Support Information

High switchable dielectric phase transition originating from distortion in inorganic–organic hybrid materials (H_2dabco-C_2H_5) [$M^{II}Cl_4$] (M = Co, Zn)

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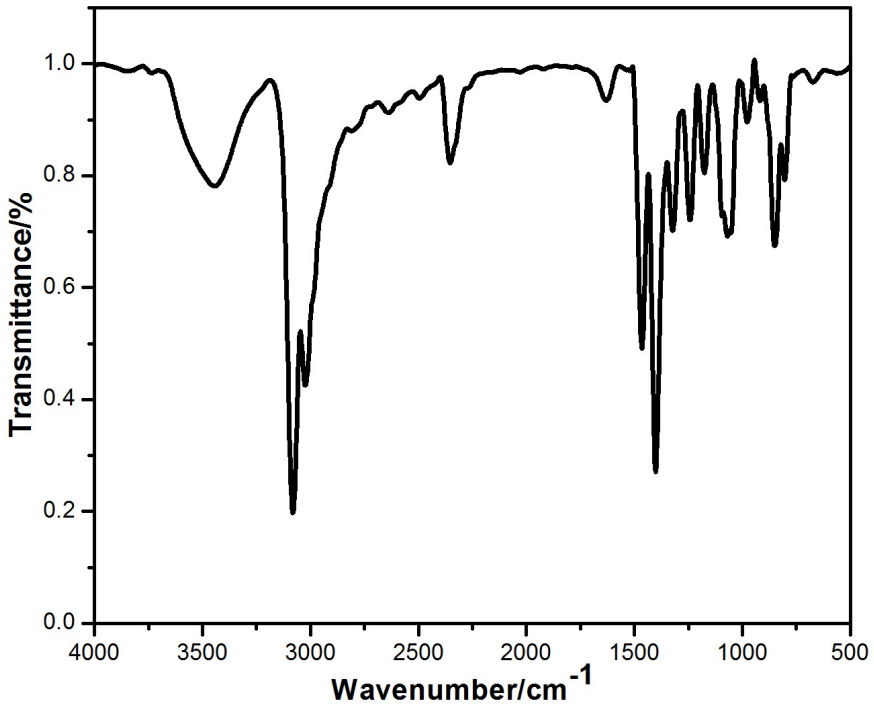

