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catena-Poly[[chloridocobalt(II)]-μ-5-(8-quinolyloxymethyl)tetrazolato-$\kappa^4N^5,O,N^1:N^4$]

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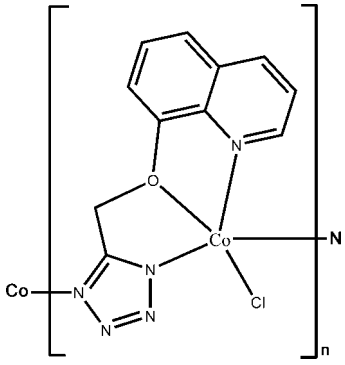
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.040; wR factor = 0.101; data-to-parameter ratio = 16.5.

In the title compound, $[Co(C_{11}H_8N_5O)Cl]_n$, the Co^{II} atom is pentacoordinated by one O atom and two N atoms from a 5-(8-quinolyloxymethyl)tetrazolate ligand, one N atom from another symmetry-related ligand, and a Cl atom. The coordination geometry can be described as slightly distorted trigonal–bipyramidal. Adjacent Co atoms are connected by the bridging tetrazole groups into a chain. The dihedral angle between the quinoline and tetrazole planes is 21.2 (1)°. The structure involves intra- and interchain C—H···N hydrogen bonds.

Related literature

For related literature, see: Luo & Ye (2008); Wang *et al.* (2005); Wang & Ye (2007); Xiong *et al.* (2002).



Experimental

Crystal data

$[Co(C_{11}H_8N_5O)Cl]$
M_r = 320.60
Monoclinic, $P2_1/c$
a = 7.0289 (11) Å
b = 8.4331 (11) Å
c = 20.220 (4) Å
β = 96.757 (10)°
V = 1190.2 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.66 mm^{-1}
T = 293 (2) K
0.20 × 0.18 × 0.14 mm

Data collection

Rigaku SCXmini CCD area-detector diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.701, T_{max} = 0.798
12192 measured reflections
2846 independent reflections
2385 reflections with $I > 2\sigma(I)$
R_{int} = 0.047

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.101
S = 1.08
2846 reflections
172 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—N1^{i}	2.049 (2)	Co1—Cl1	2.2670 (8)
Co1—N4	2.053 (2)	Co1—O1	2.3979 (18)
Co1—N5	2.066 (2)		
N1^{i}—Co1—N4	96.46 (9)	N5—Co1—Cl1	104.74 (6)
N1^{i}—Co1—N5	106.43 (8)	N1^{i}—Co1—O1	86.22 (8)
N4—Co1—N5	134.43 (8)	N4—Co1—O1	70.65 (7)
N1^{i}—Co1—Cl1	104.93 (7)	N5—Co1—O1	72.16 (7)
N4—Co1—Cl1	106.62 (7)	Cl1—Co1—O1	168.82 (6)

Symmetry code: (i) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2B···N3^{ii}	0.97	2.54	3.292 (4)	135
C8—H8A···N2^{iii}	0.93	2.52	3.398 (4)	157

Symmetry codes: (ii) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (iii) $x-1, -y+\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2140).

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supporting information

Acta Cryst. (2008). E**64**, m1006 [doi:10.1107/S1600536808020205]

catena-Poly[[chloridocobalt(II)]-μ-5-(8-quinolyloxymethyl)tetrazolato-$\kappa^4N^5,O,N^1:N^4$]

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S1. Comment

In the past five years, we have focused on the chemistry of 5-substituted tetrazoles because of their multiple coordination modes to metal ions and the construction of novel metal–organic frameworks. (Wang *et al.*, 2005; Xiong *et al.*, 2002). As part of our on going studies of the chemistry of tetrazoles, we have determined the crystal structure of the title compound.

