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Tetraethylammonium dichlorido[*N*,*N*′-(*o*-phenylene)bis(isoquinoline-2-carboxamidato)-κ^4N]cobaltate(III)

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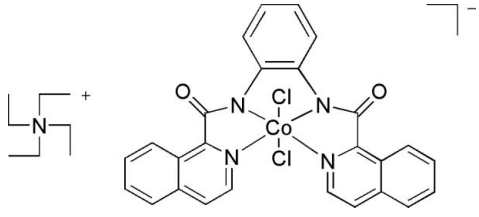
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.006 Å; R factor = 0.050; wR factor = 0.102; data-to-parameter ratio = 14.7.

In the title compound, $(C_8H_{20}N)[Co(C_{26}H_{16}N_4O_2)Cl_2]$, the four N atoms of the *N*,*N*′-(*o*-phenylene)bis(isoquinoline-2-carboxamidate) ($biqb^{2-}$) ligand form the equatorial plane of a distorted octahedral coordination environment around the Co^{III} ion, while two chloride ligands are axially coordinated. The $Co-N_{amide}$ distances are significantly shorter than the $Co-N_{pyridyl}$ distances. The dihedral angle between the two isoquinoline fused-ring systems is 25.72 (7)°. The crystal structure is stabilized, in part, by intermolecular $C_{cation}-H\cdots Cl$ and $C_{isoquinoline}-H\cdots Cl$ hydrogen bonds.

Related literature

The corresponding $[Et_4N][Co(bpb)Cl_2]$ [H_2bpb = 1,2-bis(2-pyridine-2-carboxamido)benzene] complex has distorted octahedral geometry (Seo *et al.*, 2004) with chloride axial ligands having long Co—Cl bonds.

For related literature, see: Barton & Doller (1992); Jain & Sain (2003); Kaizer *et al.* (2004); Nam *et al.* (2000, 2006); Sawyer *et al.* (1996).



Experimental

Crystal data

$(C_8H_{20}N)[Co(C_{26}H_{16}N_4O_2)Cl_2]$
M_r = 676.51
Monoclinic, $P2_1/n$
a = 12.921 (2) Å
b = 16.646 (3) Å
c = 14.022 (2) Å
β = 90.625 (4)°
V = 3015.7 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.79 mm^{-1}
T = 100 (2) K
0.15 × 0.10 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.910, T_{max} = 0.924
16659 measured reflections
5913 independent reflections
3440 reflections with $I > 2\sigma(I)$
R_{int} = 0.085

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.102
S = 0.89
5913 reflections
401 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

Table 1
Selected bond lengths (Å).

Co1—N3	1.859 (3)	Co1—N4	1.965 (3)
Co1—N2	1.877 (3)	Co1—Cl1	2.2552 (11)
Co1—N1	1.965 (3)	Co1—Cl2	2.2674 (11)

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

D—H···A	D—H	H···A	D···A	D—H···A
C53—H53B···Cl1^{i}	0.99	2.81	3.701 (4)	150
C57—H57A···Cl1^{i}	0.99	2.64	3.576 (4)	159
C55—H55B···Cl2^{ii}	0.99	2.76	3.740 (4)	172
C5—H5···Cl2^{iii}	0.95	2.77	3.501 (4)	135
C26—H26···Cl1^{i}	0.95	2.79	3.669 (4)	155

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x+\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$; (iii) $x+\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); 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: LH2427).

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supplementary materials

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Tetraethylammonium dichlorido[*N*,*N*'-(*o*-phenylene)bis(isoquinoline-2-carboxamidato)-κ^4N\]cobaltate(III)

D. N. Lee, E. Y. Lee, C. Kim, S.-J. Kim and Y. Kim

Comment

Selective hydroxylation of hydrocarbons is an important but still very difficult chemical transformation process. A great deal of effort has been made to develop efficient catalysts for the hydrocarbon oxidation in synthetic organic chemistry and industrial chemistry (Barton & Doller, 1992, Sawyer *et al.*, 1996). While much attention has been paid to heme and nonheme iron complexes due to their high catalytic activity and biological relevance (Nam *et al.*, 2000, Kaizer *et al.*, 2004), cobalt complexes have attracted less attention in the oxidation chemistry (Jain & Sain, 2003). In order to study the catalytic oxidation reactions of hydrocarbons with new cobalt complexes, we have synthesized the title complex by the reaction of cobalt(II) chloride with 1,2-bis(isoquinoline-2-carboxamido)benzene (H_2biqb).

The four N atoms of the $biqb^{2-}$ ligand form the equatorial plane of the distorted octahedral coordination geometry of the Co^{III} ion, and two chloro ligands are axially coordinated to the Co^{III} ion (Fig. 1). The two Co—N_{amide} distances are significantly shorter than the Co—$N_{pyridyl}$ distances. The anion is not planar with a dihedral angle of 25.72 (7)° between two isoqunoline rings. In the crystal structure, there are inter-molecular C(cation)-H···Cl and *C*(isoquinoline)-H···Cl hydrogen bonds as shown in Fig. 2.

