Supporting Information

Title: Construction of Co(II) Coordination Polymers Comprising Helical Units Using a Flexible Pyrazole Based Ligand

Authors: Satirtha Sengupta, Sumi Ganguli, Arijit Goswami, Sukhen Bala, Raju Mondal*

Journal: CrystEngComm

==========

Contents:

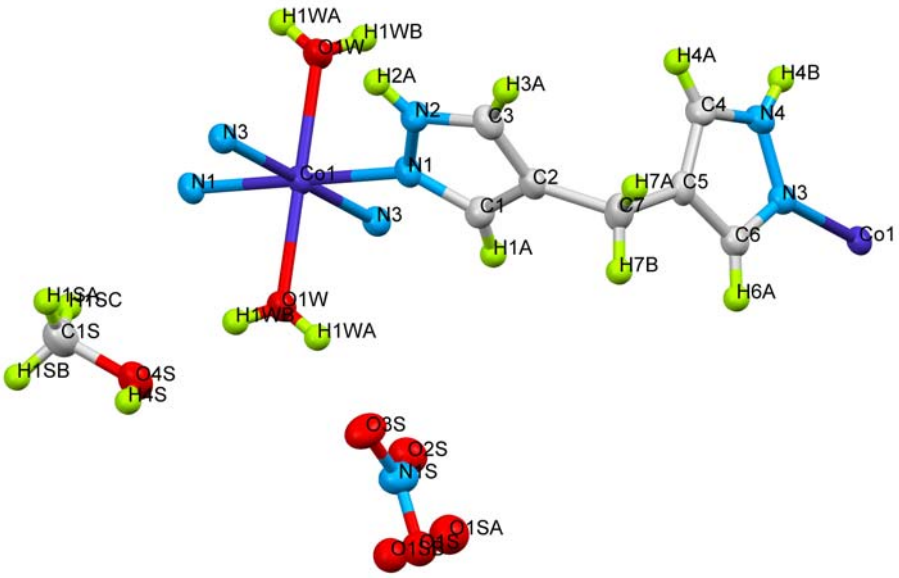

Figure SI-1. The coordination environment around the Co(II) ion of compound **1.**

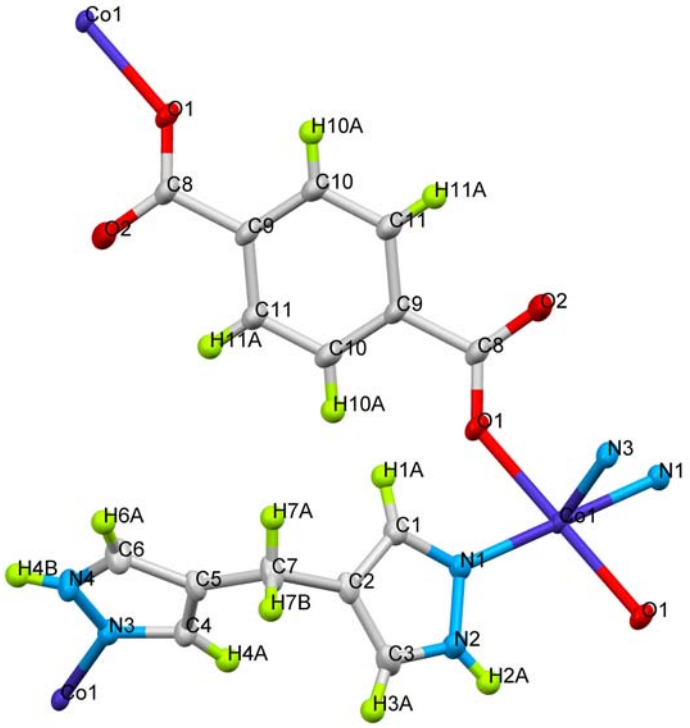

Figure SI-2. The coordination environment around the Co(II) ion of compound **2.** Disordered DMF molecule is ommited for clarity.

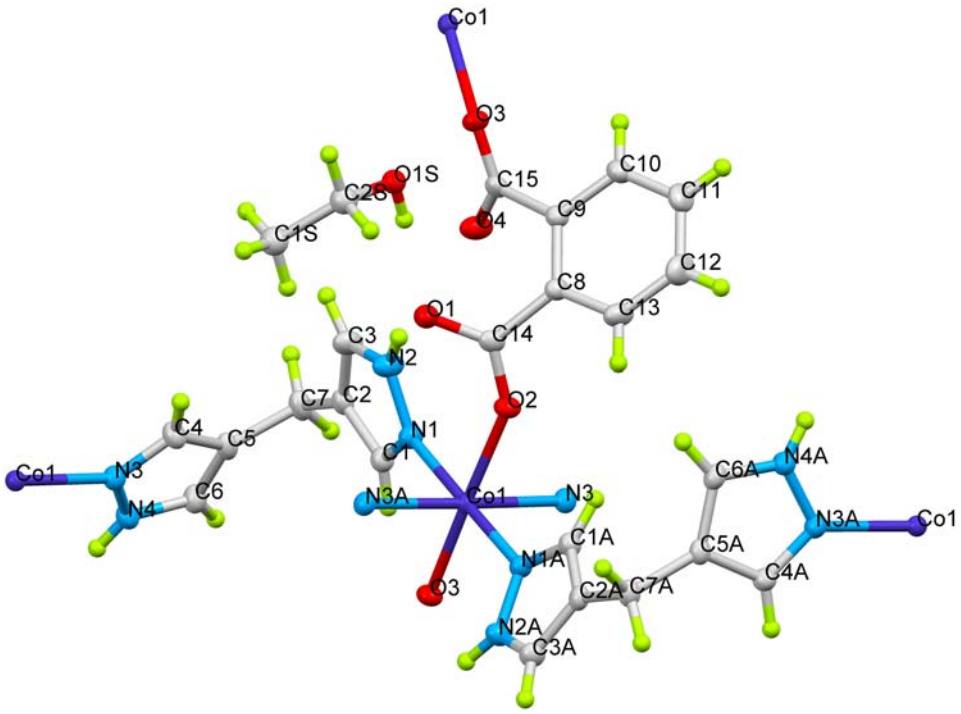

Figure SI-3. The coordination environment around the Co(II) ion of compound **3.**

