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Bis{2,4-dibromo-6-[3-(cyclohexylamino)-propyliminomethyl]phenolato}cobalt(III) perchlorate

Kun Li,[a] Shan-Shan Huang,[b]* Qin Zhou,[b] Hong Li[c] and Yun-Peng Diao[b]*

[a]College of Chemistry and Chemical Engineering, Liaoning Normal University, Dalian 116029, People's Republic of China, [b]School of Pharmacy, Dalian Medical University, Dalian 116027, People's Republic of China, and [c]College of Medical Laboratory Science, Dalian Medical University, Dalian 116027, People's Republic of China
Correspondence e-mail: dyp78@sina.com, diaoyiwen@126.com

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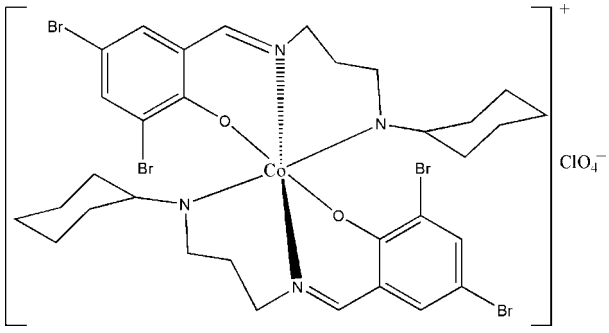
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.015 Å; R factor = 0.075; wR factor = 0.213; data-to-parameter ratio = 19.2.

In the title compound, $[Co(C_{16}H_{21}Br_2N_2O)_2]ClO_4$, a centrosymmetric mononuclear Schiff base cobalt(III) complex, the Co atom is hexacoordinated by two O and four N atoms from two Schiff base ligands, forming an octahedral geometry.

Related literature

For related literature, see: Diao (2007*a*,*b*); Diao, Huang *et al.* (2007); Diao, Shu *et al.* (2007); Hodnett & Dunn (1972); Hodnett *et al.* (1971); Sacconi *et al.* (1965); Takeuchi *et al.* (1998); Zakrzewski & Sacconi (1968).



Experimental

Crystal data

$[Co(C_{16}H_{21}Br_2N_2O)_2]ClO_4$
M_r = 992.72
Monoclinic, $P2_1/c$
a = 16.208 (3) Å
b = 12.801 (3) Å
c = 18.060 (4) Å
β = 98.91 (3)°
V = 3701.8 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.90 mm^{-1}
T = 298 (2) K
0.33 × 0.32 × 0.32 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.295, T_{max} = 0.303
(expected range = 0.203–0.208)
30784 measured reflections
8354 independent reflections
3168 reflections with $I > 2\sigma(I)$
R_{int} = 0.142

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.075
$wR(F^2)$ = 0.213
S = 0.96
8354 reflections
436 parameters
24 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.76 e Å^{-3}

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: AT2358).

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supplementary materials

Acta Cryst. (2007). E**63**, m2274 [**doi:10.1107/S1600536807037579**]

Bis{2,4-dibromo-6-[3-(cyclohexylamino)propyliminomethyl]phenolato}cobalt(III) perchlorate

K. Li, S.-S. Huang, Q. Zhou, H. Li and Y.-P. Diao

Comment

Cobalt complexes with Schiff base ligands have received much attention in recent years (Sacconi *et al.*, 1965; Zakrzewski & Sacconi, 1968). Some of the complexes have been found to have pharmacological and antitumor properties (Hodnett *et al.*, 1971; Hodnett & Dunn, 1972; Takeuchi *et al.*, 1998). We have recently reported a few transition metal complexes (Diao, Huang *et al.*, 2007; Diao, Shu *et al.*, 2007; Diao, 2007*a*,*b*). As an extension of the work on the crystal structures of such complexes, we report herein the crystal structure of the title complex.

The complex is a centrosymmetric mononuclear Schiff base cobalt(III) complex, which consists of a cobalt(III) cation and a perchlorate anion. The Co atom is hexacoordinated by two O and four N atoms from two Schiff base ligands, forming an octahedral geometry (Fig. 1).

Experimental

3,5-Dibromosalicylaldehyde (0.2 mmol, 56.0 mg), *N*-cyclohexyl-1,3-diaminopropane (0.2 mmol, 31.0 mg), and $Cu(ClO_4)\cdot 7H_2O$ (0.1 mmol, 39.0 mg) were dissolved in a methanol solution (20 ml). The mixture was stirred for half an hour at room temperature, giving a brown solution. After allowing the solution to stand in air for a week, brown block-like crystals were formed.