Experimental

For the preparation of the ligand H2biqb, a slightly modified method by Nam *et al.* was used (Nam *et al.*, 2006). To a stirred solution of 1–isoquinolinecarboxylic acid (1.73 g, 10 mmol) in pyridine (10 ml), a solution of 1,2–phenylenediamine (0.54 g, 5 mmol) in pyridine (5 ml) was added drop by drop. The solution was stirred for 15 min and triphenyl phosphite (2.70 ml, 10 mmol) was slowly added. The reaction mixture was warmed up to 393 K, and the mixture was stirred for 4 h. The volume of the solution was then reduced to 2 ml and kept in air. Crystallization from an aqueous solution afforded a pale–yellow powder, which was washed with ethanol. For the preparation of the title complex, equimolar quantities of $CoCl_2·6H_2O$ (0.12 g, 0.5 mmol) and H_2biqb (0.21 g, 0.5 mmol) were dissolved in DMF, and triethylamine (0.14 ml, 1 mmol) and tetraethylammonium chloride hydrate (0.17 g, 1 mmol) were added to the reaction solution. After the solution was refluxed for 4 h, brown precipitate was obtained. Dark brown crystals were obtained from an acetonitrile–diethyl ether solution at room temperature by slow evaporation for *X*–ray experiments.

Refinement

H atoms were placed in calculated positions with C—H distances of 0.95Å (isoquinoline and benzene), 0.99Å (methylene) and 0.98Å (methyl)·They were included in the refinement in riding–motion approximation with U_{iso}(H) = 1.2U_{eq}(C) or U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms.

Figures

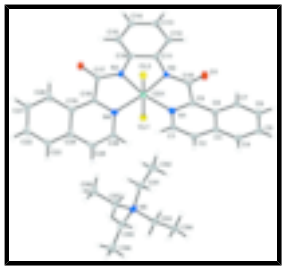


Fig. 1. The molecular structure of the title compound showing the atom-labeling scheme. Displacement ellipsoids are shown at the 50% probability level.

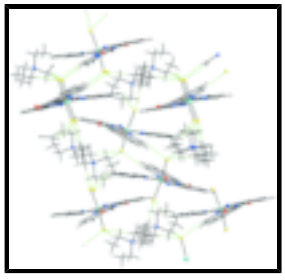


Fig. 2. Part of the crystal structure showing hydrogen bonds as dashed lines.

Tetraethylammonium dichlorido[*N*,*N*'-(*o*-phenylene)bis(isoquinoline-2-carboxamidato)- κ^4N]cobaltate(III)

Crystal data

$(C_8H_{20}N)[Co(C_{26}H_{16}N_4O_2)Cl_2]$	F_{000} = 1408
M_r = 676.51	D_x = 1.490 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 813 reflections
a = 12.921 (2) Å	θ = 2.2–17.4º
b = 16.646 (3) Å	μ = 0.79 mm^{-1}
c = 14.022 (2) Å	T = 100 (2) K
β = 90.625 (4)º	Block, dark brown
V = 3015.7 (9) Å^3	0.15 × 0.10 × 0.10 mm
Z = 4	

Data collection

Bruker SMART CCD diffractometer	5913 independent reflections
Radiation source: fine-focus sealed tube	3440 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.085
T = 100(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 1.9º
Absorption correction: multi-scan (SADABS; Bruker, 1997)	h = −15→14
T_{min} = 0.910, T_{max} = 0.924	k = −20→20
16659 measured reflections	l = −12→17

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.050$	H-atom parameters constrained
$wR(F^2) = 0.102$	$w = 1/[\sigma^2(F_o^2) + (0.0407P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.89$	$(\Delta/\sigma)_{max} = 0.001$
5913 reflections	$\Delta\rho_{max} = 0.42$ e Å^{-3}
401 parameters	$\Delta\rho_{min} = -0.43$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.36201 (4)	0.65718 (3)	0.46734 (4)	0.01553 (14)
Cl1	0.31747 (7)	0.52714 (5)	0.44809 (7)	0.0203 (2)
Cl2	0.42351 (7)	0.78286 (5)	0.49397 (7)	0.0235 (2)
N1	0.4901 (2)	0.63953 (16)	0.3961 (2)	0.0167 (7)
N2	0.3095 (2)	0.67995 (16)	0.3450 (2)	0.0138 (7)
N3	0.2300 (2)	0.68338 (16)	0.5085 (2)	0.0160 (7)
N4	0.3827 (2)	0.63030 (16)	0.6027 (2)	0.0153 (7)
O1	0.33359 (18)	0.64480 (15)	0.18733 (17)	0.0247 (6)
O2	0.12527 (18)	0.69526 (14)	0.64086 (17)	0.0204 (6)
C1	0.5880 (3)	0.6354 (2)	0.4333 (3)	0.0194 (9)
H1	0.5977	0.6389	0.5004	0.023*
C2	0.6715 (3)	0.6266 (2)	0.3770 (3)	0.0209 (9)
H2	0.7384	0.6225	0.4053	0.025*
C3	0.6608 (3)	0.6233 (2)	0.2774 (3)	0.0191 (9)
C4	0.7456 (3)	0.6157 (2)	0.2165 (3)	0.0229 (9)
H4	0.8134	0.6114	0.2429	0.027*
C5	0.7324 (3)	0.6146 (2)	0.1204 (3)	0.0241 (9)
H5	0.7908	0.6095	0.0803	0.029*