Fig. S1 IR curve of **1**

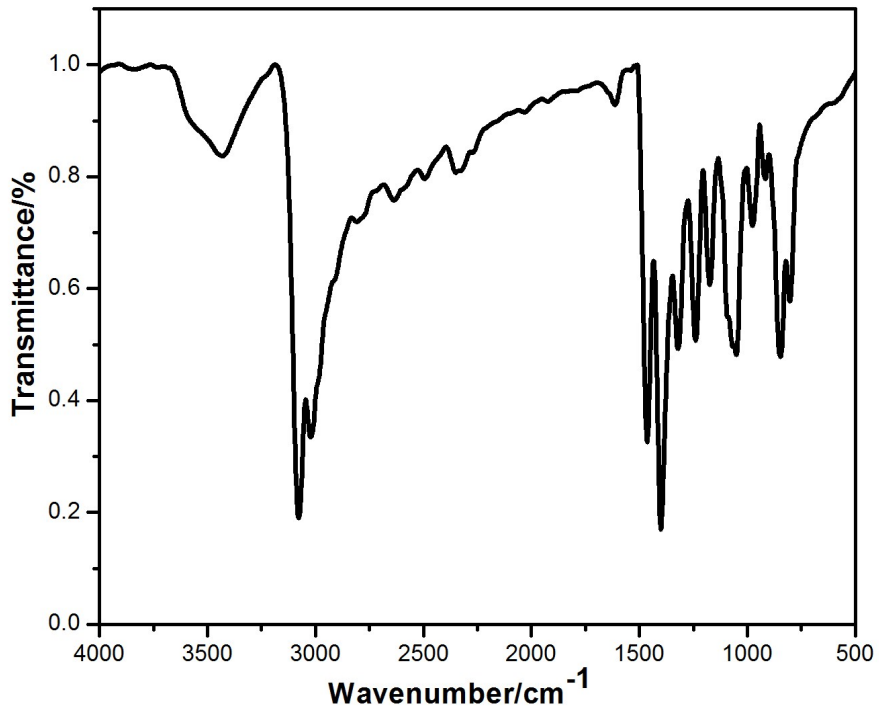

Fig. S2 IR curve of **2**

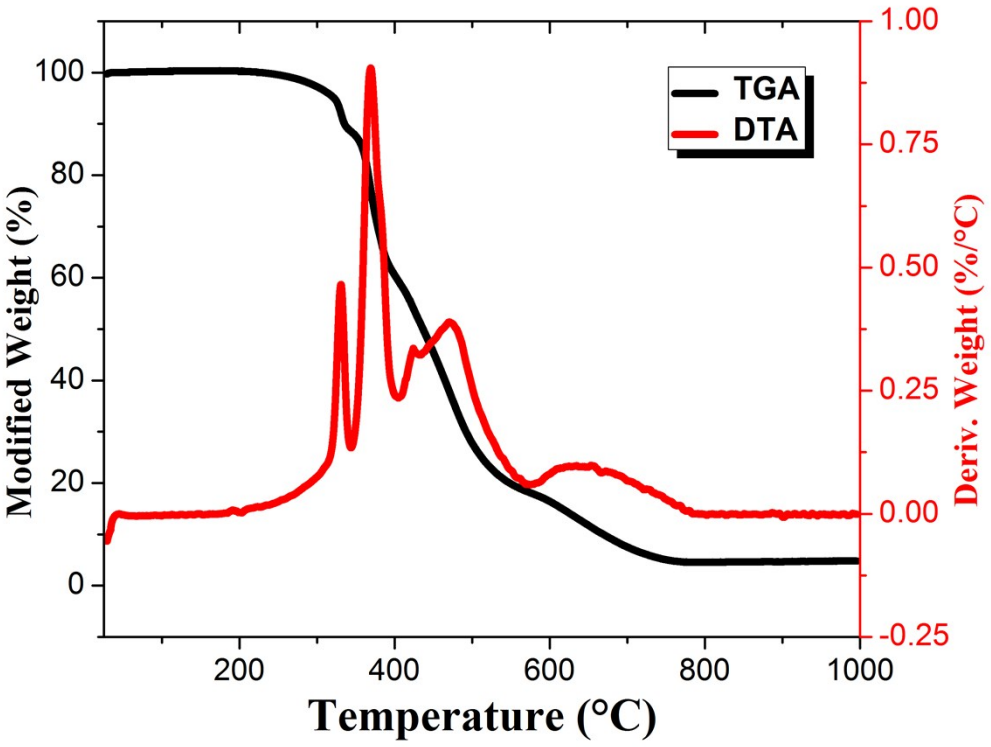

Fig. S3 TG and DTA curve of **1**

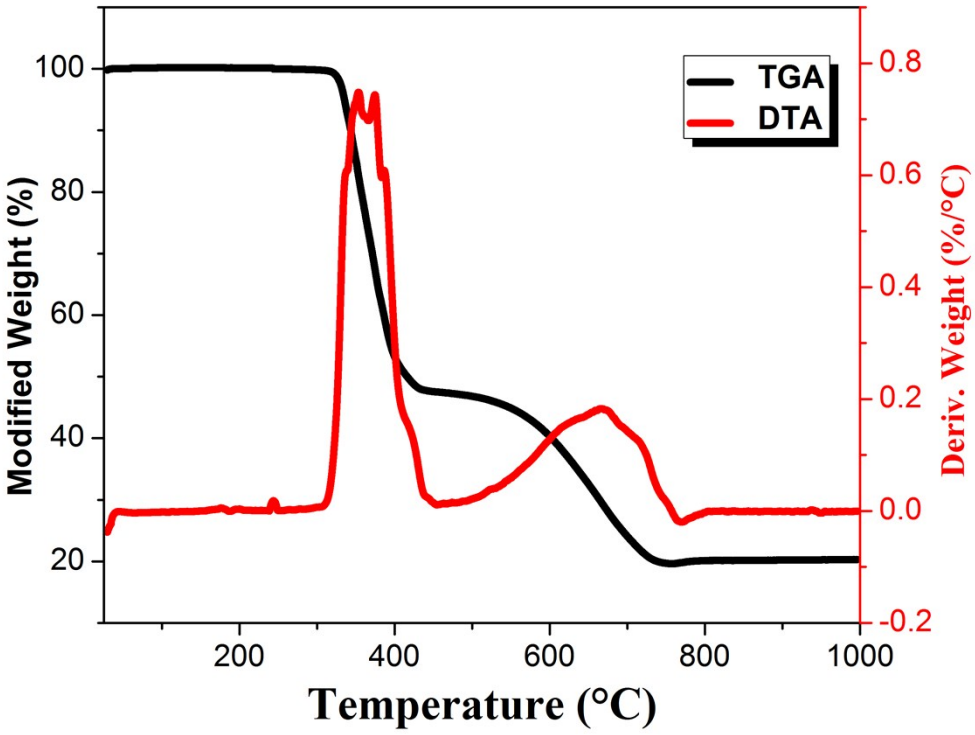

Fig. S4 TG and DTA curve of **2**