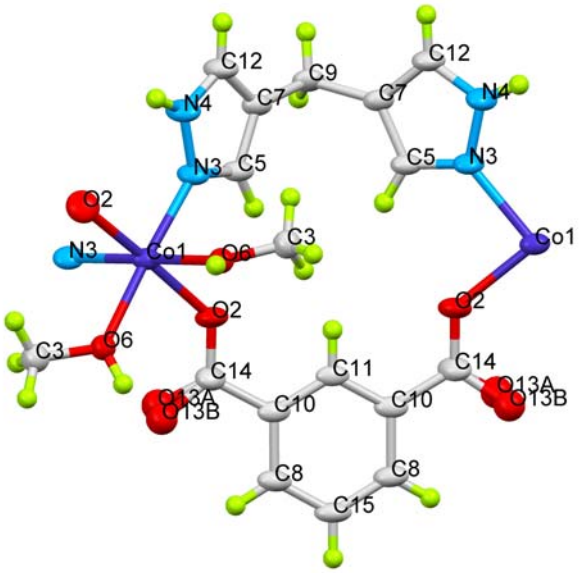

Figure SI-4. The coordination environment around the Co(II) ion of compound **4.**

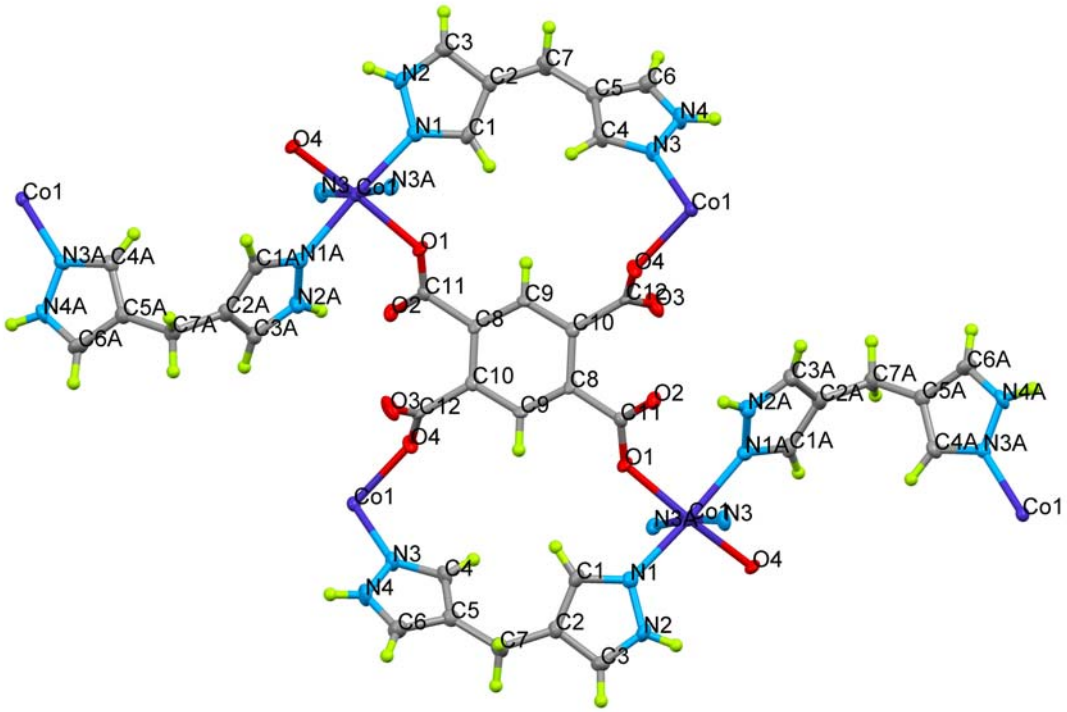

Figure SI-5. The coordination environment around the Co(II) ion of compound **5.**

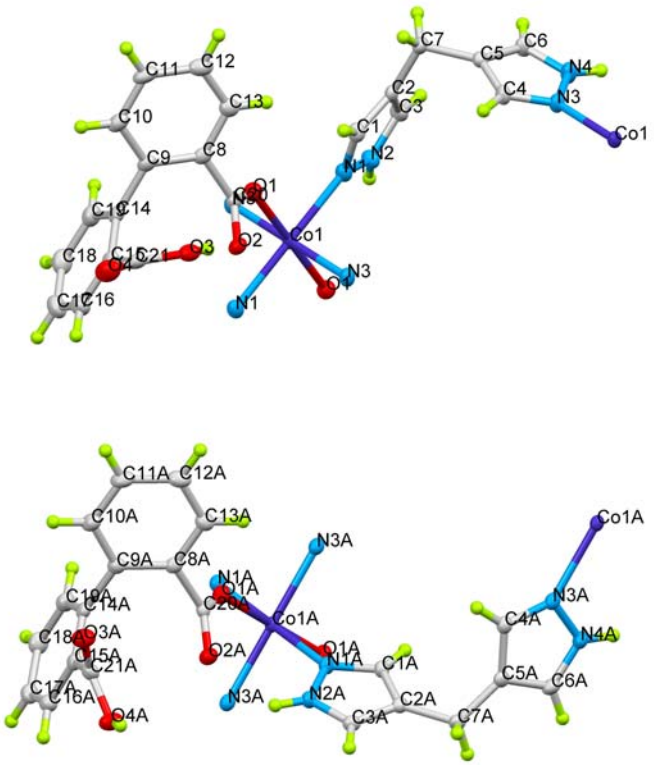

Figure SI-6. The coordination environment around the Co(II) ion of compound **6.**