In the title compound, the Co^{II} atom is penta-coordinated by one O atom and two N atoms from an 8-[(tetrazol-5-yl)methoxy]quinoline ligand, by one N atom from another symmetry-related ligand, and by one terminal Cl atom (Fig. 1). The coordination geometry can be described as slightly distorted trigonal–bipyramidal (Table 1), with three N atoms (N4, N5 and N1^{i}) [symmetry code: (i) -*x* + 1, *y* + 1/2, -*z* + 1/2] forming the equatorial palne and the O1 and Cl1 atoms occupying the axial positions. The deviation of the Co1 atom from the equatorial plane is 0.549 (1) Å. The bond angles of N4—Co1—N5, N5—Co1—N1^{i} and N4—Co1—N1^{i} are 134.43 (8), 106.43 (8) and 96.46 (9)°, respectively. Adjacent Co atoms are connected by the bridging tetrazole groups into a chain (Fig. 2). Geometric parameters of the ligand are in normal ranges (Wang & Ye, 2007). The dihedral angle between the quinoline and tetrazole planes is 21.2 (1)°. The structure involves intrachain and interchain C—H···N hydrogen bonds (Fig. 3; Table 2).

S2. Experimental

8-(1*H*-Tetrazol-5-yl)methoxy)quinoline was synthesized by using a similar procedure described previously by us (Luo & Ye, 2008). A mixture of the ligand (0.045 g, 0.2 mmol), $CoCl_2$ (0.026 g, 0.2 mmol) and water (1 ml) was sealed in a glass tube and maintained at 383 K. Purple crystals of the title compound suitable for X-ray ananlysis were obtained after 3 d.

S3. Refinement

H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 (aromatic) and 0.97 (CH_2) Å and with U_{iso}(H) = 1.2U_{eq}(C).

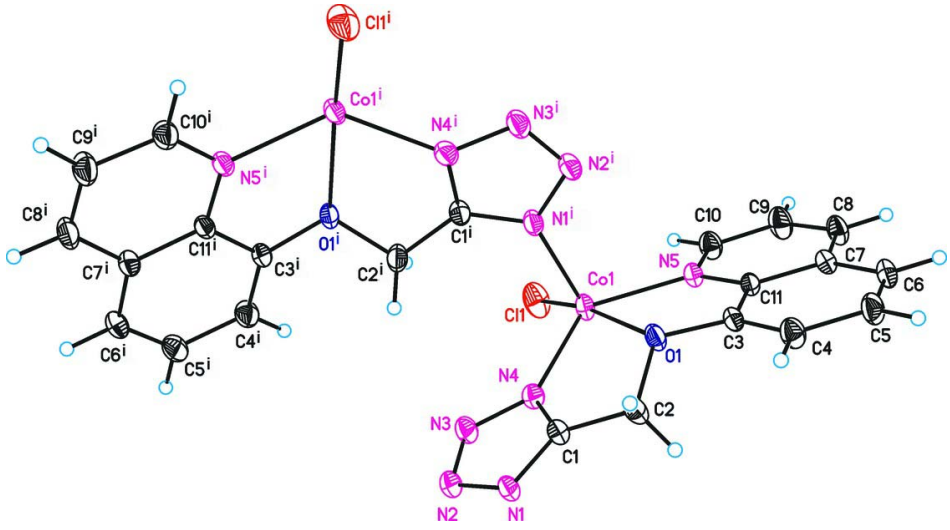

Figure 1

The structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) -*x* + 1, *y* + 1/2, -*z* + 1/2.]