Refinement

H atoms were placed in calculated positions and constrained to ride on their parent atoms, with C—H = 0.93–0.97 Å, N—H = 0.91 Å, and with U_{iso}(H) set at 1.2U_{eq}(C,*N*). The ration of observed/unique reflections is low (38%), and the value of R_{int} is 0.14, due to the poor quality of the diffraction.

Figures

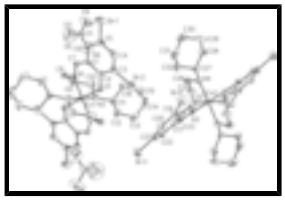


Fig. 1. Molecular structure of the complex with 30% probabily ellipsoids.

Bis{2,4-dibromo-6-[3-(cyclohexylamino)propyliminomethyl]phenolato}cobalt(III) perchlorate

Crystal data

$[Co(C_{16}H_{21}Br_2N_2O)_2]ClO_4$ F_{000} = 1976

M_r = 992.72	D_x = 1.781 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 1447 reflections
a = 16.208 (3) Å	θ = 2.3–24.5º
b = 12.801 (3) Å	μ = 4.90 mm^{-1}
c = 18.060 (4) Å	T = 298 (2) K
β = 98.91 (3)º	Block, brown
V = 3701.8 (14) Å^3	0.33 × 0.32 × 0.32 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	8354 independent reflections
Radiation source: fine-focus sealed tube	3168 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.142
T = 298(2) K	θ_{max} = 27.5º
ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	h = −21→21
T_{min} = 0.295, T_{max} = 0.303	k = −16→16
30784 measured reflections	l = −22→23

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.075	H-atom parameters constrained
$wR(F^2)$ = 0.213	$w = 1/[\sigma^2(F_o^2) + (0.0821P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.96	$(\Delta/\sigma)_{max} < 0.001$
8354 reflections	$\Delta\rho_{max}$ = 1.12 e Å^{-3}
436 parameters	$\Delta\rho_{min}$ = −0.75 e Å^{-3}
24 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2\text{sigma}(F^2)$ is used only for calculat-

ing *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	0.5000	0.5000	0.5000	0.0388 (4)
Co2	0.0000	0.0000	0.5000	0.0351 (4)
Br1	0.15360 (8)	0.79302 (11)	0.28990 (8)	0.0947 (5)
Br2	0.23554 (7)	0.37506 (9)	0.36766 (7)	0.0779 (4)
Br3	0.40645 (7)	0.02431 (11)	0.36755 (8)	0.0917 (5)
Br4	0.06878 (8)	0.13017 (10)	0.26659 (6)	0.0795 (4)
Cl1	0.35696 (18)	0.8654 (3)	0.67797 (19)	0.0731 (9)
O1	0.3871 (4)	0.4778 (4)	0.4574 (3)	0.0465 (16)
O2	0.0500 (4)	0.0608 (4)	0.4218 (3)	0.0443 (15)
O3	0.3804 (8)	0.8974 (11)	0.6126 (7)	0.175 (5)
O4	0.2889 (8)	0.9120 (11)	0.6912 (7)	0.174 (5)
O5	0.4137 (12)	0.9087 (15)	0.7300 (11)	0.256 (8)
O6	0.3674 (9)	0.7618 (13)	0.6982 (9)	0.206 (6)
N1	0.4761 (5)	0.6429 (6)	0.5224 (4)	0.0442 (19)
N2	0.4722 (5)	0.4576 (6)	0.5999 (4)	0.052 (2)
H2A	0.5201	0.4265	0.6224	0.062*
N3	0.1045 (4)	0.0001 (5)	0.5661 (4)	0.0374 (17)
N4	−0.0236 (4)	0.1438 (6)	0.5369 (4)	0.0453 (19)
H4A	−0.0719	0.1322	0.5553	0.054*
C1	0.3510 (5)	0.6588 (7)	0.4321 (5)	0.044 (2)
C2	0.3363 (6)	0.5496 (8)	0.4234 (5)	0.046 (2)
C3	0.2619 (6)	0.5196 (7)	0.3778 (6)	0.053 (3)
C4	0.2069 (6)	0.5910 (9)	0.3389 (5)	0.059 (3)
H4	0.1574	0.5690	0.3101	0.071*
C5	0.2281 (7)	0.6968 (9)	0.3443 (6)	0.064 (3)
C6	0.2971 (6)	0.7307 (8)	0.3913 (6)	0.054 (3)
H6	0.3083	0.8019	0.3963	0.064*
C7	0.4161 (6)	0.6962 (7)	0.4881 (5)	0.045 (2)
H7	0.4144	0.7666	0.5006	0.054*
C8	0.5282 (6)	0.6920 (8)	0.5894 (5)	0.056 (3)
H8A	0.5066	0.7610	0.5976	0.068*
H8B	0.5851	0.7000	0.5798	0.068*
C9	0.5282 (8)	0.6267 (9)	0.6591 (6)	0.078 (4)
H9A	0.5209	0.6726	0.7003	0.094*
H9B	0.5823	0.5933	0.6715	0.094*
C10	0.4603 (7)	0.5423 (8)	0.6518 (6)	0.070 (3)
H10A	0.4586	0.5125	0.7010	0.084*
H10B	0.4066	0.5749	0.6352	0.084*
C11	0.4077 (6)	0.3707 (7)	0.5978 (5)	0.046 (2)
H11	0.4015	0.3405	0.5474	0.055*
C12	0.4408 (7)	0.2828 (8)	0.6527 (6)	0.071 (3)
H12A	0.4481	0.3086	0.7038	0.085*

