-N(1)-Co(1)	119.33(15)
C(1)-O(1)-Co(1)	125.64(14)
C(15)-O(2)-Co(1)#5	115.51(15)
C(1)-O(3)-Co(1)#2	123.60(15)
C(15)-O(4)-Co(1)#6	132.41(14)

Symmetry transformations used to generate equivalent atoms

#1 -x+2/3,-y+1/3,-z-2/3 #2 -x+2/3,-y+1/3,-z+1/3 #3 -y+2/3,x-y+1/3,z+1/3
#4 y,-x+y,-z #5 -x+y+1/3,-x+2/3,z-1/3
#6x-y,x,-z

Compound 3

Co(1)-O(3)	2.046(4)
Co(1)-O(5)	2.083(5)
Co(1)-O(1)	2.103(4)
Co(1)-N(3)	2.142(5)
Co(1)-N(1)	2.166(5)
Co(1)-O(2)	2.236(4)
Co(2)-O(7)	1.991(4)
Co(2)-O(8)	2.018(4)
Co(2)-N(5)	2.048(5)
Co(2)-N(7)	2.055(5)
O(13)-C(15)	1.382(7)
O(13)-C(14)	1.425(8)
O(2)-C(28)	1.267(7)
O(3)-C(10)	1.257(7)
O(14)-C(13)	1.372(7)
O(14)-C(14)	1.407(7)

O(7)-C(21)	1.278(7)	O(1)-Co(1)-N(3)	93.08(19)
O(1)-C(28)	1.257(7)	O(3)-Co(1)-N(1)	87.58(17)
O(8)-C(32)	1.279(7)	O(5)-Co(1)-N(1)	95.4(2)
O(6)-C(21)	1.221(7)	O(1)-Co(1)-N(1)	89.89(18)
N(1)-C(1)	1.337(8)	N(3)-Co(1)-N(1)	176.07(19)
N(1)-C(5)	1.341(7)	O(3)-Co(1)-O(2)	98.14(16)
N(5)-C(33)	1.333(8)	O(5)-Co(1)-O(2)	163.16(18)
N(5)-C(37)	1.335(8)	O(1)-Co(1)-O(2)	60.63(15)
O(9)-C(32)	1.233(7)	N(3)-Co(1)-O(2)	86.97(18)
O(4)-C(10)	1.255(7)	N(1)-Co(1)-O(2)	92.27(17)
N(3)-C(22)	1.317(8)	O(7)-Co(2)-O(8)	96.15(17)
N(3)-C(26)	1.342(8)	O(7)-Co(2)-N(5)	112.20(19)
N(7)-C(48)	1.334(8)	O(8)-Co(2)-N(5)	117.07(19)
N(7)-C(45)	1.341(8)	O(7)-Co(2)-N(7)	100.35(19)
N(6)-C(36)	1.364(8)	O(8)-Co(2)-N(7)	104.97(19)
N(6)-C(38)	1.437(8)	N(5)-Co(2)-N(7)	121.9(2)
N(2)-C(6)	1.446(9)	C(21)-O(7)-Co(2)	113.0(4)
N(4)-C(27)	1.439(11)	C(28)-O(1)-Co(1)	92.3(3)
		C(32)-O(8)-Co(2)	99.1(4)
		C(1)-N(1)-Co(1)	122.7(4)
O(3)-Co(1)-O(5)	97.16(18)	C(5)-N(1)-Co(1)	119.2(4)
O(3)-Co(1)-O(1)	158.52(16)	O(9)-C(32)-O(8)	121.5(5)
O(5)-Co(1)-O(1)	104.32(18)	O(9)-C(32)-C(19)#1	119.4(5)
O(3)-Co(1)-N(3)	88.72(18)	O(8)-C(32)-C(19)#1	119.1(5)
O(5)-Co(1)-N(3)	86.4(2)	C(36)-N(6)-C(38)	124.0(6)

Symmetry transformations used to generate equivalent atoms:
#1 x+1,y,z #2 x-1,y,z #3 -x+2,-y,-z+1
#4 -x+1,-y+1,-z #5 -x,-y+3,-z+1

******************************End of supporting Information*********************