C6	0.6330 (3)	0.6208 (2)	0.0800 (3)	0.0238 (9)
H6	0.6247	0.6200	0.0126	0.029*
C7	0.5475 (3)	0.6281 (2)	0.1367 (3)	0.0193 (9)
H7	0.4806	0.6323	0.1083	0.023*
C8	0.5586 (3)	0.6295 (2)	0.2369 (3)	0.0162 (8)
C9	0.4755 (3)	0.6390 (2)	0.3014 (3)	0.0170 (9)
C10	0.3649 (3)	0.6539 (2)	0.2705 (3)	0.0170 (8)
C11	0.2027 (3)	0.6964 (2)	0.3431 (3)	0.0162 (8)
C12	0.1406 (3)	0.70987 (19)	0.2625 (3)	0.0178 (9)
H12	0.1705	0.7097	0.2009	0.021*
C13	0.0357 (3)	0.7234 (2)	0.2724 (3)	0.0195 (9)
H13	−0.0065	0.7323	0.2174	0.023*
C14	−0.0084 (3)	0.7241 (2)	0.3624 (3)	0.0178 (9)
H14	−0.0807	0.7327	0.3685	0.021*
C15	0.0525 (3)	0.7121 (2)	0.4438 (3)	0.0205 (9)
H15	0.0220	0.7133	0.5051	0.025*
C16	0.1581 (3)	0.69848 (19)	0.4351 (3)	0.0153 (8)
C17	0.2091 (3)	0.6808 (2)	0.6022 (3)	0.0156 (8)
C18	0.3032 (3)	0.6515 (2)	0.6576 (2)	0.0136 (8)
C19	0.3040 (3)	0.63931 (19)	0.7576 (3)	0.0157 (8)
C20	0.2256 (3)	0.6671 (2)	0.8204 (3)	0.0197 (9)
H20	0.1676	0.6953	0.7950	0.024*
C21	0.2325 (3)	0.6540 (2)	0.9165 (3)	0.0241 (9)
H21	0.1798	0.6736	0.9572	0.029*
C22	0.3169 (3)	0.6118 (2)	0.9555 (3)	0.0248 (10)
H22	0.3204	0.6022	1.0223	0.030*
C23	0.3939 (3)	0.5843 (2)	0.8982 (3)	0.0206 (9)
H23	0.4508	0.5560	0.9255	0.025*
C24	0.3900 (3)	0.5975 (2)	0.7989 (3)	0.0168 (9)
C25	0.4678 (3)	0.5711 (2)	0.7364 (3)	0.0195 (9)
H25	0.5244	0.5407	0.7608	0.023*
C26	0.4627 (3)	0.58839 (19)	0.6426 (3)	0.0172 (9)
H26	0.5171	0.5706	0.6027	0.021*
N5	0.9072 (2)	0.54941 (17)	0.7444 (2)	0.0207 (8)
C51	0.9003 (3)	0.6357 (2)	0.7087 (3)	0.0259 (10)
H51A	0.8780	0.6702	0.7622	0.031*
H51B	0.9705	0.6534	0.6904	0.031*
C52	0.8280 (3)	0.6497 (2)	0.6252 (3)	0.0344 (11)
H52A	0.8498	0.6168	0.5711	0.052*
H52B	0.8298	0.7066	0.6073	0.052*
H52C	0.7574	0.6349	0.6431	0.052*
C53	0.9412 (3)	0.4925 (2)	0.6655 (3)	0.0220 (9)
H53A	0.9425	0.4372	0.6914	0.026*
H53B	0.8884	0.4939	0.6138	0.026*
C54	1.0459 (3)	0.5102 (2)	0.6225 (3)	0.0240 (10)
H54A	1.0443	0.5632	0.5921	0.036*
H54B	1.0621	0.4692	0.5748	0.036*
H54C	1.0991	0.5098	0.6729	0.036*
C55	0.9856 (3)	0.5497 (2)	0.8262 (3)	0.0290 (10)