H12B	0.4945	0.2585	0.6422	0.085*
C13	0.3771 (9)	0.1920 (8)	0.6434 (7)	0.089 (4)
H13A	0.3740	0.1624	0.5936	0.107*
H13B	0.3958	0.1376	0.6795	0.107*
C14	0.2907 (10)	0.2297 (12)	0.6549 (8)	0.114 (6)
H14A	0.2515	0.1720	0.6475	0.136*
H14B	0.2928	0.2549	0.7058	0.136*
C15	0.2627 (8)	0.3127 (10)	0.6025 (8)	0.090 (4)
H15A	0.2078	0.3356	0.6107	0.108*
H15B	0.2575	0.2854	0.5519	0.108*
C16	0.3215 (6)	0.4068 (8)	0.6094 (7)	0.076 (3)
H16A	0.3007	0.4589	0.5721	0.091*
H16B	0.3242	0.4382	0.6586	0.091*
C17	0.1947 (6)	0.0204 (6)	0.4686 (5)	0.044 (2)
C18	0.1278 (6)	0.0523 (7)	0.4124 (5)	0.045 (2)
C19	0.1514 (6)	0.0796 (7)	0.3438 (5)	0.048 (2)
C20	0.2327 (8)	0.0718 (8)	0.3306 (6)	0.070 (3)
H20	0.2460	0.0901	0.2840	0.084*
C21	0.2949 (6)	0.0365 (8)	0.3870 (7)	0.060 (3)
C22	0.2758 (6)	0.0135 (7)	0.4557 (6)	0.053 (3)
H22	0.3177	−0.0070	0.4942	0.064*
C23	0.1772 (5)	0.0054 (7)	0.5443 (5)	0.045 (2)
H23	0.2233	−0.0012	0.5816	0.054*
C24	0.1034 (6)	0.0094 (7)	0.6471 (5)	0.049 (2)
H24A	0.1603	0.0145	0.6731	0.059*
H24B	0.0785	−0.0530	0.6647	0.059*
C25	0.0551 (7)	0.1031 (8)	0.6650 (5)	0.061 (3)
H25A	0.0881	0.1397	0.7064	0.073*
H25B	0.0048	0.0788	0.6825	0.073*
C26	0.0299 (7)	0.1804 (8)	0.6032 (5)	0.063 (3)
H26A	0.0020	0.2381	0.6237	0.076*
H26B	0.0805	0.2079	0.5879	0.076*
C27	−0.0514 (5)	0.2239 (6)	0.4777 (5)	0.040 (2)
H27	−0.0680	0.1866	0.4303	0.048*
C28	−0.1276 (6)	0.2791 (8)	0.4964 (6)	0.063 (3)
H28A	−0.1133	0.3175	0.5430	0.076*
H28B	−0.1703	0.2283	0.5030	0.076*
C29	−0.1616 (8)	0.3557 (10)	0.4322 (7)	0.095 (4)
H29A	−0.1818	0.3163	0.3871	0.113*
H29B	−0.2081	0.3948	0.4460	0.113*
C30	−0.0944 (10)	0.4309 (10)	0.4163 (8)	0.105 (5)
H30A	−0.1159	0.4736	0.3733	0.126*
H30B	−0.0796	0.4768	0.4590	0.126*
C31	−0.0177 (8)	0.3742 (9)	0.4010 (7)	0.083 (4)
H31A	0.0250	0.4245	0.3938	0.100*
H31B	−0.0311	0.3338	0.3553	0.100*
C32	0.0156 (6)	0.3016 (8)	0.4656 (6)	0.067 (3)
H32A	0.0644	0.2648	0.4542	0.080*
H32B	0.0320	0.3421	0.5109	0.080*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0420 (10)	0.0357 (10)	0.0374 (10)	0.0002 (8)	0.0021 (8)	−0.0028 (8)
Co2	0.0375 (9)	0.0342 (9)	0.0329 (10)	0.0023 (7)	0.0031 (7)	−0.0017 (8)
Br1	0.0855 (9)	0.0993 (10)	0.0913 (10)	0.0441 (8)	−0.0112 (8)	0.0101 (8)
Br2	0.0671 (8)	0.0720 (8)	0.0864 (9)	−0.0146 (6)	−0.0138 (6)	−0.0125 (7)
Br3	0.0655 (8)	0.1031 (11)	0.1179 (12)	−0.0095 (7)	0.0496 (8)	−0.0105 (8)
Br4	0.0935 (9)	0.0932 (9)	0.0530 (7)	0.0052 (7)	0.0156 (6)	0.0266 (7)
Cl1	0.0549 (18)	0.088 (2)	0.077 (2)	0.0211 (16)	0.0111 (16)	0.0037 (18)