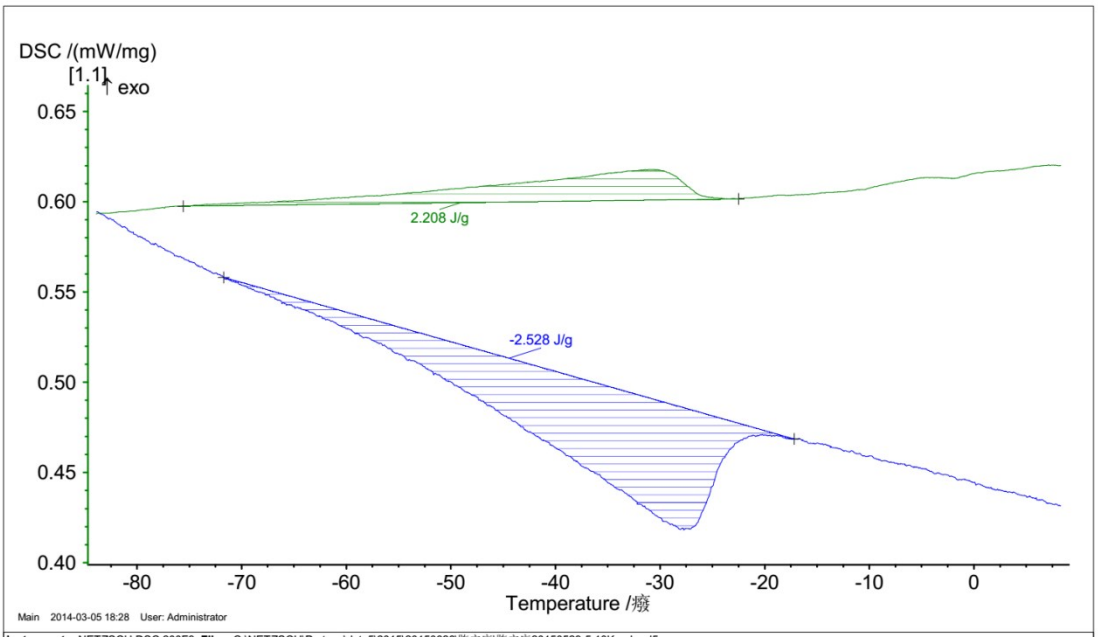

Fig. S5 the DSC of **1**

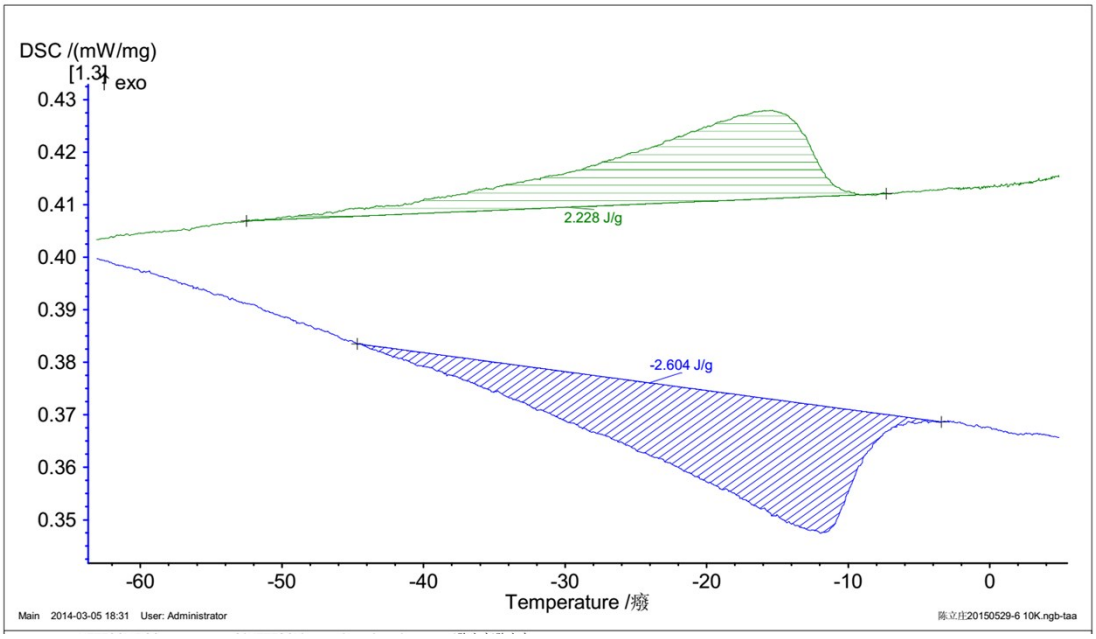

Fig. S6 the DSC of **2**

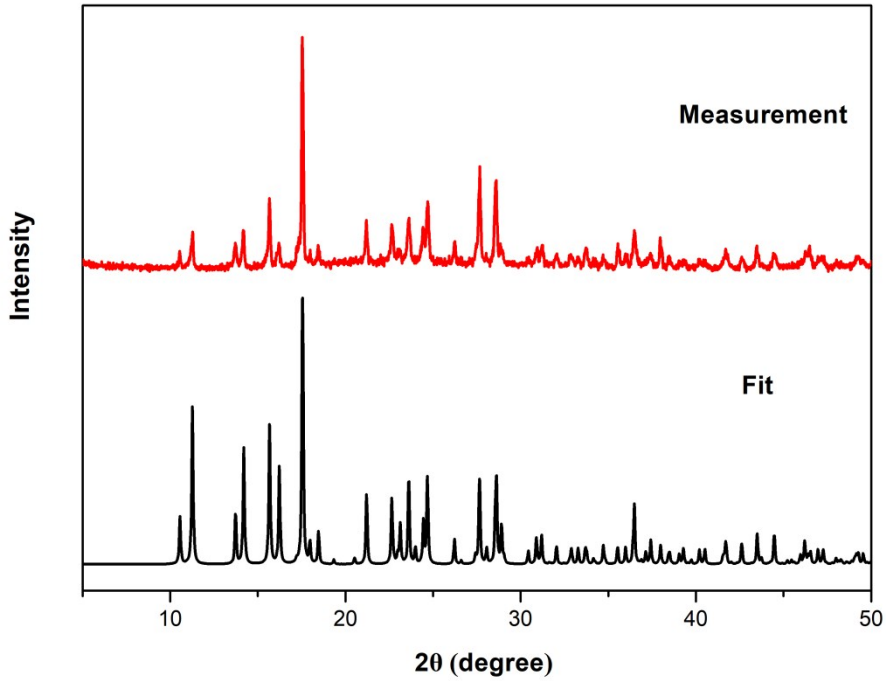

Fig. S7 PXRD pattern of compound **1** measured at