H55A	1.0535	0.5669	0.8012	0.035*
H55B	0.9639	0.5901	0.8738	0.035*
C56	0.9994 (3)	0.4697 (2)	0.8761 (3)	0.0363 (11)
H56A	0.9344	0.4544	0.9066	0.055*
H56B	1.0542	0.4742	0.9246	0.055*
H56C	1.0184	0.4286	0.8294	0.055*
C57	0.8029 (3)	0.5188 (2)	0.7762 (3)	0.0215 (9)
H57A	0.7559	0.5170	0.7200	0.026*
H57B	0.8115	0.4631	0.7995	0.026*
C58	0.7518 (3)	0.5675 (2)	0.8531 (3)	0.0283 (10)
H58A	0.7995	0.5734	0.9075	0.042*
H58B	0.6888	0.5399	0.8739	0.042*
H58C	0.7337	0.6206	0.8281	0.042*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0159 (3)	0.0166 (3)	0.0141 (3)	0.0011 (2)	0.0008 (2)	−0.0001 (2)
Cl1	0.0210 (5)	0.0199 (5)	0.0200 (5)	0.0001 (4)	−0.0003 (4)	0.0000 (4)
Cl2	0.0269 (6)	0.0211 (5)	0.0226 (6)	0.0003 (4)	0.0024 (4)	0.0002 (4)
N1	0.0166 (17)	0.0153 (17)	0.0182 (18)	−0.0005 (13)	−0.0015 (13)	0.0003 (14)
N2	0.0152 (17)	0.0142 (16)	0.0122 (17)	−0.0006 (13)	0.0028 (13)	0.0046 (13)
N3	0.0162 (17)	0.0181 (17)	0.0137 (18)	0.0010 (13)	0.0032 (13)	−0.0008 (14)
N4	0.0165 (17)	0.0105 (16)	0.0189 (18)	−0.0012 (13)	−0.0007 (14)	0.0002 (13)
O1	0.0240 (15)	0.0355 (17)	0.0145 (15)	0.0012 (13)	−0.0005 (12)	−0.0026 (13)
O2	0.0184 (15)	0.0237 (15)	0.0192 (15)	0.0001 (12)	0.0050 (12)	0.0008 (12)
C1	0.019 (2)	0.025 (2)	0.014 (2)	−0.0001 (17)	−0.0027 (17)	0.0014 (17)
C2	0.017 (2)	0.024 (2)	0.022 (2)	0.0020 (17)	−0.0023 (18)	0.0044 (18)
C3	0.021 (2)	0.016 (2)	0.020 (2)	0.0001 (17)	0.0050 (17)	0.0026 (17)
C4	0.015 (2)	0.025 (2)	0.028 (3)	0.0023 (18)	0.0026 (18)	0.0024 (19)
C5	0.020 (2)	0.022 (2)	0.031 (3)	0.0033 (18)	0.0093 (19)	0.0036 (19)
C6	0.030 (2)	0.020 (2)	0.021 (2)	−0.0023 (19)	0.0082 (19)	0.0003 (18)
C7	0.026 (2)	0.015 (2)	0.017 (2)	0.0027 (17)	0.0004 (18)	0.0037 (17)
C8	0.014 (2)	0.0089 (18)	0.025 (2)	−0.0007 (15)	0.0062 (17)	0.0038 (17)
C9	0.021 (2)	0.014 (2)	0.016 (2)	−0.0003 (16)	0.0020 (17)	−0.0005 (16)
C10	0.018 (2)	0.0136 (19)	0.019 (2)	−0.0051 (17)	0.0004 (17)	0.0055 (18)
C11	0.018 (2)	0.017 (2)	0.014 (2)	0.0006 (16)	−0.0006 (16)	−0.0053 (17)
C12	0.024 (2)	0.014 (2)	0.015 (2)	−0.0007 (17)	0.0026 (17)	−0.0017 (16)
C13	0.017 (2)	0.019 (2)	0.022 (2)	0.0026 (17)	−0.0056 (17)	−0.0016 (18)
C14	0.015 (2)	0.014 (2)	0.024 (2)	0.0019 (16)	−0.0040 (17)	−0.0001 (17)
C15	0.027 (2)	0.018 (2)	0.017 (2)	0.0034 (17)	0.0029 (17)	0.0009 (17)
C16	0.017 (2)	0.0096 (19)	0.020 (2)	0.0019 (16)	−0.0010 (16)	0.0007 (17)
C17	0.021 (2)	0.0092 (19)	0.017 (2)	−0.0023 (16)	0.0022 (17)	0.0031 (16)
C18	0.015 (2)	0.0093 (18)	0.016 (2)	0.0007 (16)	0.0002 (16)	0.0012 (16)
C19	0.024 (2)	0.0096 (19)	0.014 (2)	−0.0057 (16)	−0.0017 (16)	0.0010 (16)
C20	0.023 (2)	0.020 (2)	0.016 (2)	−0.0042 (18)	0.0033 (17)	−0.0008 (18)
C21	0.031 (2)	0.023 (2)	0.018 (2)	−0.0042 (19)	0.0071 (18)	−0.0033 (19)
C22	0.037 (3)	0.024 (2)	0.014 (2)	−0.0088 (19)	0.0039 (19)	−0.0001 (18)

C23	0.020 (2)	0.021 (2)	0.021 (2)	−0.0058 (17)	−0.0048 (18)	0.0065 (19)
C24	0.024 (2)	0.0086 (19)	0.018 (2)	−0.0074 (16)	0.0007 (17)	−0.0012 (16)
C25	0.019 (2)	0.020 (2)	0.019 (2)	0.0008 (17)	−0.0052 (17)	0.0016 (18)
C26	0.020 (2)	0.0109 (19)	0.021 (2)	0.0004 (16)	0.0017 (17)	−0.0008 (17)
N5	0.0215 (18)	0.0186 (17)	0.0219 (19)	0.0028 (14)	0.0034 (14)	−0.0076 (15)
C51	0.024 (2)	0.019 (2)	0.036 (3)	−0.0016 (18)	0.0102 (19)	−0.0051 (19)
C52	0.037 (3)	0.021 (2)	0.045 (3)	0.004 (2)	0.007 (2)	0.003 (2)
C53	0.027 (2)	0.017 (2)	0.022 (2)	0.0025 (17)	0.0027 (18)	−0.0064 (18)
C54	0.025 (2)	0.019 (2)	0.027 (2)	0.0052 (18)	0.0011 (18)	−0.0072 (19)
C55	0.017 (2)	0.040 (3)	0.030 (3)	0.0039 (19)	−0.0034 (18)	−0.020 (2)
C56	0.034 (3)	0.047 (3)	0.028 (3)	0.013 (2)	−0.008 (2)	−0.013 (2)
C57	0.017 (2)	0.025 (2)	0.022 (2)	−0.0045 (17)	0.0036 (17)	−0.0028 (18)
C58	0.020 (2)	0.039 (3)	0.025 (3)	0.0012 (19)	0.0027 (18)	−0.010 (2)