O1	0.053 (4)	0.039 (4)	0.046 (4)	−0.002 (3)	0.000 (3)	0.000 (3)
O2	0.052 (4)	0.046 (4)	0.036 (4)	0.000 (3)	0.009 (3)	0.005 (3)
O3	0.189 (8)	0.200 (9)	0.152 (8)	0.061 (7)	0.080 (7)	0.013 (7)
O4	0.147 (7)	0.231 (9)	0.156 (8)	0.089 (7)	0.065 (6)	0.045 (7)
O5	0.248 (11)	0.246 (11)	0.256 (11)	−0.018 (9)	−0.018 (9)	−0.007 (9)
O6	0.214 (9)	0.169 (9)	0.239 (10)	−0.003 (8)	0.040 (8)	0.021 (8)
N1	0.042 (5)	0.041 (5)	0.050 (5)	0.002 (4)	0.007 (4)	−0.008 (4)
N2	0.067 (5)	0.040 (5)	0.048 (5)	0.001 (4)	0.008 (4)	0.001 (4)
N3	0.042 (4)	0.032 (4)	0.035 (4)	0.007 (3)	−0.004 (3)	−0.006 (3)
N4	0.048 (5)	0.051 (5)	0.034 (4)	0.005 (4)	−0.001 (4)	−0.007 (4)
C1	0.041 (5)	0.044 (6)	0.047 (6)	0.007 (5)	0.010 (5)	−0.001 (5)
C2	0.049 (6)	0.050 (6)	0.039 (6)	−0.002 (5)	0.008 (5)	−0.004 (5)
C3	0.048 (6)	0.051 (7)	0.059 (7)	−0.002 (5)	0.001 (5)	0.000 (5)
C4	0.046 (6)	0.088 (9)	0.043 (6)	−0.002 (6)	0.000 (5)	−0.013 (6)
C5	0.062 (7)	0.066 (8)	0.062 (8)	0.030 (6)	0.006 (6)	0.014 (6)
C6	0.056 (7)	0.041 (6)	0.065 (7)	0.015 (5)	0.016 (6)	0.002 (5)
C7	0.044 (6)	0.033 (5)	0.060 (7)	−0.001 (5)	0.016 (5)	−0.010 (5)
C8	0.062 (7)	0.052 (7)	0.052 (7)	0.001 (5)	−0.001 (5)	−0.016 (5)
C9	0.105 (10)	0.073 (8)	0.054 (8)	−0.006 (7)	0.002 (7)	−0.022 (6)
C10	0.095 (9)	0.075 (8)	0.045 (7)	−0.012 (7)	0.026 (6)	−0.012 (6)
C11	0.055 (6)	0.045 (6)	0.036 (5)	−0.005 (5)	0.004 (4)	0.014 (5)
C12	0.089 (8)	0.054 (7)	0.064 (7)	−0.015 (6)	−0.004 (6)	0.011 (6)
C13	0.153 (13)	0.038 (7)	0.066 (8)	−0.009 (8)	−0.014 (9)	0.010 (6)
C14	0.141 (14)	0.101 (12)	0.118 (12)	−0.083 (11)	0.078 (11)	−0.030 (10)
C15	0.085 (9)	0.072 (9)	0.119 (12)	−0.022 (7)	0.036 (8)	0.015 (9)
C16	0.052 (7)	0.073 (8)	0.107 (10)	0.011 (6)	0.026 (7)	0.003 (7)
C17	0.056 (6)	0.032 (5)	0.043 (6)	0.003 (4)	0.006 (5)	−0.003 (4)
C18	0.063 (7)	0.028 (5)	0.044 (6)	−0.002 (5)	0.007 (5)	−0.006 (4)
C19	0.065 (7)	0.050 (6)	0.035 (6)	−0.004 (5)	0.019 (5)	0.006 (5)
C20	0.091 (9)	0.069 (8)	0.064 (8)	−0.012 (7)	0.052 (7)	−0.007 (6)
C21	0.046 (6)	0.066 (7)	0.071 (8)	−0.011 (5)	0.018 (6)	−0.002 (6)
C22	0.049 (6)	0.040 (6)	0.072 (8)	−0.008 (5)	0.017 (5)	−0.015 (5)
C23	0.031 (5)	0.042 (6)	0.058 (7)	−0.007 (4)	−0.005 (5)	−0.002 (5)
C24	0.055 (6)	0.053 (6)	0.037 (6)	0.010 (5)	−0.003 (5)	0.003 (5)
C25	0.081 (8)	0.061 (7)	0.036 (6)	0.013 (6)	−0.009 (5)	−0.008 (5)
C26	0.082 (8)	0.054 (7)	0.048 (7)	0.017 (6)	−0.006 (6)	−0.013 (5)
C27	0.051 (6)	0.029 (5)	0.041 (6)	0.001 (4)	0.006 (4)	−0.007 (4)