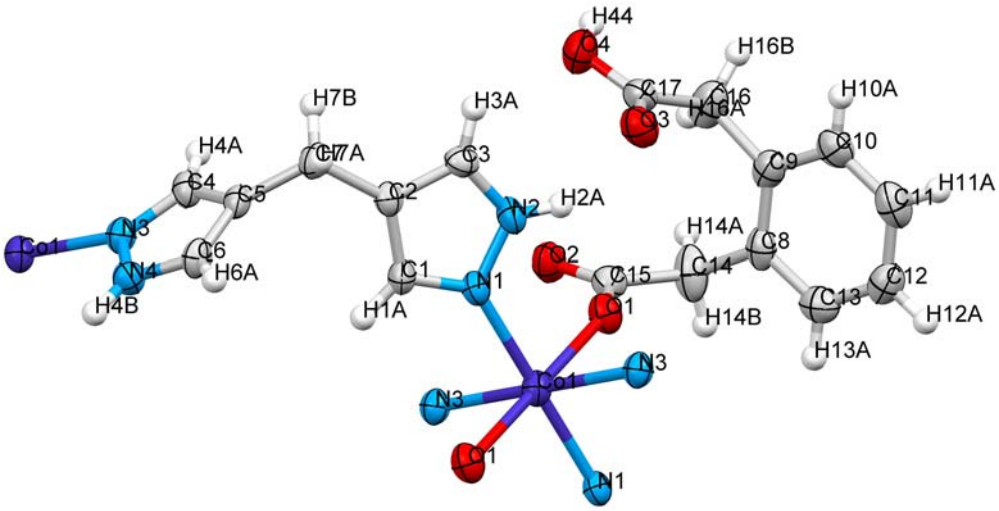

Figure SI-7. The coordination environment around the Co(II) ion of compound **7.**

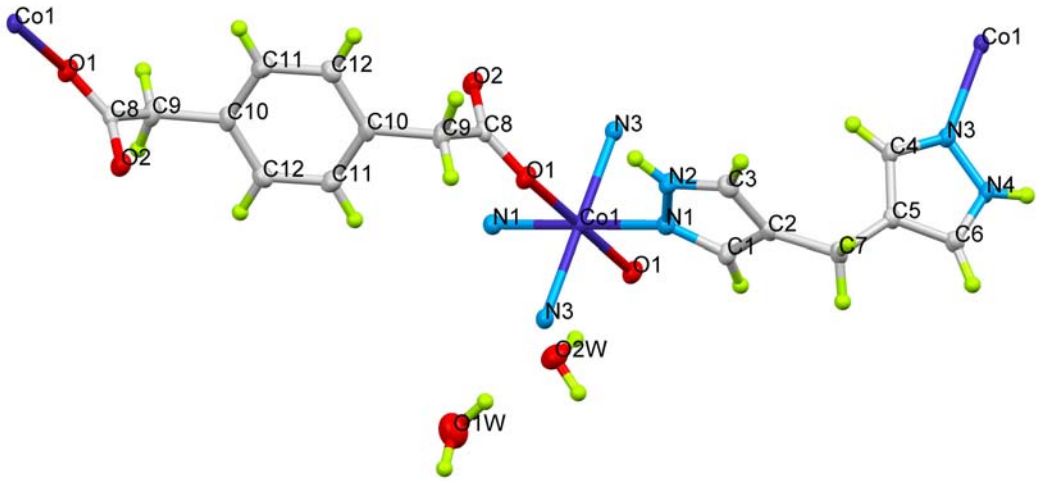

Figure SI-8. The coordination environment around the Co(II) ion of compound **8.**

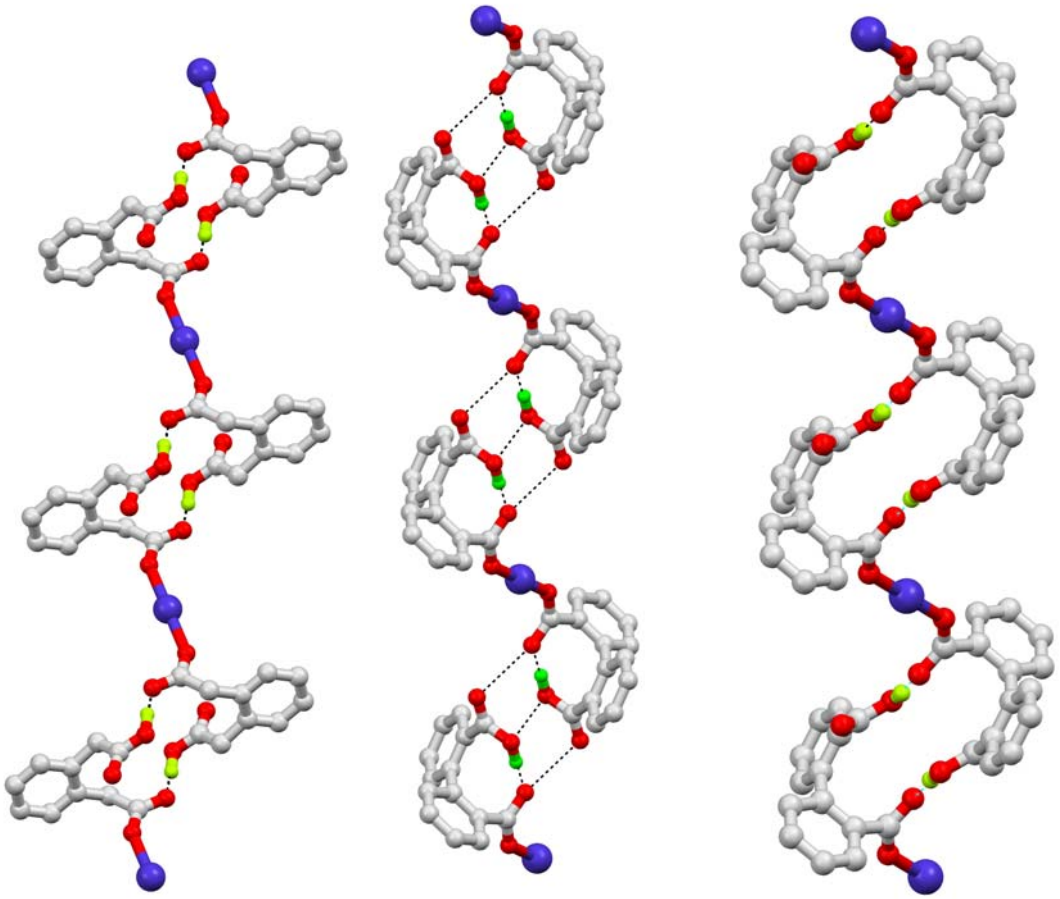

Figure SI-9. Depiction of hydrogen bonded helical motifs formed in compounds **6** and **7**.