Geometric parameters (Å, °)

Co1—N3	1.859 (3)	C18—C19	1.417 (5)
Co1—N2	1.877 (3)	C19—C24	1.428 (5)
Co1—N1	1.965 (3)	C19—C20	1.428 (5)
Co1—N4	1.965 (3)	C20—C21	1.367 (5)
Co1—Cl1	2.2552 (11)	C20—H20	0.9500
Co1—Cl2	2.2674 (11)	C21—C22	1.404 (5)
N1—C9	1.340 (4)	C21—H21	0.9500
N1—C1	1.363 (4)	C22—C23	1.365 (5)
N2—C10	1.345 (4)	C22—H22	0.9500
N2—C11	1.407 (4)	C23—C24	1.410 (5)
N3—C17	1.344 (4)	C23—H23	0.9500
N3—C16	1.402 (4)	C24—C25	1.410 (5)
N4—C18	1.338 (4)	C25—C26	1.348 (5)
N4—C26	1.362 (4)	C25—H25	0.9500
O1—C10	1.239 (4)	C26—H26	0.9500
O2—C17	1.241 (4)	N5—C57	1.512 (4)
C1—C2	1.352 (5)	N5—C55	1.522 (4)
C1—H1	0.9500	N5—C51	1.523 (4)
C2—C3	1.403 (5)	N5—C53	1.524 (4)
C2—H2	0.9500	C51—C52	1.508 (5)
C3—C4	1.402 (5)	C51—H51A	0.9900
C3—C8	1.435 (5)	C51—H51B	0.9900
C4—C5	1.355 (5)	C52—H52A	0.9800
C4—H4	0.9500	C52—H52B	0.9800
C5—C6	1.401 (5)	C52—H52C	0.9800
C5—H5	0.9500	C53—C54	1.516 (5)
C6—C7	1.373 (5)	C53—H53A	0.9900
C6—H6	0.9500	C53—H53B	0.9900
C7—C8	1.412 (5)	C54—H54A	0.9800
C7—H7	0.9500	C54—H54B	0.9800
C8—C9	1.420 (5)	C54—H54C	0.9800
C9—C10	1.509 (5)	C55—C56	1.515 (5)
C11—C12	1.397 (5)	C55—H55A	0.9900

C11—C16	1.418 (5)	C55—H55B	0.9900
C12—C13	1.383 (5)	C56—H56A	0.9800
C12—H12	0.9500	C56—H56B	0.9800
C13—C14	1.391 (5)	C56—H56C	0.9800
C13—H13	0.9500	C57—C58	1.507 (5)
C14—C15	1.393 (4)	C57—H57A	0.9900
C14—H14	0.9500	C57—H57B	0.9900
C15—C16	1.389 (5)	C58—H58A	0.9800
C15—H15	0.9500	C58—H58B	0.9800
C17—C18	1.516 (5)	C58—H58C	0.9800
N3—Co1—N2	85.00 (12)	C19—C18—C17	123.4 (3)
N3—Co1—N1	166.97 (12)	C18—C19—C24	118.0 (3)
N2—Co1—N1	82.18 (12)	C18—C19—C20	124.5 (3)
N3—Co1—N4	82.49 (12)	C24—C19—C20	117.5 (3)
N2—Co1—N4	166.62 (12)	C21—C20—C19	121.2 (3)
N1—Co1—N4	110.48 (12)	C21—C20—H20	119.4
N3—Co1—Cl1	91.63 (9)	C19—C20—H20	119.4
N2—Co1—Cl1	89.73 (9)	C20—C21—C22	120.4 (4)
N1—Co1—Cl1	90.64 (8)	C20—C21—H21	119.8
N4—Co1—Cl1	85.93 (8)	C22—C21—H21	119.8
N3—Co1—Cl2	93.07 (9)	C23—C22—C21	120.5 (4)
N2—Co1—Cl2	94.97 (9)	C23—C22—H22	119.8
N1—Co1—Cl2	85.75 (8)	C21—C22—H22	119.8
N4—Co1—Cl2	90.41 (8)	C22—C23—C24	120.7 (3)
Cl1—Co1—Cl2	173.62 (4)	C22—C23—H23	119.6
C9—N1—C1	119.9 (3)	C24—C23—H23	119.6
C9—N1—Co1	113.2 (2)	C25—C24—C23	123.1 (3)
C1—N1—Co1	126.6 (3)	C25—C24—C19	117.1 (3)
C10—N2—C11	125.4 (3)	C23—C24—C19	119.7 (3)
C10—N2—Co1	117.0 (2)	C26—C25—C24	120.8 (3)
C11—N2—Co1	113.6 (2)	C26—C25—H25	119.6
C17—N3—C16	125.8 (3)	C24—C25—H25	119.6
C17—N3—Co1	119.4 (2)	C25—C26—N4	122.6 (3)
C16—N3—Co1	114.6 (2)	C25—C26—H26	118.7
C18—N4—C26	118.9 (3)	N4—C26—H26	118.7
C18—N4—Co1	113.5 (2)	C57—N5—C55	111.5 (3)
C26—N4—Co1	127.5 (3)	C57—N5—C51	111.4 (3)
C2—C1—N1	121.7 (3)	C55—N5—C51	106.3 (3)
C2—C1—H1	119.2	C57—N5—C53	105.6 (3)
N1—C1—H1	119.2	C55—N5—C53	110.7 (3)
C1—C2—C3	121.0 (3)	C51—N5—C53	111.3 (3)
C1—C2—H2	119.5	C52—C51—N5	115.8 (3)
C3—C2—H2	119.5	C52—C51—H51A	108.3
C4—C3—C2	122.7 (3)	N5—C51—H51A	108.3
C4—C3—C8	119.2 (3)	C52—C51—H51B	108.3
C2—C3—C8	118.1 (3)	N5—C51—H51B	108.3
C5—C4—C3	121.0 (3)	H51A—C51—H51B	107.4
C5—C4—H4	119.5	C51—C52—H52A	109.5
C3—C4—H4	119.5	C51—C52—H52B	109.5