C28	0.061 (7)	0.067 (7)	0.066 (7)	0.007 (6)	0.023 (6)	−0.011 (6)
C29	0.103 (10)	0.096 (11)	0.084 (10)	0.060 (9)	0.012 (8)	0.005 (8)
C30	0.143 (14)	0.055 (9)	0.112 (12)	0.016 (9)	0.003 (10)	0.040 (8)
C31	0.100 (10)	0.064 (8)	0.082 (9)	−0.022 (7)	0.001 (8)	0.022 (7)
C32	0.070 (8)	0.065 (8)	0.063 (7)	−0.018 (6)	0.006 (6)	0.008 (6)

Geometric parameters (Å, °)

Co1—O1	1.894 (6)	C11—C12	1.541 (12)
Co1—O1^{i}	1.894 (6)	C11—H11	0.9800
Co1—N1	1.926 (7)	C12—C13	1.546 (14)
Co1—N1^{i}	1.926 (7)	C12—H12A	0.9700
Co1—N2^{i}	2.002 (7)	C12—H12B	0.9700
Co1—N2	2.002 (7)	C13—C14	1.526 (17)
Co2—O2^{ii}	1.900 (6)	C13—H13A	0.9700
Co2—O2	1.900 (6)	C13—H13B	0.9700
Co2—N3^{ii}	1.915 (7)	C14—C15	1.449 (18)
Co2—N3	1.915 (7)	C14—H14A	0.9700
Co2—N4^{ii}	2.014 (7)	C14—H14B	0.9700
Co2—N4	2.014 (7)	C15—C16	1.529 (15)
Br1—C5	1.889 (9)	C15—H15A	0.9700
Br2—C3	1.901 (9)	C15—H15B	0.9700
Br3—C21	1.900 (10)	C16—H16A	0.9700
Br4—C19	1.891 (10)	C16—H16B	0.9700
Cl1—O4	1.309 (11)	C17—C22	1.372 (12)
Cl1—O5	1.330 (18)	C17—C18	1.425 (12)
Cl1—O3	1.359 (12)	C17—C23	1.452 (13)
Cl1—O6	1.380 (15)	C18—C19	1.397 (12)
O1—C2	1.319 (10)	C19—C20	1.379 (13)
O2—C18	1.303 (10)	C20—C21	1.394 (14)
N1—C7	1.268 (10)	C20—H20	0.9300
N1—C8	1.503 (11)	C21—C22	1.358 (14)
N2—C10	1.465 (12)	C22—H22	0.9300
N2—C11	1.522 (11)	C23—H23	0.9300
N2—H2A	0.9100	C24—C25	1.495 (12)
N3—C23	1.300 (10)	C24—H24A	0.9700
N3—C24	1.470 (11)	C24—H24B	0.9700
N4—C26	1.443 (11)	C25—C26	1.500 (13)
N4—C27	1.500 (10)	C25—H25A	0.9700
N4—H4A	0.9100	C25—H25B	0.9700
C1—C6	1.397 (12)	C26—H26A	0.9700
C1—C2	1.423 (12)	C26—H26B	0.9700
C1—C7	1.427 (12)	C27—C28	1.507 (12)
C2—C3	1.405 (12)	C27—C32	1.513 (12)
C3—C4	1.389 (13)	C27—H27	0.9800
C4—C5	1.397 (14)	C28—C29	1.553 (14)
C4—H4	0.9300	C28—H28A	0.9700
C5—C6	1.368 (13)	C28—H28B	0.9700