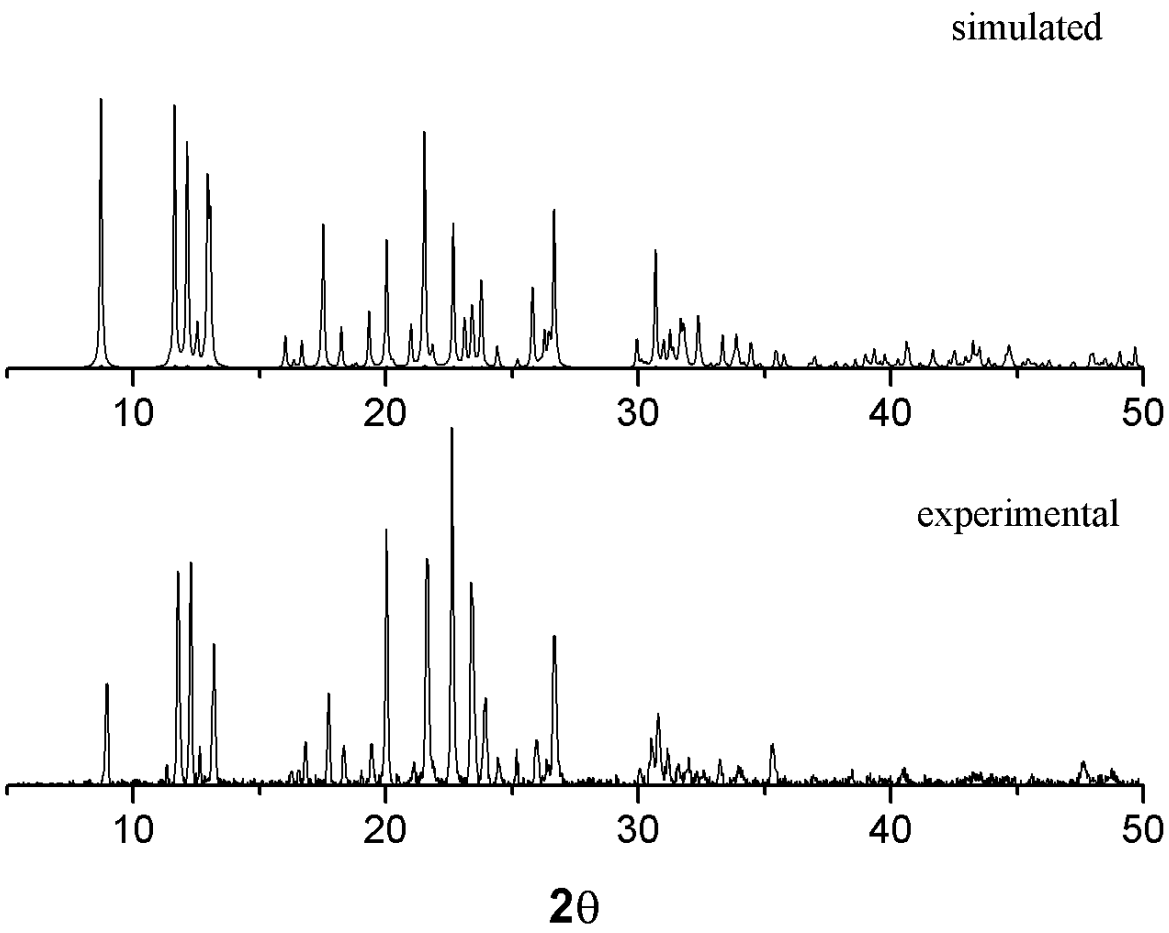

Figure SI-10. The PXRD of compound **2**.