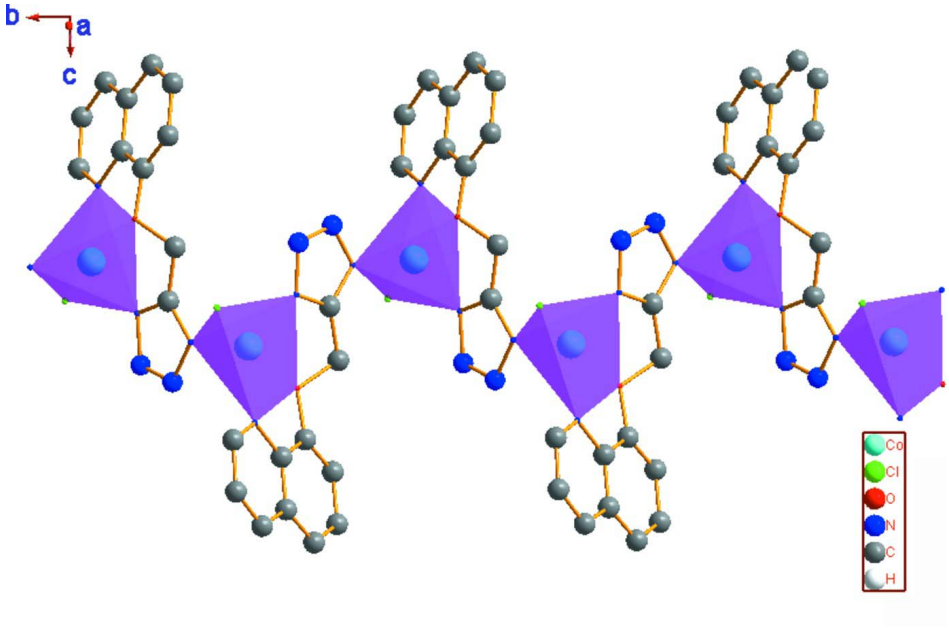

Figure 2

A polyhedral drawing of the chain in the title compound.

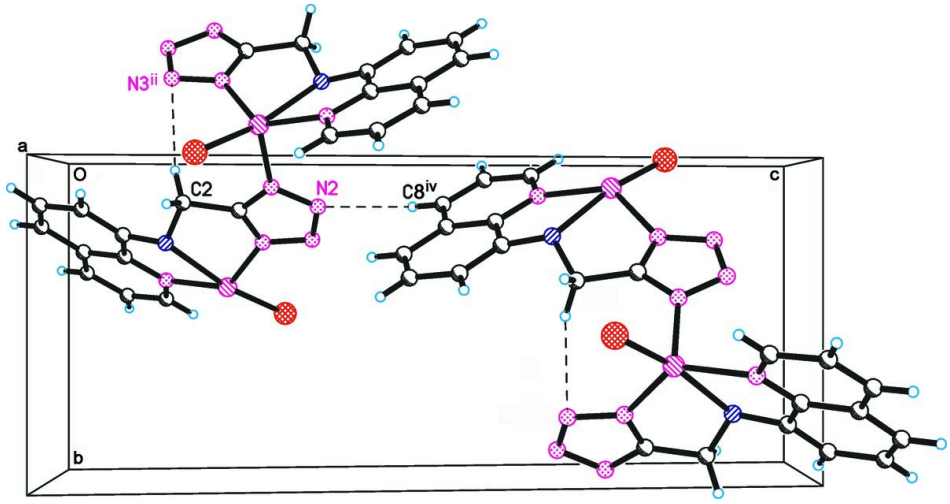

Figure 3

Crystal packing of the title compound viewed along the *a*-axis. Dashed lines denote hydrogen bonds. [Symmetry codes: (ii) -*x* + 1, *y* - 1/2, -*z* + 1/2; (iv) *x* + 1, -*y* + 1/2, *z* + 1/2.]

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Crystal data

$[Co(C_{11}H_8N_5O)Cl]$
M_r = 320.60
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 7.0289 (11) Å
b = 8.4331 (11) Å
c = 20.220 (4) Å
β = 96.757 (10)°
V = 1190.2 (3) Å^3
Z = 4
$F(000)$ = 644
D_x = 1.789 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2846 reflections
θ = 2.6–27.9°
μ = 1.66 mm^{-1}
T = 293 K
Prism, purple
0.20 × 0.18 × 0.14 mm

Data collection

Rigaku SCXmini CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.701, T_{max} = 0.798
12192 measured reflections
2846 independent reflections
2385 reflections with $I > 2\sigma(I)$
R_{int} = 0.047
θ_{max} = 27.9°, θ_{min} = 2.6°
h = −9→9
k = −11→11
l = −26→26