C4—C5—C6	120.4 (4)	H52A—C52—H52B	109.5
C4—C5—H5	119.8	C51—C52—H52C	109.5
C6—C5—H5	119.8	H52A—C52—H52C	109.5
C7—C6—C5	120.8 (4)	H52B—C52—H52C	109.5
C7—C6—H6	119.6	C54—C53—N5	115.7 (3)
C5—C6—H6	119.6	C54—C53—H53A	108.4
C6—C7—C8	120.2 (3)	N5—C53—H53A	108.4
C6—C7—H7	119.9	C54—C53—H53B	108.4
C8—C7—H7	119.9	N5—C53—H53B	108.4
C7—C8—C9	124.5 (3)	H53A—C53—H53B	107.4
C7—C8—C3	118.4 (3)	C53—C54—H54A	109.5
C9—C8—C3	117.1 (3)	C53—C54—H54B	109.5
N1—C9—C8	122.2 (3)	H54A—C54—H54B	109.5
N1—C9—C10	114.0 (3)	C53—C54—H54C	109.5
C8—C9—C10	123.7 (3)	H54A—C54—H54C	109.5
O1—C10—N2	126.8 (3)	H54B—C54—H54C	109.5
O1—C10—C9	123.3 (3)	C56—C55—N5	114.8 (3)
N2—C10—C9	109.9 (3)	C56—C55—H55A	108.6
C12—C11—N2	126.9 (3)	N5—C55—H55A	108.6
C12—C11—C16	119.8 (3)	C56—C55—H55B	108.6
N2—C11—C16	113.3 (3)	N5—C55—H55B	108.6
C13—C12—C11	120.0 (3)	H55A—C55—H55B	107.6
C13—C12—H12	120.0	C55—C56—H56A	109.5
C11—C12—H12	120.0	C55—C56—H56B	109.5
C12—C13—C14	120.2 (3)	H56A—C56—H56B	109.5
C12—C13—H13	119.9	C55—C56—H56C	109.5
C14—C13—H13	119.9	H56A—C56—H56C	109.5
C13—C14—C15	120.6 (3)	H56B—C56—H56C	109.5
C13—C14—H14	119.7	C58—C57—N5	115.4 (3)
C15—C14—H14	119.7	C58—C57—H57A	108.4
C16—C15—C14	119.8 (4)	N5—C57—H57A	108.4
C16—C15—H15	120.1	C58—C57—H57B	108.4
C14—C15—H15	120.1	N5—C57—H57B	108.4
C15—C16—N3	127.4 (3)	H57A—C57—H57B	107.5
C15—C16—C11	119.5 (3)	C57—C58—H58A	109.5
N3—C16—C11	113.0 (3)	C57—C58—H58B	109.5
O2—C17—N3	127.3 (3)	H58A—C58—H58B	109.5
O2—C17—C18	122.5 (3)	C57—C58—H58C	109.5
N3—C17—C18	110.0 (3)	H58A—C58—H58C	109.5
N4—C18—C19	122.3 (3)	H58B—C58—H58C	109.5
N4—C18—C17	114.0 (3)		
N3—Co1—N1—C9	−20.2 (6)	N1—C9—C10—O1	−169.8 (3)
N2—Co1—N1—C9	−9.8 (2)	C8—C9—C10—O1	13.5 (5)
N4—Co1—N1—C9	165.7 (2)	N1—C9—C10—N2	12.1 (4)
Cl1—Co1—N1—C9	79.8 (2)	C8—C9—C10—N2	−164.6 (3)
Cl2—Co1—N1—C9	−105.4 (2)	C10—N2—C11—C12	−18.5 (5)
N3—Co1—N1—C1	153.6 (5)	Co1—N2—C11—C12	−175.3 (3)
N2—Co1—N1—C1	164.1 (3)	C10—N2—C11—C16	161.4 (3)
N4—Co1—N1—C1	−20.4 (3)	Co1—N2—C11—C16	4.6 (4)