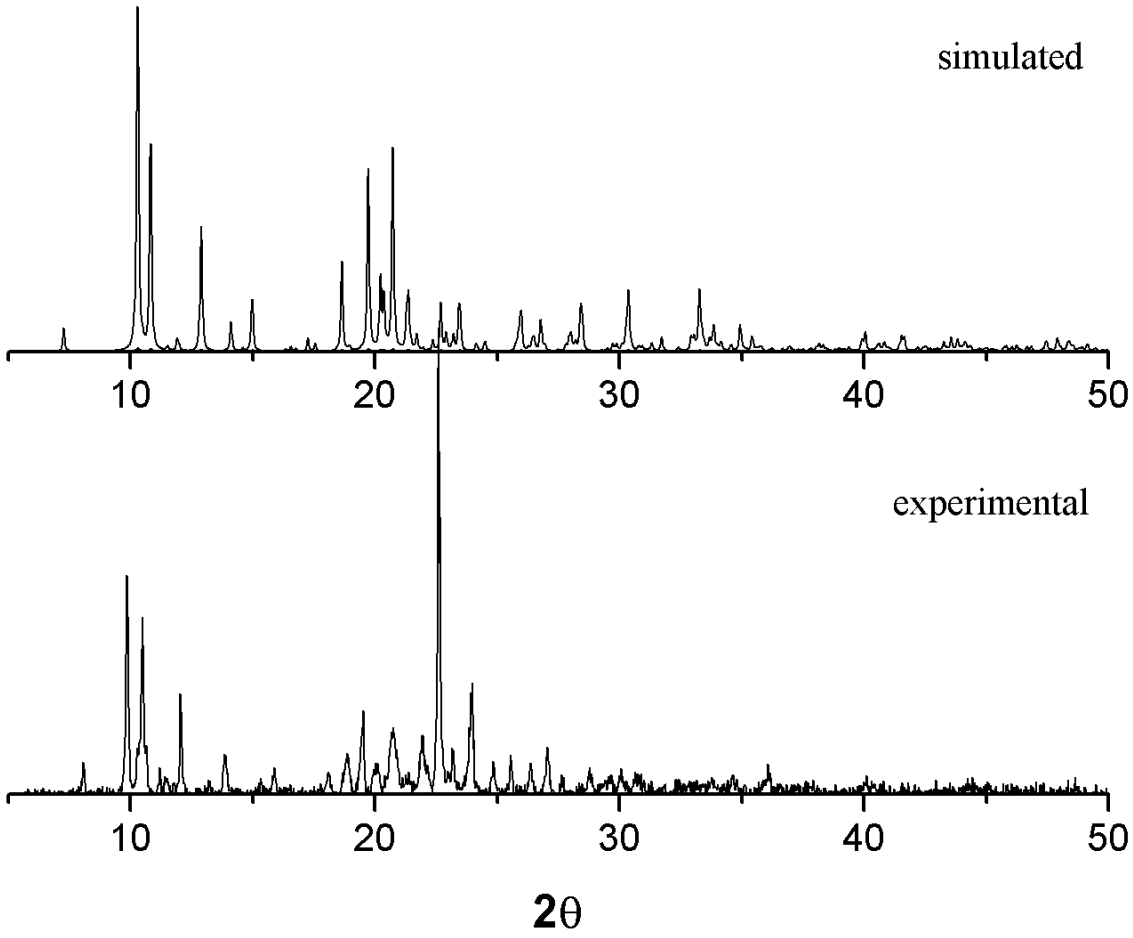

Figure SI-11. The PXRD of compound **3**.

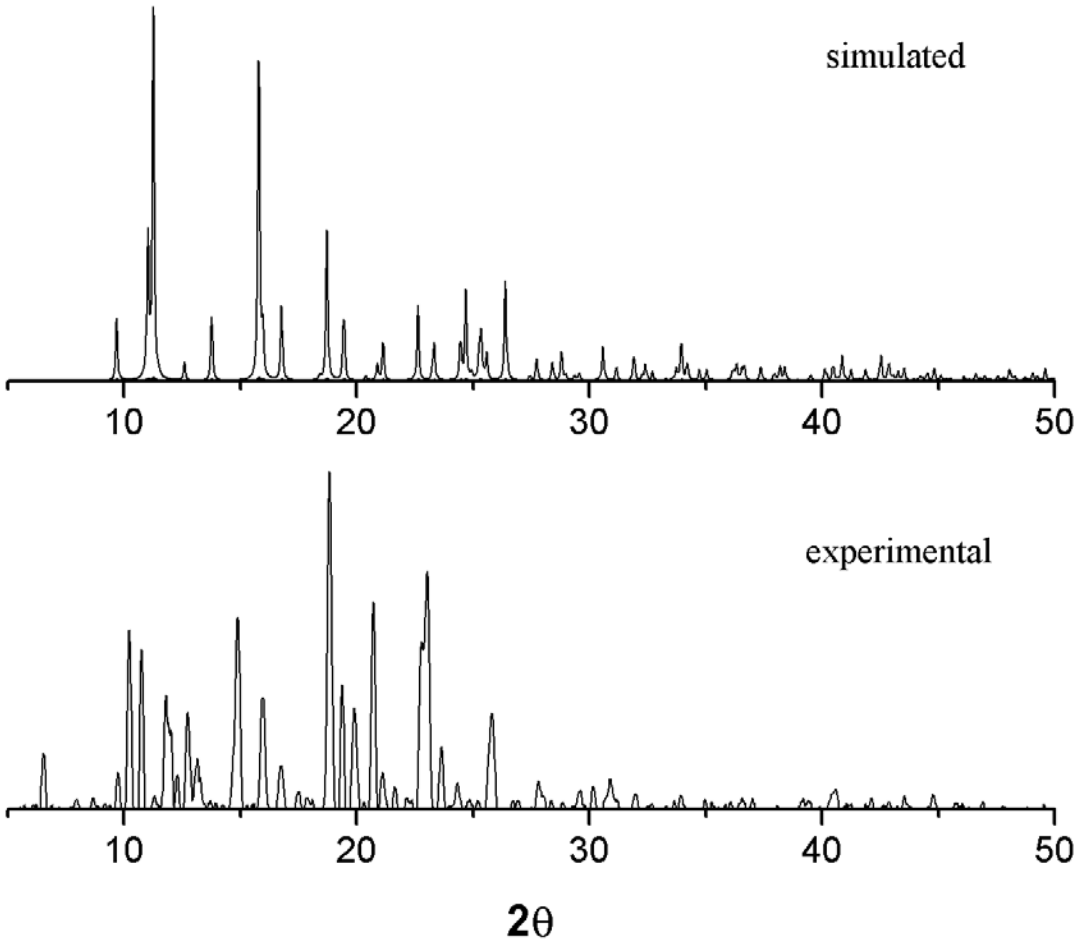

Figure SI-12. The PXRD of compound **4**.

