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Bis{2,4-dibromo-6-[(2-phenylethyl)-iminomethyl]phenolato-κ^2N,O}cobalt(II)

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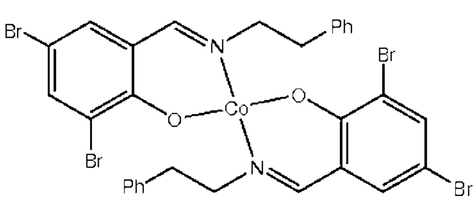
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.006 Å; R factor = 0.032; wR factor = 0.108; data-to-parameter ratio = 16.2.

In the title complex, $[Co(C_{15}H_{12}Br_2NO)_2]$, the Co^{II} atom is four-coordinated by two N,O-bidentate chelate Schiff base ligands, displaying a flattened tetrahedral coordination environment. The Co^{II} atom occupies a special position on a twofold rotation axis. In the crystal, molecules are linked *via* weak C—H⋯Br interactions.

Related literature

For background to vitamin B12, see: Randaccio *et al.* (2010). For the antitumour activity of Schiff base–metal complexes, see: Ren *et al.* (2002) and for their anti-microbial activity, see: Panneerselvam *et al.* (2005). For related structures, see: Chen *et al.* (2010); Li *et al.* (2010); Jiang *et al.* (2008); For standard bond lengths, see: Allen *et al.* (1987).



Experimental

Crystal data

$[Co(C_{15}H_{12}Br_2NO)_2]$
M_r = 823.08
Monoclinic, $C2/c$
a = 22.5087 (16) Å
b = 4.8717 (4) Å
c = 28.864 (2) Å
β = 111.505 (1)°
V = 2944.8 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 6.04 mm^{-1}
T = 291 K
0.24 × 0.23 × 0.22 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000) T_{min} = 0.325, T_{max} = 0.350
14453 measured reflections
2876 independent reflections
2478 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.108
S = 1.01
2876 reflections
177 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.79 e Å^{-3}
$\Delta\rho_{min}$ = −0.78 e Å^{-3}

Table 1
Selected bond lengths (Å).

Co1—O1	1.916 (2)	Co1—N1	1.986 (3)

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C7—H7⋯Br2^{i}	0.93	3.01	3.940 (3)	173
C8—H8B⋯Br1^{ii}	0.97	2.93	3.814 (3)	151
C9—H9B⋯Br2^{iii}	0.97	2.94	3.854 (3)	157

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT-Plus* (Bruker, 2000); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); 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: BR2176).

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supplementary materials

Acta Cryst. (2011). E**67**, m1642 [**doi:10.1107/S160053681104459X**]

Bis{2,4-dibromo-6-[(2-phenylethyl)iminomethyl]phenolato-κ^2*N*,*O*}cobalt(II)

Y. Yin, J. Wang, Y. Zhao and L. Huang

Comment

Cobalt is an important life-required element. For example, vitamin B12, also called cobalamin, is a water soluble vitamin with a key role in the normal functioning of the brain and nervous system, and for the formation of blood (Randaccio *et al.*, 2010). In addition, the Schiff base metal complexes generally possess antitumour activities (Ren *et al.*, 2002) and antimicrobial activities (Panneerselvam *et al.*, 2005). By taking the biological importance of element cobalt into account, we synthesized the title complex with the bidentate N,O-donor Schiff base ligands (Scheme I).

In the title compound, the Co^{II} atom occupies a special position on a twofold rotation axis to form a distorted tetrahedral coordination sphere. Cobalt(II) atom is four-coordinated by two imino N atoms and two phenolic O atoms from two bidentate Schiff-base ligands derived from the condensation of 3,5-dibromosalicylaldehyde and 2-phenylethylamine (Fig. 1). All bond lengths are within normal ranges (Allen *et al.*, 1987). The C7═N1 bond length of 1.284 (4) Å is within the range of 1.256 (14)–1.310 (15) Å observed in the analogous tetrahedral Co(II) species (Chen *et al.*, 2010; Li *et al.*, 2010). The Co–O and Co–N bond distances of 1.916 (2) and 1.986 (3) Å are also similar to those of 1.935 (2) and 2.006 (3) Å previously reported in the related cobalt(II) complex of a Schiff base ligand derived from the condensation of 3,5-dibromosalicylaldehyde and benzylamine (Jiang *et al.*, 2008).