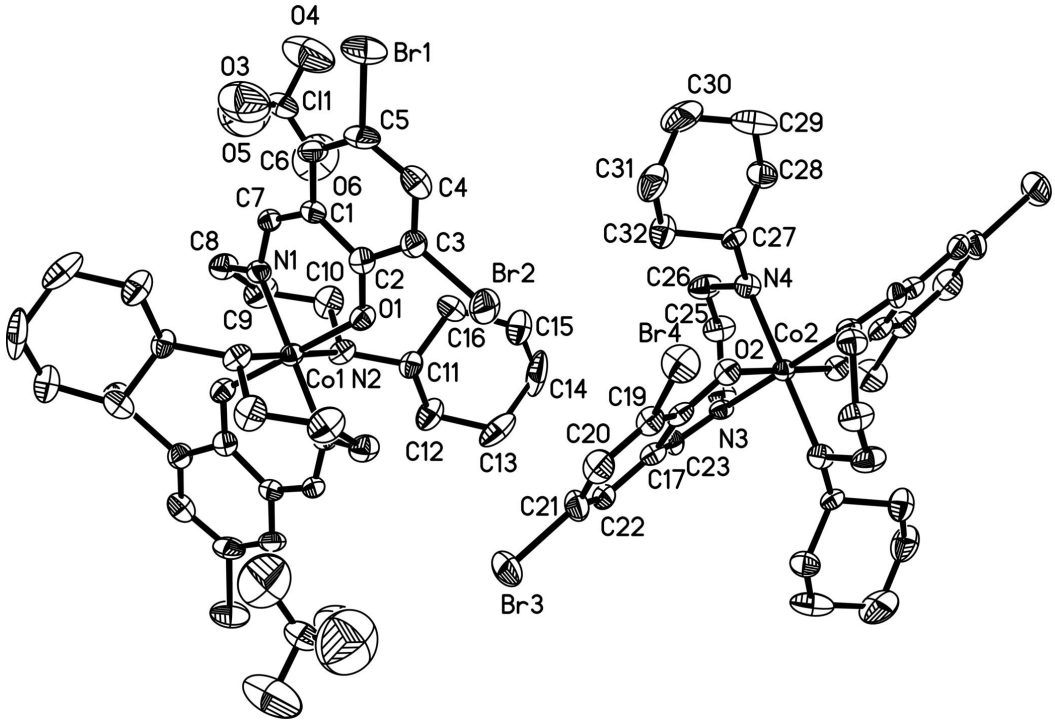
C6—H6	0.9300	C29—C30	1.513 (17)
C7—H7	0.9300	C29—H29A	0.9700
C8—C9	1.510 (14)	C29—H29B	0.9700
C8—H8A	0.9700	C30—C31	1.501 (16)
C8—H8B	0.9700	C30—H30A	0.9700
C9—C10	1.534 (14)	C30—H30B	0.9700
C9—H9A	0.9700	C31—C32	1.523 (14)
C9—H9B	0.9700	C31—H31A	0.9700
C10—H10A	0.9700	C31—H31B	0.9700
C10—H10B	0.9700	C32—H32A	0.9700
C11—C16	1.518 (12)	C32—H32B	0.9700
O1—Co1—O1^{i}	180.00 (16)	C13—C12—H12A	110.0
O1—Co1—N1	90.8 (3)	C11—C12—H12B	110.0
O1^{i}—Co1—N1	89.2 (3)	C13—C12—H12B	110.0
O1—Co1—N1^{i}	89.2 (3)	H12A—C12—H12B	108.4
O1^{i}—Co1—N1^{i}	90.8 (3)	C14—C13—C12	111.0 (10)
N1—Co1—N1^{i}	180.000 (1)	C14—C13—H13A	109.4
O1—Co1—N2^{i}	90.7 (3)	C12—C13—H13A	109.4
O1^{i}—Co1—N2^{i}	89.3 (3)	C14—C13—H13B	109.4
N1—Co1—N2^{i}	90.7 (3)	C12—C13—H13B	109.4
N1^{i}—Co1—N2^{i}	89.3 (3)	H13A—C13—H13B	108.0
O1—Co1—N2	89.3 (3)	C15—C14—C13	110.1 (10)
O1^{i}—Co1—N2	90.7 (3)	C15—C14—H14A	109.6
N1—Co1—N2	89.3 (3)	C13—C14—H14A	109.6
N1^{i}—Co1—N2	90.7 (3)	C15—C14—H14B	109.6
N2^{i}—Co1—N2	180.000 (2)	C13—C14—H14B	109.6
O2^{ii}—Co2—O2	180.000 (1)	H14A—C14—H14B	108.2
O2^{ii}—Co2—N3^{ii}	91.4 (3)	C14—C15—C16	113.4 (11)
O2—Co2—N3^{ii}	88.6 (3)	C14—C15—H15A	108.9
O2^{ii}—Co2—N3	88.6 (3)	C16—C15—H15A	108.9
O2—Co2—N3	91.4 (3)	C14—C15—H15B	108.9
N3^{ii}—Co2—N3	180.000 (1)	C16—C15—H15B	108.9
O2^{ii}—Co2—N4^{ii}	89.8 (3)	H15A—C15—H15B	107.7
O2—Co2—N4^{ii}	90.2 (3)	C11—C16—C15	108.9 (9)
N3^{ii}—Co2—N4^{ii}	89.3 (3)	C11—C16—H16A	109.9
N3—Co2—N4^{ii}	90.7 (3)	C15—C16—H16A	109.9
O2^{ii}—Co2—N4	90.2 (3)	C11—C16—H16B	109.9
O2—Co2—N4	89.8 (3)	C15—C16—H16B	109.9
N3^{ii}—Co2—N4	90.7 (3)	H16A—C16—H16B	108.3
N3—Co2—N4	89.3 (3)	C22—C17—C18	122.8 (9)
N4^{ii}—Co2—N4	180.0 (4)	C22—C17—C23	118.9 (9)
O4—Cl1—O5	101.0 (11)	C18—C17—C23	118.0 (8)
O4—Cl1—O3	112.3 (8)	O2—C18—C19	119.9 (9)
O5—Cl1—O3	103.5 (11)	O2—C18—C17	125.2 (8)