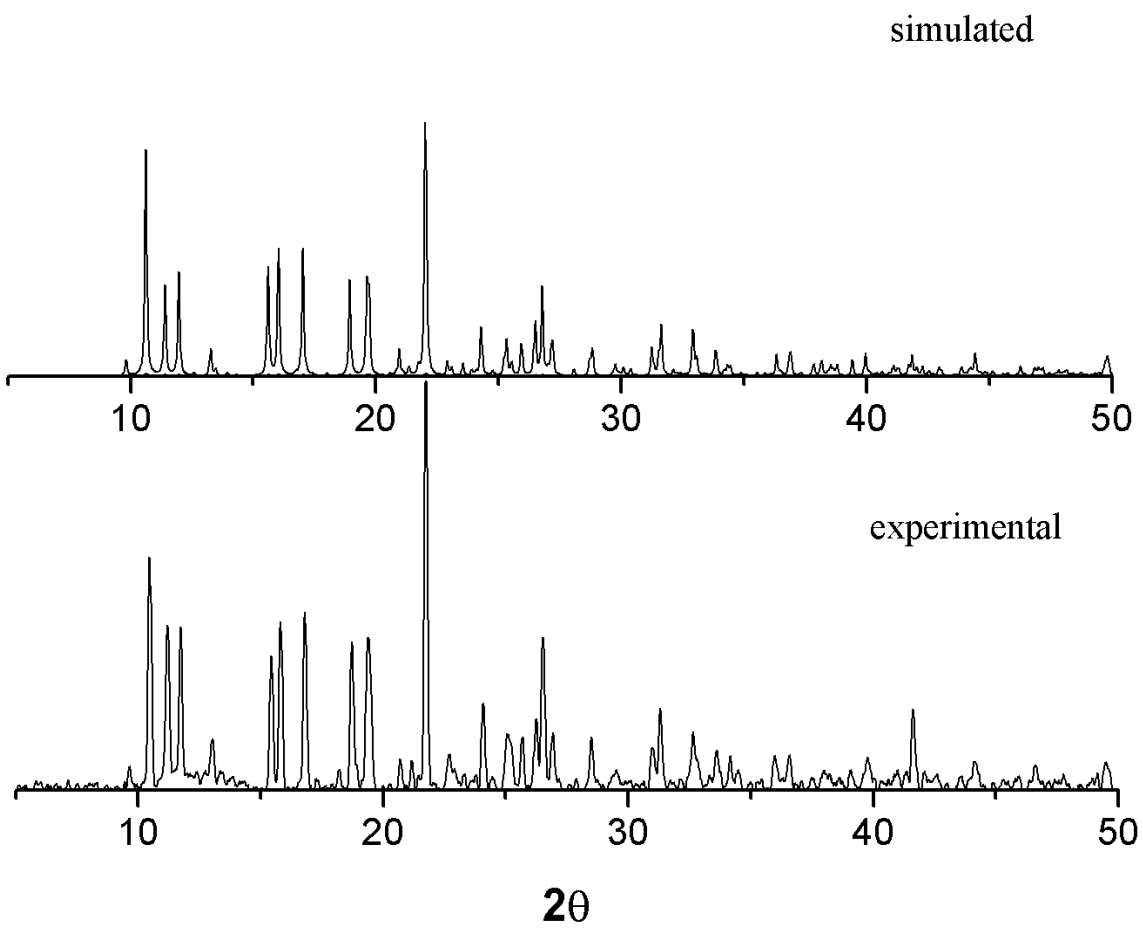

Figure SI-13. The PXRD of compound **5**.

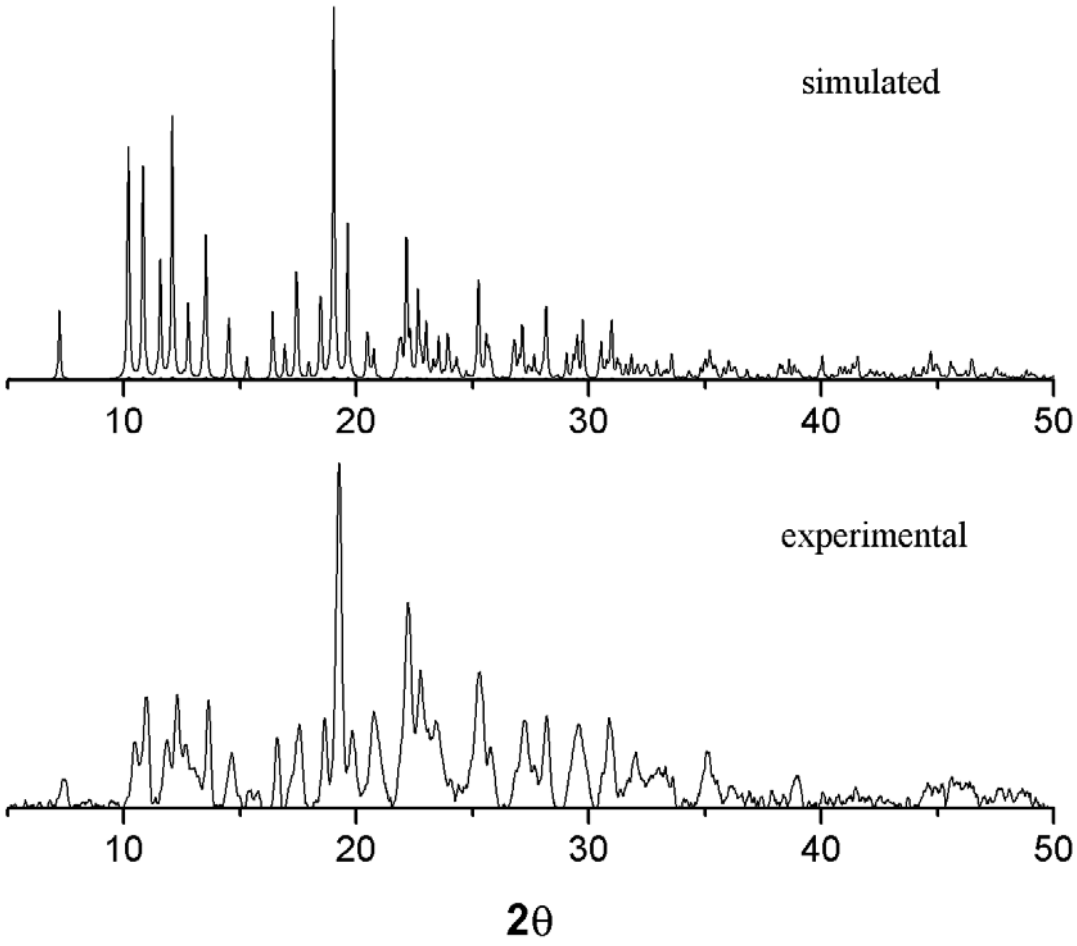

Figure SI-14. The PXRD of compound **6**.