RT, compared with the simulated data based on the single crystal structure

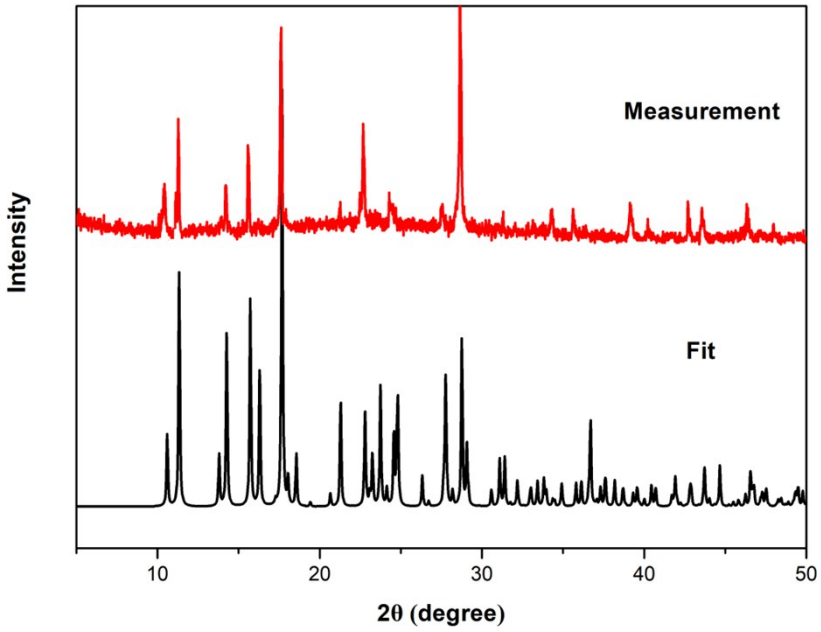

Fig. S8 PXRD pattern of compound **2** measured at RT, compared with the simulated data based on the single crystal structure