Cl1—Co1—N1—C1	−106.3 (3)	N2—C11—C12—C13	178.4 (3)
Cl2—Co1—N1—C1	68.4 (3)	C16—C11—C12—C13	−1.5 (5)
N3—Co1—N2—C10	−164.5 (3)	C11—C12—C13—C14	0.3 (5)
N1—Co1—N2—C10	17.9 (2)	C12—C13—C14—C15	0.8 (5)
N4—Co1—N2—C10	−143.7 (5)	C13—C14—C15—C16	−0.8 (5)
Cl1—Co1—N2—C10	−72.8 (2)	C14—C15—C16—N3	−178.2 (3)
Cl2—Co1—N2—C10	102.9 (2)	C14—C15—C16—C11	−0.4 (5)
N3—Co1—N2—C11	−5.6 (2)	C17—N3—C16—C15	−1.2 (5)
N1—Co1—N2—C11	176.7 (2)	Co1—N3—C16—C15	173.7 (3)
N4—Co1—N2—C11	15.2 (6)	C17—N3—C16—C11	−179.2 (3)
Cl1—Co1—N2—C11	86.1 (2)	Co1—N3—C16—C11	−4.3 (4)
Cl2—Co1—N2—C11	−98.3 (2)	C12—C11—C16—C15	1.5 (5)
N2—Co1—N3—C17	−179.2 (3)	N2—C11—C16—C15	−178.4 (3)
N1—Co1—N3—C17	−168.8 (4)	C12—C11—C16—N3	179.7 (3)
N4—Co1—N3—C17	5.5 (2)	N2—C11—C16—N3	−0.3 (4)
Cl1—Co1—N3—C17	91.2 (2)	C16—N3—C17—O2	−4.2 (6)
Cl2—Co1—N3—C17	−84.5 (2)	Co1—N3—C17—O2	−178.9 (3)
N2—Co1—N3—C16	5.5 (2)	C16—N3—C17—C18	172.1 (3)
N1—Co1—N3—C16	15.9 (7)	Co1—N3—C17—C18	−2.6 (4)
N4—Co1—N3—C16	−169.7 (2)	C26—N4—C18—C19	6.7 (5)
Cl1—Co1—N3—C16	−84.1 (2)	Co1—N4—C18—C19	−178.3 (2)
Cl2—Co1—N3—C16	100.2 (2)	C26—N4—C18—C17	−167.0 (3)
N3—Co1—N4—C18	−7.5 (2)	Co1—N4—C18—C17	8.0 (3)
N2—Co1—N4—C18	−28.3 (6)	O2—C17—C18—N4	172.7 (3)
N1—Co1—N4—C18	171.2 (2)	N3—C17—C18—N4	−3.8 (4)
Cl1—Co1—N4—C18	−99.7 (2)	O2—C17—C18—C19	−0.9 (5)
Cl2—Co1—N4—C18	85.6 (2)	N3—C17—C18—C19	−177.4 (3)
N3—Co1—N4—C26	167.0 (3)	N4—C18—C19—C24	−4.7 (5)
N2—Co1—N4—C26	146.1 (5)	C17—C18—C19—C24	168.4 (3)
N1—Co1—N4—C26	−14.4 (3)	N4—C18—C19—C20	174.2 (3)
Cl1—Co1—N4—C26	74.8 (3)	C17—C18—C19—C20	−12.7 (5)
Cl2—Co1—N4—C26	−100.0 (3)	C18—C19—C20—C21	−179.1 (3)
C9—N1—C1—C2	−3.5 (5)	C24—C19—C20—C21	−0.2 (5)
Co1—N1—C1—C2	−177.0 (3)	C19—C20—C21—C22	−0.7 (5)
N1—C1—C2—C3	1.7 (5)	C20—C21—C22—C23	1.0 (6)
C1—C2—C3—C4	178.8 (3)	C21—C22—C23—C24	−0.3 (5)
C1—C2—C3—C8	−0.1 (5)	C22—C23—C24—C25	179.5 (3)
C2—C3—C4—C5	−178.6 (3)	C22—C23—C24—C19	−0.7 (5)
C8—C3—C4—C5	0.3 (5)	C18—C19—C24—C25	−0.3 (5)
C3—C4—C5—C6	−0.1 (5)	C20—C19—C24—C25	−179.3 (3)
C4—C5—C6—C7	−0.1 (5)	C18—C19—C24—C23	179.9 (3)
C5—C6—C7—C8	0.0 (5)	C20—C19—C24—C23	0.9 (5)
C6—C7—C8—C9	178.3 (3)	C23—C24—C25—C26	−177.0 (3)
C6—C7—C8—C3	0.2 (5)	C19—C24—C25—C26	3.2 (5)
C4—C3—C8—C7	−0.3 (5)	C24—C25—C26—N4	−1.3 (5)
C2—C3—C8—C7	178.6 (3)	C18—N4—C26—C25	−3.7 (5)
C4—C3—C8—C9	−178.6 (3)	Co1—N4—C26—C25	−177.9 (2)
C2—C3—C8—C9	0.3 (5)	C57—N5—C51—C52	−59.6 (4)
C1—N1—C9—C8	3.8 (5)	C55—N5—C51—C52	178.7 (3)