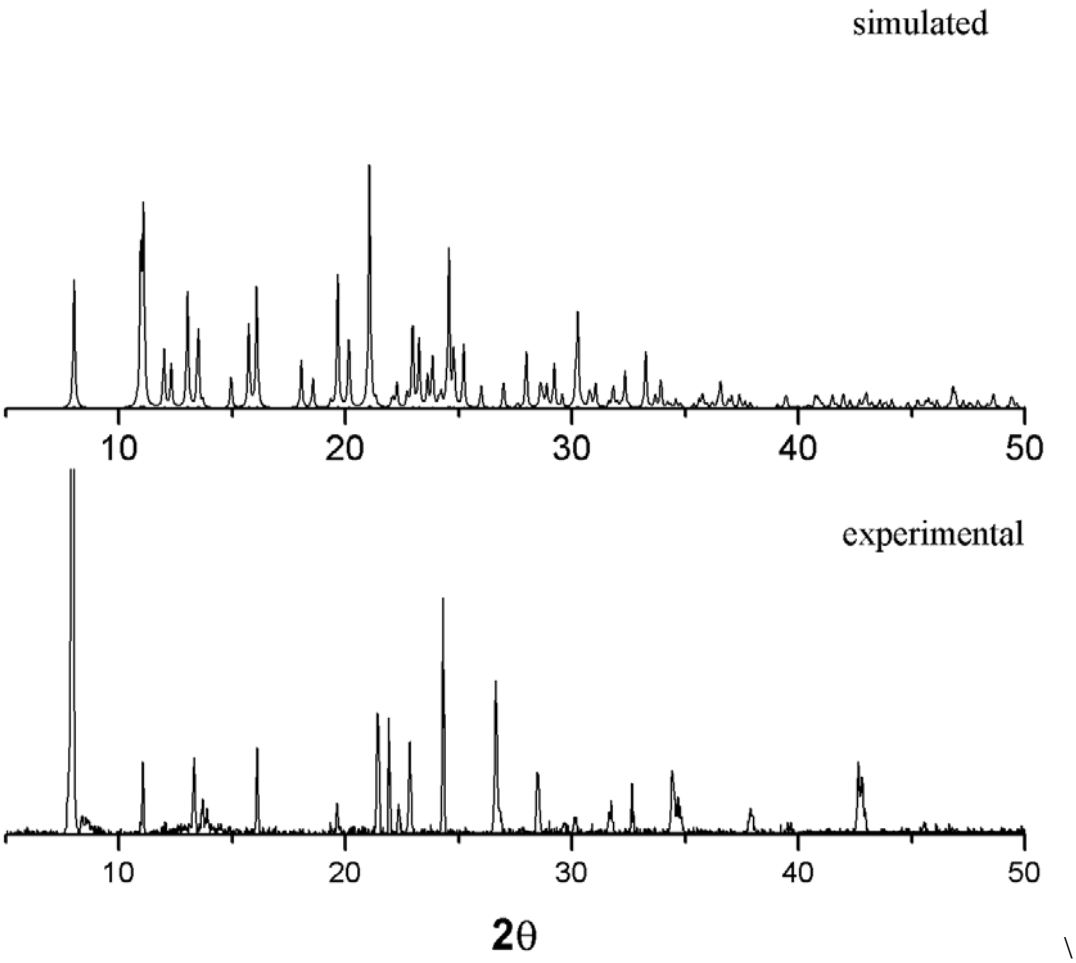

Figure SI-15. The PXRD of compound **7**.

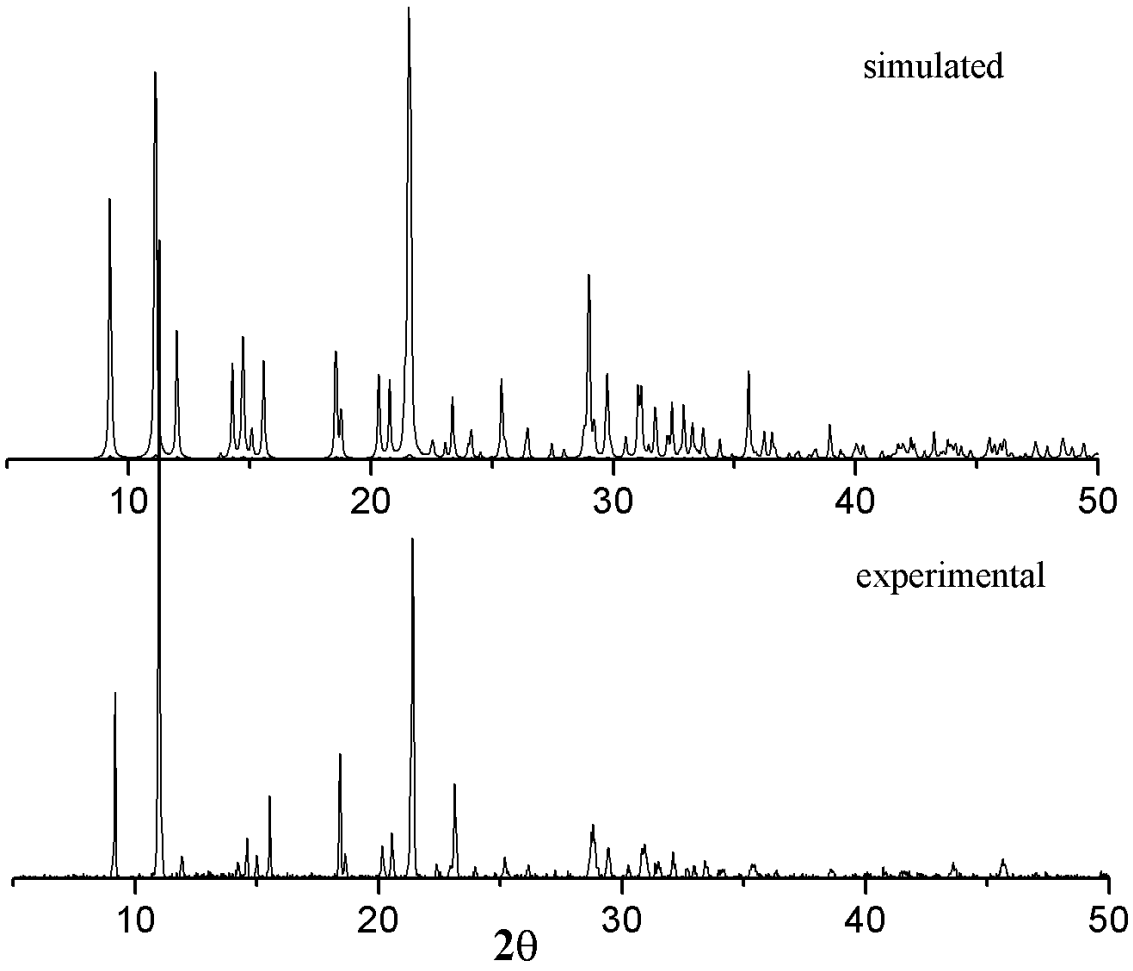

Figure SI-16. The PXRD of compound **8**.