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.101
S = 1.08
2846 reflections
172 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0449P)^2 + 0.5457P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.39$ e Å^{-3}
$\Delta\rho_{min} = -0.37$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.19156 (5)	0.40223 (4)	0.221382 (16)	0.02932 (13)
C1	0.5028 (3)	0.1574 (3)	0.24542 (12)	0.0287 (5)
C2	0.4852 (4)	0.1332 (4)	0.17171 (13)	0.0380 (6)
H2A	0.6097	0.1391	0.1556	0.046*
H2B	0.4281	0.0310	0.1596	0.046*
C3	0.2568 (4)	0.2342 (3)	0.08430 (11)	0.0279 (5)
C4	0.3194 (4)	0.1528 (4)	0.03257 (13)	0.0376 (6)
H4A	0.4403	0.1065	0.0375	0.045*
C5	0.1997 (4)	0.1392 (4)	−0.02832 (13)	0.0404 (7)
H5A	0.2424	0.0841	−0.0636	0.049*
C6	0.0216 (4)	0.2065 (3)	−0.03590 (13)	0.0369 (6)
H6A	−0.0553	0.1978	−0.0764	0.044*
C7	−0.0466 (4)	0.2890 (3)	0.01735 (12)	0.0303 (5)
C8	−0.2301 (4)	0.3590 (4)	0.01327 (14)	0.0403 (6)
H8A	−0.3132	0.3524	−0.0260	0.048*
C9	−0.2846 (4)	0.4360 (4)	0.06704 (15)	0.0454 (7)
H9A	−0.4052	0.4825	0.0647	0.054*
C10	−0.1581 (4)	0.4453 (4)	0.12616 (14)	0.0375 (6)
H10A	−0.1980	0.4984	0.1624	0.045*
C11	0.0727 (3)	0.3037 (3)	0.07850 (11)	0.0253 (5)
N1	0.6256 (3)	0.0865 (3)	0.29043 (10)	0.0303 (5)
N2	0.5887 (3)	0.1467 (3)	0.34993 (10)	0.0362 (5)
N3	0.4486 (3)	0.2482 (3)	0.34007 (11)	0.0359 (5)
N4	0.3906 (3)	0.2574 (3)	0.27357 (10)	0.0309 (5)
N5	0.0151 (3)	0.3818 (2)	0.13259 (10)	0.0272 (4)
Cl1	−0.00233 (11)	0.49197 (11)	0.29524 (4)	0.0531 (2)
O1	0.3637 (3)	0.2596 (2)	0.14477 (8)	0.0324 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0282 (2)	0.0378 (2)	0.02076 (19)	0.00290 (14)	−0.00200 (13)	−0.00415 (14)
C1	0.0287 (12)	0.0331 (13)	0.0232 (12)	0.0014 (10)	−0.0014 (9)	0.0009 (10)
C2	0.0440 (16)	0.0439 (16)	0.0246 (13)	0.0178 (12)	−0.0024 (11)	0.0015 (12)
C3	0.0333 (13)	0.0308 (12)	0.0183 (11)	0.0017 (10)	−0.0019 (9)	0.0010 (10)
C4	0.0387 (15)	0.0451 (15)	0.0286 (13)	0.0113 (12)	0.0018 (11)	−0.0043 (12)
C5	0.0511 (17)	0.0481 (16)	0.0221 (13)	0.0060 (13)	0.0041 (11)	−0.0077 (12)
C6	0.0450 (15)	0.0441 (16)	0.0197 (12)	0.0004 (12)	−0.0036 (11)	−0.0027 (11)
C7	0.0346 (13)	0.0333 (13)	0.0217 (12)	−0.0004 (10)	−0.0026 (10)	0.0012 (10)
C8	0.0356 (15)	0.0532 (17)	0.0287 (14)	0.0039 (12)	−0.0099 (11)	−0.0020 (13)
C9	0.0330 (14)	0.063 (2)	0.0376 (16)	0.0142 (13)	−0.0065 (12)	−0.0070 (14)

C10	0.0343 (14)	0.0457 (16)	0.0312 (14)	0.0101 (12)	−0.0011 (11)	−0.0056 (12)
C11	0.0283 (12)	0.0278 (12)	0.0189 (11)	−0.0020 (9)	−0.0010 (9)	0.0001 (9)
N1	0.0345 (11)	0.0343 (11)	0.0204 (10)	−0.0012 (9)	−0.0031 (8)	0.0026 (8)
N2	0.0473 (14)	0.0382 (12)	0.0214 (11)	−0.0021 (10)	−0.0027 (9)	0.0010 (9)
N3	0.0448 (13)	0.0405 (13)	0.0216 (10)	−0.0018 (10)	0.0005 (9)	0.0005 (9)
N4	0.0357 (12)	0.0329 (11)	0.0235 (10)	−0.0008 (9)	0.0012 (9)	−0.0010 (9)
N5	0.0286 (10)	0.0318 (11)	0.0205 (10)	0.0008 (8)	−0.0008 (8)	−0.0019 (8)
Cl1	0.0478 (4)	0.0800 (6)	0.0326 (4)	0.0160 (4)	0.0090 (3)	−0.0097 (4)
O1	0.0347 (10)	0.0374 (10)	0.0227 (9)	0.0098 (7)	−0.0072 (7)	−0.0021 (8)