In the crystal structure, the molecules are linked *via* weak C–H···Br interactions (Fig.2).

Experimental

3,5-Dibromosalicylaldehyde (560 mg, 2 mmol) and 2-phenylethylamine (242 mg, 2 mmol) were dissolved in a methanol solution (25 mL).The mixture was stirred at room temperature for 1 h to give an orange solution, which was added to a methanol solution (15 mL) of $Co(NO_3)_2.6H_2O$ (280 mg, 1 mmol). The mixture was stirred for another 25 min at room temperature to give a red solution and then filtered. The filtrate was kept in air for 7 days, forming red blocky crystals. The crystals were isolated and dried in a vacuum desiccator containing anhydrous $CaCl_2$, in about 64% yield. Anal. Calcd for $C_{30}H_{24}Br_4CoN_2O_2$: C, 43.78; H, 2.94; N, 3.40. Found: C, 43.66; H, 2.99; N, 3.31%. IR (KBr, cm^{-1}): 3423, 2909, 2361, 1614, 1502, 1433, 1410, 1310, 1210, 1152, 865, 749, 703, 486, 437.

Refinement

All the H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93 and 0.97 Å, and with $U_{iso}(H) = 1.2U_{eq}(carrier)$.

Figures

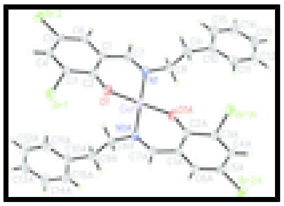

Fig. 1. The structure of the title compound, with the atom numbering scheme of the unique atoms (30% probability ellipsoids).

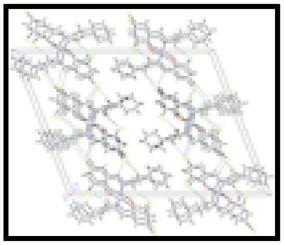

Fig. 2. Partial packing view showing the chain formed through weak C–H···Br interactions.

Bis{2,4-dibromo-6-[(2-phenylethyl)iminomethyl]phenolato- κ^2N,O}cobalt(II)

Crystal data

$[Co(C_{15}H_{12}Br_2NO)_2]$	$F(000) = 1604$
$M_r = 823.08$	$D_x = 1.857$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -C 2yc	Cell parameters from 5864 reflections
$a = 22.5087$ (16) Å	$\theta = 2.9–28.1°$
$b = 4.8717$ (4) Å	$\mu = 6.04$ mm^{-1}
$c = 28.864$ (2) Å	$T = 291$ K
$\beta = 111.505$ (1)°	Block, red
$V = 2944.8$ (4) Å^3	0.24 × 0.23 × 0.22 mm
$Z = 4$	

Data collection

Bruker SMART APEX CCD diffractometer	2876 independent reflections
Radiation source: fine-focus sealed tube	2478 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.031$
φ and ω scans	$\theta_{max} = 26.0°$, $\theta_{min} = 1.9°$
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)	$h = -27 \rightarrow 27$
$T_{min} = 0.325$, $T_{max} = 0.350$	$k = -6 \rightarrow 6$
14453 measured reflections	$l = -35 \rightarrow 35$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map