Table SI-1: Selected Bond Lengths (A^o) and Angles (^{o}) for Compounds **1-5**

Compound 1

Co_1-O_{1W}	2.120(2)	O_{1W}-Co_1-N_1	92.79(9)
Co_1-N_1	2.121(2)	N_1-Co_1-N_1	180.00(15)
Co_1-N_3	2.141(2)	O_{1W}-Co_1-N_3	87.08(9)
O_{1W}-Co_1-O_{1W}	180.00(8)	N_1-Co_1-N_3	92.31(9)
O_{1W}-Co_1-N_1	87.21(9)	N_3-Co_1-N_3	180.00(9)

Compound 2

Co_1-O_1	2.1208(13)	O_1-Co_1-O_1	180.00(8)
Co_1-N_1	2.1497(16)	O_1-Co_1-N_3	88.35(6)
Co_1-N_3	2.1219(16)	O_1-Co_1-N_3	91.65(6)
		N_3-Co_1-N_3	180.00(9)
		O_1-Co_1-N_1	83.63(6)
		O_1-Co_1-N_1	96.37(6)
		N_3-Co_1-N_1	87.60(6)
		N_3-Co_1-N_1	92.40(6)

Compound 3

Co_1-O_3	2.0936(11)	O_2-Co_1-N_{3A}	93.25(5)
Co_1-O_2	2.1128(11)	N_3-Co_1-N_{3A}	178.01(5)
Co_1-N_3	2.1218(13)	O_3-Co_1-N_{1A}	95.76(5)
Co_1-N_{3A}	2.1321(13)	O_2-Co_1-N_{1A}	86.84(5)
Co_1-N_{1A}	2.1419(13)	N_3-Co_1-N_{1A}	91.34(5)
Co_1-N_1	2.1638(14)	N_{3A}-Co_1-N_{1A}	90.64(5)
		O_3-Co_1-N_1	85.61(5)
O_3-Co_1-O_2	175.28(4)	O_2-Co_1-N_1	91.83(5)
O_3-Co_1-N_3	89.33(5)	N_3-Co_1-N_1	89.22(5)
O_2-Co_1-N_3	86.67(5)	N_{3A}-Co_1-N_1	88.80(5)
O_3-Co_1-N_{3A}	90.67(5)	N_{1A}-Co_1-N_1	178.52(5)

Compound 4

Co_1-O_2	2.0960(19)	N_3-Co_1-N_3	93.74(12)
Co_1-N_3	2.100(2)	O_2-Co_1-O_6	89.57(10)
Co_1-O_6	2.132(2)	O_2-Co_1-O_6	86.50(10)
O_2-Co_1-O_2	174.44(10)	N_3-Co_1-O_6	177.10(10)
O_2-Co_1-N_3	88.02(7)	N_3-Co_1-O_6	88.11(9)
O_2-Co_1-N_3	95.79(8)	O_6-Co_1-O_6	90.13(14)

Compound 5

Co_1-O_4	2.096(3)	O_1-Co_1-N_{3A}	85.88(11)
Co_1-O_1	2.100(2)	N_3-Co_1-N_{3A}	173.79(13)
Co_1-N_3	2.107(3)	O_4-Co_1-N_1	101.97(12)
Co_1-N_{3A}	2.123(3)	O_1-Co_1-N_1	83.47(11)
Co_1-N_1	2.173(3)	N_3-Co_1-N_1	89.79(13)
Co_1-N_{1A}	2.178(3)	N_{3A}-Co_1-N_1	86.05(13)
O_4-Co_1-O_1	169.67(12)	O_4-Co_1-N_{1A}	82.97(11)
O_4-Co_1-N_3	90.61(12)	O_1-Co_1-N_{1A}	92.26(11)
O_1-Co_1-N_3	98.24(12)	N_3-Co_1-N_{1A}	86.23(13)
O_4-Co_1-N_{3A}	85.75(11)	N_{3A}-Co_1-N_{1A}	98.30(13)
		N_1-Co_1-N_{1A}	173.70(13)

Table SI-2: Selected Bond Lengths (A^o) and Angles (^{o}) for Compounds **6**-**8**

Compound 6				**Compound 7**			
Co_1-N_3	2.1310(11)	N_1-Co_1-N_1	180.00(8)	Co_1-N_1	2.107(3)	N_1-Co_1-N_1	180.0(3)
Co_1-N_1	2.1371(11)	N_3-Co_1-O_1	87.13(4)	Co_1-O_1	2.141(3)	N_1-Co_1-O_1	87.97(11)
Co_1-O_1	2.1437(10)	N_3-Co_1-O_1	92.87(4)	Co_1-N_3	2.155(3)	N_1-Co_1-O_1	92.03(11)
Co_{1A}-O_{1A}	2.0858(9)	N_1-Co_1-O_1	94.80(4)			N_1-Co_1-N_3	88.32(11)
Co_{1A}-N_{1A}	2.1177(11)	N_1-Co_1-O_1	85.20(4)			N_1-Co_1-N_3	91.68(11)
Co_{1A}-N_{3A}	2.1938(11)	O_1-Co_1-O_1	180.00(6)			O_1-Co_1-N_3	82.76(11)
N_3-Co_1-N_3	180.00(5)	O_{1A}-Co_{1A}-N_{1A}	94.63(4)			O_1-Co_1-N_3	97.24(11)
N_3-Co_1-N_1	90.07(4)	O_{1A}-Co_{1A}-N_{1A}	85.37(4)			N_3-Co_1-N_3	180.00(18)
N_3-Co_1-N_1	89.93(4)	O_{1A}-Co_{1A}-N_{3A}	94.79(4)				
		O_{1A}-Co_{1A}-N_{3A}	85.21(4)				
		N_{1A}-Co_{1A}-N_{3A}	87.78(4)				

Compound 8			
Co_1-O_1	2.1045(13)	O_1-Co_1-O_1	180.00(8)
Co_1-N_3	2.1227(15)	O_1-Co_1-N_3	92.51(6)
Co_1-N_1	2.1504(15)	O_1-Co_1-N3	87.49(6)
		N_3-Co_1-N_3	180.00(12)
		O_1-Co_1-N_1	92.55(5)
		O_1-Co_1-N_1	87.45(5)
		N_3-Co_1-N_1	92.19(6)
		N_3-Co_1-N_1	87.81(6)
		N_1-Co_1-N_1	180.00(6)