Geometric parameters (Å, º)

Co1—N1^{i}	2.049 (2)	C5—H5A	0.9300
Co1—N4	2.053 (2)	C6—C7	1.413 (4)
Co1—N5	2.066 (2)	C6—H6A	0.9300
Co1—Cl1	2.2670 (8)	C7—C8	1.412 (4)
Co1—O1	2.3979 (18)	C7—C11	1.415 (3)
C1—N1	1.321 (3)	C8—C9	1.360 (4)
C1—N4	1.327 (3)	C8—H8A	0.9300
C1—C2	1.495 (3)	C9—C10	1.406 (4)
C2—O1	1.433 (3)	C9—H9A	0.9300
C2—H2A	0.9700	C10—N5	1.322 (3)
C2—H2B	0.9700	C10—H10A	0.9300
C3—C4	1.366 (3)	C11—N5	1.378 (3)
C3—O1	1.375 (3)	N1—N2	1.359 (3)
C3—C11	1.413 (3)	N1—Co1^{ii}	2.049 (2)
C4—C5	1.412 (4)	N2—N3	1.302 (3)
C4—H4A	0.9300	N3—N4	1.361 (3)
C5—C6	1.366 (4)		
N1^{i}—Co1—N4	96.46 (9)	C7—C6—H6A	119.7
N1^{i}—Co1—N5	106.43 (8)	C8—C7—C6	123.4 (2)
N4—Co1—N5	134.43 (8)	C8—C7—C11	117.3 (2)
N1^{i}—Co1—Cl1	104.93 (7)	C6—C7—C11	119.3 (2)
N4—Co1—Cl1	106.62 (7)	C9—C8—C7	119.6 (2)
N5—Co1—Cl1	104.74 (6)	C9—C8—H8A	120.2
N1^{i}—Co1—O1	86.22 (8)	C7—C8—H8A	120.2
N4—Co1—O1	70.65 (7)	C8—C9—C10	119.8 (3)
N5—Co1—O1	72.16 (7)	C8—C9—H9A	120.1
Cl1—Co1—O1	168.82 (6)	C10—C9—H9A	120.1
N1—C1—N4	111.4 (2)	N5—C10—C9	123.0 (3)
N1—C1—C2	126.6 (2)	N5—C10—H10A	118.5
N4—C1—C2	122.1 (2)	C9—C10—H10A	118.5
O1—C2—C1	104.7 (2)	N5—C11—C3	119.0 (2)
O1—C2—H2A	110.8	N5—C11—C7	122.4 (2)
C1—C2—H2A	110.8	C3—C11—C7	118.6 (2)
O1—C2—H2B	110.8	C1—N1—N2	105.3 (2)
C1—C2—H2B	110.8	C1—N1—Co1^{ii}	129.11 (17)

H2A—C2—H2B	108.9	N2—N1—Co1^{ii}	125.07 (16)
C4—C3—O1	124.6 (2)	N3—N2—N1	109.3 (2)
C4—C3—C11	121.3 (2)	N2—N3—N4	108.8 (2)
O1—C3—C11	114.1 (2)	C1—N4—N3	105.3 (2)
C3—C4—C5	119.7 (3)	C1—N4—Co1	124.09 (17)
C3—C4—H4A	120.1	N3—N4—Co1	130.42 (17)
C5—C4—H4A	120.1	C10—N5—C11	117.9 (2)
C6—C5—C4	120.6 (2)	C10—N5—Co1	120.22 (17)
C6—C5—H5A	119.7	C11—N5—Co1	121.84 (16)
C4—C5—H5A	119.7	C3—O1—C2	117.5 (2)
C5—C6—C7	120.5 (2)	C3—O1—Co1	112.87 (14)
C5—C6—H6A	119.7	C2—O1—Co1	116.81 (15)

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+1/2; (ii) −*x*+1, *y*−1/2, −*z*+1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2*B*···N3^{ii}	0.97	2.54	3.292 (4)	135
C8—H8*A*···N2^{iii}	0.93	2.52	3.398 (4)	157

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