$R[F^2 > 2\sigma(F^2)] = 0.032$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.108$	H-atom parameters constrained
$S = 1.01$	$w = 1/[\sigma^2(F_o^2) + (0.082P)^2 + 0.812P]$ where $P = (F_o^2 + 2F_c^2)/3$
2876 reflections	$(\Delta/\sigma)_{max} < 0.001$
177 parameters	$\Delta\rho_{max} = 0.79$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.78$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 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}
C1	0.12749 (15)	0.3862 (7)	0.22685 (12)	0.0389 (7)
C2	0.08497 (15)	0.5880 (6)	0.19768 (11)	0.0367 (7)
C3	0.09703 (15)	0.6772 (6)	0.15481 (11)	0.0365 (6)
C4	0.14508 (15)	0.5753 (6)	0.14172 (12)	0.0409 (7)
H4	0.1509	0.6379	0.1132	0.049*
C5	0.18509 (15)	0.3773 (7)	0.17151 (12)	0.0430 (7)
C6	0.17739 (16)	0.2844 (7)	0.21350 (12)	0.0435 (8)
H6	0.2052	0.1534	0.2333	0.052*
C7	0.12310 (17)	0.2717 (7)	0.27173 (12)	0.0431 (7)
H7	0.1561	0.1560	0.2903	0.052*
C8	0.08535 (19)	0.1846 (8)	0.33657 (12)	0.0492 (8)
H8A	0.1125	0.0239	0.3418	0.059*
H8B	0.0438	0.1257	0.3358	0.059*
C9	0.1142 (2)	0.3836 (9)	0.37889 (14)	0.0656 (11)
H9A	0.0876	0.5464	0.3729	0.079*
H9B	0.1560	0.4390	0.3799	0.079*
C10	0.12060 (19)	0.2619 (7)	0.42885 (13)	0.0503 (9)
C11	0.0790 (2)	0.3341 (10)	0.45192 (14)	0.0613 (10)
H11	0.0479	0.4661	0.4374	0.074*
C12	0.0828 (3)	0.2136 (10)	0.49615 (16)	0.0701 (12)
H12	0.0536	0.2616	0.5107	0.084*
C13	0.1281 (3)	0.0287 (10)	0.51828 (15)	0.0702 (12)
H13	0.1309	−0.0479	0.5485	0.084*
C14	0.1703 (3)	−0.0485 (13)	0.49693 (19)	0.0972 (19)

H14	0.2012	−0.1803	0.5121	0.117*
C15	0.1668 (2)	0.0710 (11)	0.45224 (17)	0.0773 (14)
H15	0.1962	0.0209	0.4380	0.093*
Br1	0.040636 (17)	0.94006 (7)	0.113456 (12)	0.04757 (15)
Br2	0.250012 (17)	0.22456 (9)	0.151646 (14)	0.05805 (16)
Co1	0.0000	0.52246 (15)	0.2500	0.04521 (19)
N1	0.07834 (13)	0.3134 (6)	0.28853 (10)	0.0425 (6)
O1	0.03706 (12)	0.6888 (5)	0.20677 (9)	0.0468 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0389 (16)	0.0510 (18)	0.0320 (16)	−0.0033 (13)	0.0192 (13)	−0.0013 (13)
C2	0.0394 (16)	0.0439 (17)	0.0338 (16)	−0.0048 (12)	0.0219 (13)	−0.0012 (12)
C3	0.0406 (16)	0.0432 (16)	0.0303 (15)	−0.0029 (13)	0.0182 (13)	0.0005 (12)
C4	0.0460 (18)	0.0523 (19)	0.0324 (16)	−0.0078 (15)	0.0239 (14)	−0.0023 (13)
C5	0.0360 (16)	0.0589 (19)	0.0414 (18)	−0.0039 (14)	0.0226 (14)	−0.0086 (15)
C6	0.0364 (16)	0.059 (2)	0.0370 (17)	0.0031 (14)	0.0155 (14)	0.0028 (14)
C7	0.0444 (18)	0.0548 (19)	0.0336 (16)	0.0020 (14)	0.0184 (14)	0.0063 (14)
C8	0.054 (2)	0.064 (2)	0.0345 (17)	−0.0061 (17)	0.0213 (15)	0.0100 (15)
C9	0.091 (3)	0.069 (2)	0.038 (2)	−0.021 (2)	0.026 (2)	0.0042 (17)
C10	0.062 (2)	0.057 (2)	0.0324 (17)	−0.0141 (17)	0.0174 (16)	−0.0011 (14)
C11	0.067 (2)	0.074 (3)	0.040 (2)	0.005 (2)	0.0150 (18)	0.0093 (18)
C12	0.089 (3)	0.087 (3)	0.044 (2)	0.001 (3)	0.035 (2)	−0.004 (2)
C13	0.095 (3)	0.083 (3)	0.036 (2)	0.004 (3)	0.027 (2)	0.0095 (19)
C14	0.114 (4)	0.133 (5)	0.050 (3)	0.052 (4)	0.036 (3)	0.032 (3)
C15	0.076 (3)	0.116 (4)	0.047 (2)	0.022 (3)	0.032 (2)	0.013 (2)
Br1	0.0584 (2)	0.0515 (2)	0.0413 (2)	0.00711 (15)	0.02841 (17)	0.00863 (13)
Br2	0.0447 (2)	0.0830 (3)	0.0575 (3)	0.00539 (17)	0.03169 (19)	−0.00833 (18)
Co1	0.0441 (4)	0.0638 (4)	0.0359 (4)	0.000	0.0243 (3)	0.000
N1	0.0470 (16)	0.0554 (16)	0.0312 (14)	−0.0017 (13)	0.0216 (12)	0.0052 (12)
O1	0.0522 (14)	0.0575 (14)	0.0442 (13)	0.0103 (11)	0.0337 (11)	0.0089 (11)