O4—Cl1—O6	117.5 (9)	C19—C18—C17	114.9 (9)
O5—Cl1—O6	99.8 (10)	C20—C19—C18	122.4 (10)
O3—Cl1—O6	118.8 (9)	C20—C19—Br4	118.9 (8)
C2—O1—Co1	125.3 (6)	C18—C19—Br4	118.7 (8)
C18—O2—Co2	126.5 (6)	C19—C20—C21	120.0 (9)
C7—N1—C8	117.5 (8)	C19—C20—H20	120.0
C7—N1—Co1	124.9 (6)	C21—C20—H20	120.0
C8—N1—Co1	117.4 (6)	C22—C21—C20	119.8 (10)
C10—N2—C11	113.5 (8)	C22—C21—Br3	120.6 (9)
C10—N2—Co1	116.5 (6)	C20—C21—Br3	119.6 (9)
C11—N2—Co1	115.1 (5)	C21—C22—C17	120.1 (10)
C10—N2—H2A	103.1	C21—C22—H22	120.0
C11—N2—H2A	103.1	C17—C22—H22	120.0
Co1—N2—H2A	103.1	N3—C23—C17	127.7 (8)
C23—N3—C24	116.7 (7)	N3—C23—H23	116.2
C23—N3—Co2	124.5 (6)	C17—C23—H23	116.2
C24—N3—Co2	118.3 (6)	N3—C24—C25	111.6 (7)
C26—N4—C27	116.5 (7)	N3—C24—H24A	109.3
C26—N4—Co2	116.8 (6)	C25—C24—H24A	109.3
C27—N4—Co2	116.1 (5)	N3—C24—H24B	109.3
C26—N4—H4A	101.0	C25—C24—H24B	109.3
C27—N4—H4A	101.0	H24A—C24—H24B	108.0
Co2—N4—H4A	101.0	C24—C25—C26	117.3 (8)
C6—C1—C2	120.6 (9)	C24—C25—H25A	108.0
C6—C1—C7	119.0 (9)	C26—C25—H25A	108.0
C2—C1—C7	120.0 (8)	C24—C25—H25B	108.0
O1—C2—C3	120.0 (8)	C26—C25—H25B	108.0
O1—C2—C1	123.5 (8)	H25A—C25—H25B	107.2
C3—C2—C1	116.5 (9)	N4—C26—C25	117.6 (8)
C4—C3—C2	122.9 (9)	N4—C26—H26A	107.9
C4—C3—Br2	118.3 (8)	C25—C26—H26A	107.9
C2—C3—Br2	118.8 (7)	N4—C26—H26B	107.9
C3—C4—C5	118.1 (9)	C25—C26—H26B	107.9
C3—C4—H4	120.9	H26A—C26—H26B	107.2
C5—C4—H4	120.9	N4—C27—C28	109.1 (7)
C6—C5—C4	121.3 (9)	N4—C27—C32	114.1 (7)
C6—C5—Br1	120.8 (9)	C28—C27—C32	110.8 (8)
C4—C5—Br1	117.8 (8)	N4—C27—H27	107.5
C5—C6—C1	120.2 (9)	C28—C27—H27	107.5
C5—C6—H6	119.9	C32—C27—H27	107.5
C1—C6—H6	119.9	C27—C28—C29	109.7 (8)
N1—C7—C1	126.4 (8)	C27—C28—H28A	109.7
N1—C7—H7	116.8	C29—C28—H28A	109.7
C1—C7—H7	116.8	C27—C28—H28B	109.7
N1—C8—C9	111.5 (8)	C29—C28—H28B	109.7
N1—C8—H8A	109.3	H28A—C28—H28B	108.2
C9—C8—H8A	109.3	C30—C29—C28	111.1 (10)
N1—C8—H8B	109.3	C30—C29—H29A	109.4
C9—C8—H8B	109.3	C28—C29—H29A	109.4