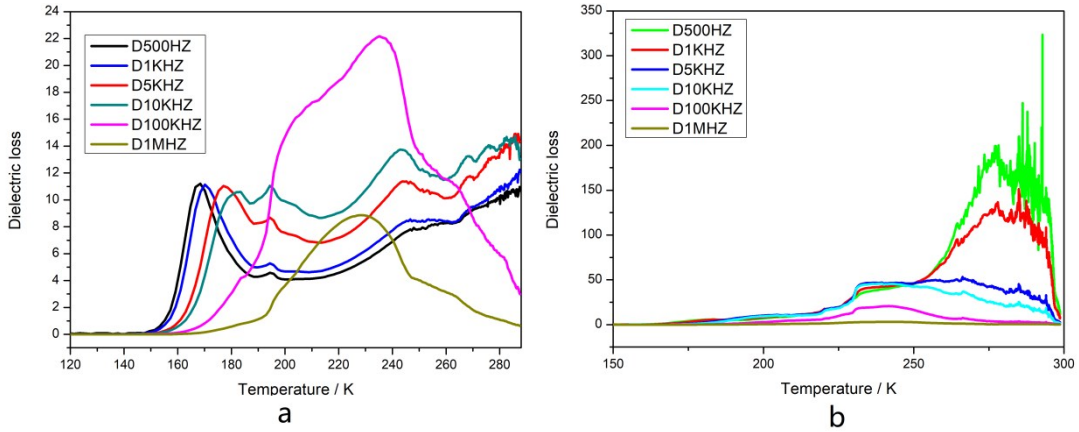

Fig. S9 The dielectric dissipation factors of two compounds on heating recorded at different frequencies: (a) of **1**; (b) of **2**

Table S1. Selected Bond Lengths (Å) and Bond Angles (°) of compound **1** (296 K and 203 K)

296 K					
Bond	Dist.	Bond	Dist.	Bond	Dist.
Zn(1)-Cl(3)	2.266(2)	Zn(1)-Cl(1)	2.2907(18)	Zn(1)-Cl(2)	2.2930(14)
Zn(1)-Cl(2)$^{\#1}$	2.2930(14)	N(1)-C(4)	1.501(9)	N(1)-C(2)	1.501(10)
N(1)-C(3)$^{\#1}$	1.508(6)	N(1)-C(3)	1.508(6)	N(2)-C(5)$^{\#1}$	1.506(7)
C(2)-C(1)	1.430(15)				
Angle	(°)	Angle	(°)	Angle	(°)
Cl(3)-Zn(1)-Cl(1)	108.45(8)	Cl(3)-Zn(1)-Cl(2)$^{\#1}$	110.15(5)	Cl(1)-Zn(1)-Cl(2)$^{\#1}$	113.49(5)

Cl(3)-Zn(1)-Cl(2)	110.15(5)	Cl(1)-Zn(1)-Cl(2)	113.49(5)	Cl(2)-Zn(1)-Cl(2)$^{\#1}$	100.93(8)
C(4)-N(1)-C(2)	111.2(6)	C(4)-N(1)-C(3)$^{\#1}$	108.7(4)	C(2)-N(1)-C(3)	109.7(4)
C(3)-N(1)-C(3)$^{\#1}$	108.8(6)	C(6)-N(2)-C(5)$^{\#1}$	109.2(4)	C(6)-N(2)-C(5)	109.2(4)
C(5)-N(2)-C(5)$^{\#1}$	110.4(7)	C(1)-C(2)-C(1)$^{\#1}$	102.8(14)		
203 K					
Bond	Dist.	Bond	Dist.	Bond	Dist.
Zn(1)-Cl(5)	2.258(3)	Zn(1)-Cl(3)	2.287(3)	Zn(1)-Cl(4)	2.298(3)
Zn(1)-Cl(2)	2.302(2)	N(1)-C(3)	1.483(14)	N(1)-(C1)	1.506(13)
N(1)-C(4)	1.524(13)				
Angle	(°)	Angle	(°)	Angle	(°)
Cl(5)-Zn(1)-Cl(3)	112.51(12)	Cl(5)-Zn(1)-Cl(4)	108.11(12)	Cl(3)-Zn(1)-Cl(4)	100.80(9)
Cl(5)-Zn(1)-Cl(2)	108.15(10)	Cl(3)-Zn(1)-Cl(2)	111.88(10)	Cl(4)-Zn(1)-Cl(2)	115.32(10)
C(3)-N(1)-C(1)	112.0(8)	C(3)-N(1)-C(4)	109.9(8)	C(1)-N(1)-C(4)	107.5(8)
C(7)-N(11)-C(5)	112.2(10)	C(7)-N(11)-C(2)	110.1(9)	C(5)-N(11)-C(2)	107.4(8)