Geometric parameters (Å, °)

C1—C6	1.405 (5)	C9—C10	1.516 (5)
C1—C2	1.415 (5)	C9—H9A	0.9700
C1—C7	1.447 (4)	C9—H9B	0.9700
C2—O1	1.296 (4)	C10—C15	1.374 (6)
C2—C3	1.428 (4)	C10—C11	1.378 (6)
C3—C4	1.363 (4)	C11—C12	1.379 (6)
C3—Br1	1.888 (3)	C11—H11	0.9300
C4—C5	1.383 (5)	C12—C13	1.335 (7)
C4—H4	0.9300	C12—H12	0.9300
C5—C6	1.363 (5)	C13—C14	1.360 (7)
C5—Br2	1.906 (3)	C13—H13	0.9300
C6—H6	0.9300	C14—C15	1.391 (7)
C7—N1	1.284 (4)	C14—H14	0.9300
C7—H7	0.9300	C15—H15	0.9300

C8—N1	1.477 (4)	Co1—O1	1.916 (2)
C8—C9	1.507 (5)	Co1—O1^{i}	1.916 (2)
C8—H8A	0.9700	Co1—N1	1.986 (3)
C8—H8B	0.9700	Co1—N1^{i}	1.986 (3)
C6—C1—C2	121.1 (3)	C10—C9—H9B	109.1
C6—C1—C7	115.7 (3)	H9A—C9—H9B	107.8
C2—C1—C7	123.2 (3)	C15—C10—C11	117.4 (3)
O1—C2—C1	125.0 (3)	C15—C10—C9	121.6 (4)
O1—C2—C3	119.8 (3)	C11—C10—C9	121.0 (4)
C1—C2—C3	115.2 (3)	C10—C11—C12	121.1 (4)
C4—C3—C2	123.5 (3)	C10—C11—H11	119.5
C4—C3—Br1	119.3 (2)	C12—C11—H11	119.5
C2—C3—Br1	117.2 (2)	C13—C12—C11	120.5 (4)
C3—C4—C5	118.9 (3)	C13—C12—H12	119.8
C3—C4—H4	120.5	C11—C12—H12	119.8
C5—C4—H4	120.5	C12—C13—C14	120.5 (4)
C6—C5—C4	121.2 (3)	C12—C13—H13	119.8
C6—C5—Br2	120.0 (3)	C14—C13—H13	119.8
C4—C5—Br2	118.8 (2)	C13—C14—C15	119.5 (5)
C5—C6—C1	120.1 (3)	C13—C14—H14	120.2
C5—C6—H6	119.9	C15—C14—H14	120.2
C1—C6—H6	119.9	C10—C15—C14	121.0 (5)
N1—C7—C1	126.7 (3)	C10—C15—H15	119.5
N1—C7—H7	116.7	C14—C15—H15	119.5
C1—C7—H7	116.7	O1—Co1—O1^{i}	129.98 (15)
N1—C8—C9	110.7 (3)	O1—Co1—N1	94.15 (10)
N1—C8—H8A	109.5	O1^{i}—Co1—N1	111.18 (11)
C9—C8—H8A	109.5	O1—Co1—N1^{i}	111.18 (11)
N1—C8—H8B	109.5	O1^{i}—Co1—N1^{i}	94.14 (10)
C9—C8—H8B	109.5	N1—Co1—N1^{i}	118.31 (17)
H8A—C8—H8B	108.1	C7—N1—C8	117.3 (3)
C8—C9—C10	112.5 (3)	C7—N1—Co1	121.9 (2)
C8—C9—H9A	109.1	C8—N1—Co1	120.7 (2)
C10—C9—H9A	109.1	C2—O1—Co1	124.4 (2)
C8—C9—H9B	109.1		