H8A—C8—H8B	108.0	C30—C29—H29B	109.4
C8—C9—C10	114.3 (9)	C28—C29—H29B	109.4
C8—C9—H9A	108.7	H29A—C29—H29B	108.0
C10—C9—H9A	108.7	C31—C30—C29	111.6 (10)
C8—C9—H9B	108.7	C31—C30—H30A	109.3
C10—C9—H9B	108.7	C29—C30—H30A	109.3
H9A—C9—H9B	107.6	C31—C30—H30B	109.3
N2—C10—C9	114.3 (9)	C29—C30—H30B	109.3
N2—C10—H10A	108.7	H30A—C30—H30B	108.0
C9—C10—H10A	108.7	C30—C31—C32	111.1 (10)
N2—C10—H10B	108.7	C30—C31—H31A	109.4
C9—C10—H10B	108.7	C32—C31—H31A	109.4
H10A—C10—H10B	107.6	C30—C31—H31B	109.4
C16—C11—N2	114.7 (8)	C32—C31—H31B	109.4
C16—C11—C12	111.7 (8)	H31A—C31—H31B	108.0
N2—C11—C12	110.4 (7)	C27—C32—C31	109.5 (8)
C16—C11—H11	106.5	C27—C32—H32A	109.8
N2—C11—H11	106.5	C31—C32—H32A	109.8
C12—C11—H11	106.5	C27—C32—H32B	109.8
C11—C12—C13	108.6 (8)	C31—C32—H32B	109.8
C11—C12—H12A	110.0	H32A—C32—H32B	108.2

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

Fig. 1


O4
Br1
O3
Cl1
C5
O5
C6
O6
C4
C7
C1
C3
C8
N1
C10
C2
Br2
C9
O1
C16
C15
Co1
N2
C11
C14
C12
C13
C30
C29
C31
C28
C32
C27
C26
N4
C25
Br4
O2
Co2
C19
C20
N3
C17
C23
C21
C22
Br3