At 296K, symmetry codes: $^{\#1}$ x, 0.5-y, z.

Table S2. Selected Bond Lengths (Å) and Bond Angles (°) of compound **2** (296 K and 233 K)

296 K					
Bond	Dist.	Bond	Dist.	Bond	Dist.
Co(1)-Cl(4)	2.2535(17)	Co(1)-Cl(1)	2.2656(15)	Co(1)-Cl(2)$^{\#1}$	2.2750(11)
Co(1)-Cl(2)	2.2750(11)	N(1)-C(3)	1.499(6)	N(1)-C(3)	1.501(4)
N(1)-C(4)	1.501(4)	N(1)-C(4)$^{\#1}$	1.501(4)	N(1)-C(2)	1.514(7)
Angle	(°)	Angle	(°)	Angle	(°)
Cl(4)-Co(1)-Cl(1)	107.44(6)	Cl(4)-Co(1)-Cl(2)$^{\#1}$	110.58(4)	Cl(1)-Co(1)-Cl(2)$^{\#1}$	113.81(4)
Cl(4)-Co(1)-Cl(2)	110.58(4)	Cl(1)-Co(1)-Cl(2)	113.81(4)	Cl(2)-Co(1)-Cl(2)$^{\#1}$	100.57(6)
C(3)-N(1)-C(4)	109.0(3)	C(3)-N(1)-C(4)$^{\#1}$	109.0(3)	C(4)-N(1)-C(4)$^{\#1}$	108.2(4)
C(2)-N(1)-C(3)	110.9(4)	C(2)-N(1)-C(4)	109.8(3)	C(2)-N(1)-C(4)$^{\#1}$	109.8(3)
C(6)-N(6)-C(5)$^{\#1}$	108.8(3)	C(6)-N(6)-C(5)	108.8(3)	C(5)-N(6)-C(5)$^{\#1}$	111.1(5)
C(1)-C(2)-C(1)$^{\#1}$	102.0(10)				
233 K					
Bond	Dist.	Bond	Dist.	Bond	Dist.
Co(1)-Cl(4)	2.259(4)	Co(1)-Cl(1)	2.274(3)	Co(1)-Cl(2)	2.278(4)
Co(1)-Cl(3)	2.291(4)	N(1)-C(5)	1.475(15)	N(1)-C(3)	1.477(16)
N(1)-C(1)	1.511(12)	N(2)-C(4)	1.487(14)	N(2)-C(4)	1.513(15)
N(2)-C(7)	1.521(14)	N(2)-C(6)	1.526(16)		
Angle	(°)	Angle	(°)	Angle	(°)
Cl(4)-Co(1)-Cl(1)	107.03(12)	Cl(4)-Co(1)-Cl(2)	112.84(15)	Cl(1)-Co(1)-Cl(2)	112.25(14)
Cl(4)-Co(1)-Cl(3)	108.58(15)	Cl(1)-Co(1)-Cl(3)	115.60(13)	Cl(2)-Co(1)-Cl(3)	100.59(14)
C(5)-N(1)-C(3)	111.9(10)	C(5)-N(1)-C(1)	109.7(9)	C(3)-N(1)-C(1)	109.1(9)
C(2)-N(2)-C(4)	109.9(9)	C(2)-N(2)-C(7)	110.8(8)	C(4)-N(2)-C(7)	109.2(9)
C(2)-N(2)-C(6)	109.0(9)	C(4)-N(2)-C(6)	107.6(8)		

At 296K, symmetry codes: [#1] x, 0.5-y, z.