Symmetry codes: (i) $-x$, y, $-z+1/2$.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···Br2^{ii}	0.93	3.01	3.940 (3)	173.
C8—H8B···Br1^{iii}	0.97	2.93	3.814 (3)	151.
C9—H9B···Br2^{iv}	0.97	2.94	3.854 (3)	157.

Symmetry codes: (ii) $-x+1/2$, $y-1/2$, $-z+1/2$; (iii) $-x$, $y-1$, $-z+1/2$; (iv) $-x+1/2$, $y+1/2$, $-z+1/2$.

Fig. 1

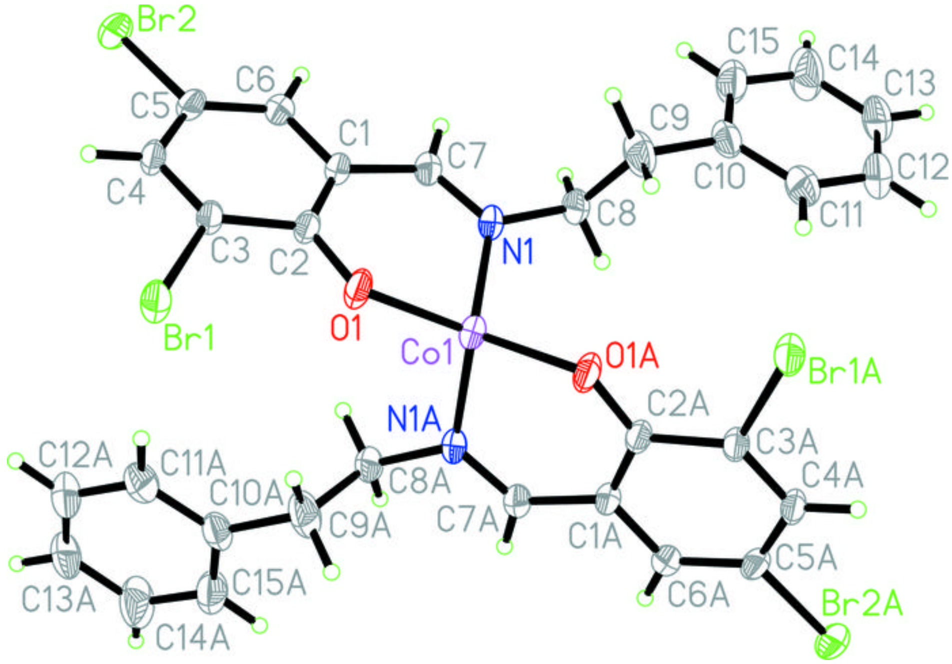
Br2
C6
C5
C1
C7
C9
C15
C14
C13
C4
C10
C12
C8
C3
C2
N1
C11
O1
Br1
Co1
O1A
Br1A
C2A
N1A
C3A
C12A
C11A
C4A
C10A
C8A
C9A
C7A
C1A
C5A
C15A
C6A
C13A
C14A
Br2A

Fig. 2