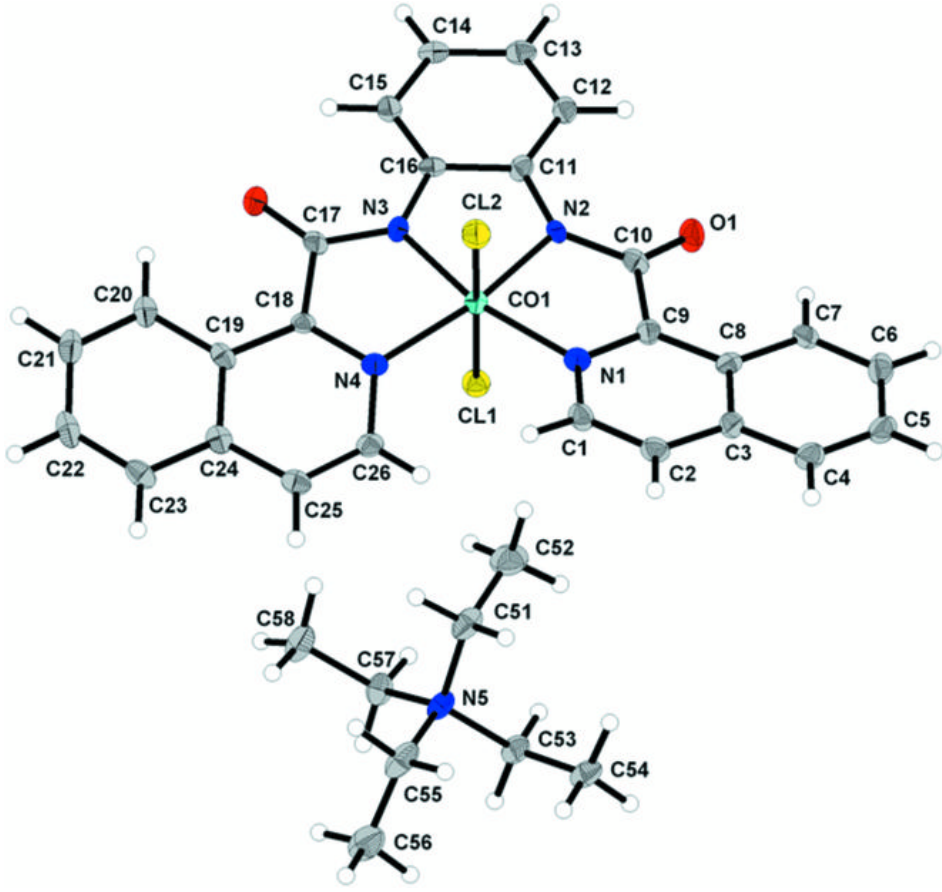
Co1—N1—C9—C8	178.1 (3)	C53—N5—C51—C52	58.0 (4)
C1—N1—C9—C10	−173.0 (3)	C57—N5—C53—C54	−179.1 (3)
Co1—N1—C9—C10	1.3 (3)	C55—N5—C53—C54	−58.2 (4)
C7—C8—C9—N1	179.7 (3)	C51—N5—C53—C54	59.8 (4)
C3—C8—C9—N1	−2.2 (5)	C57—N5—C55—C56	54.9 (4)
C7—C8—C9—C10	−3.9 (5)	C51—N5—C55—C56	176.5 (3)
C3—C8—C9—C10	174.3 (3)	C53—N5—C55—C56	−62.4 (4)
C11—N2—C10—O1	4.9 (6)	C55—N5—C57—C58	61.2 (4)
Co1—N2—C10—O1	161.0 (3)	C51—N5—C57—C58	−57.4 (4)
C11—N2—C10—C9	−177.1 (3)	C53—N5—C57—C58	−178.5 (3)
Co1—N2—C10—C9	−21.0 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C53—H53B···Cl1^{i}	0.99	2.81	3.701 (4)	150
C57—H57A···Cl1^{i}	0.99	2.64	3.576 (4)	159
C55—H55B···Cl2^{ii}	0.99	2.76	3.740 (4)	172
C5—H5···Cl2^{iii}	0.95	2.77	3.501 (4)	135
C26—H26···Cl1^{i}	0.95	2.79	3.669 (4)	155

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) *x*+1/2, −*y*+3/2, *z*+1/2; (iii) *x*+1/2, −*y*+3/2, *z*−1/2.

Fig. 1


C14
C13
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C51
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C57
N5
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C54
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C56

Fig. 2