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Bis[2,4-dibromo-6-(*n*-propyliminomethyl)phenolato-κ^2N,O]cobalt(II)

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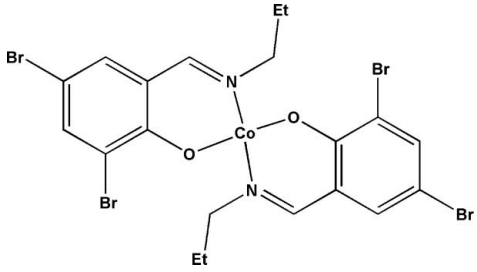
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.030; wR factor = 0.065; data-to-parameter ratio = 17.1.

In the title complex, $[Co(C_{10}H_{10}Br_2NO)_2]$, the Co^{II} atom lies on a twofold rotation axis, the N_2O_2 units having distorted tetrahedral coordination environments comprising two bidentate chelate 2,4-dibromo-6-(*n*-propyliminomethyl)phenolate Schiff base ligands [Co—N = 1.989 (3) Å, Co—O = 1.924 (2) Å and O/N—Co—O/N = 94.53 (10)–125.40 (15)°]. In the crystal structure, the molecules are linked *via* weak intermolecular C—H···O hydrogen bonds [3.334 (5) Å] and there are also short inversion-related intermolecular Br···Br contacts [3.4263 (6) Å]

Related literature

For related compounds, see: Bermejo *et al.* (1996); Chen *et al.* (2007); Li & Wang (2007); Li *et al.* (2008); Maneiro *et al.* (2001); Qiu *et al.* (2007); Yuan *et al.* (2007). For standard bond-length values, see: Allen *et al.* (1987).



Experimental

Crystal data

$[Co(C_{10}H_{10}Br_2NO)_2]$
M_r = 698.91
Monoclinic, $C2/c$
a = 24.3684 (10) Å
b = 4.8555 (2) Å
c = 21.8132 (10) Å
β = 115.523 (4)°
V = 2329.08 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 7.62 mm^{-1}
T = 296 K
0.32 × 0.22 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.097, T_{max} = 0.218
6076 measured reflections
2270 independent reflections
1657 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.065
S = 1.00
2270 reflections
133 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.50 e Å^{-3}

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXL97* (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: ZS2053).

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supporting information

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Bis[2,4-dibromo-6-(*n*-propyliminomethyl)phenolato-κ^2N,O]cobalt(II)

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S1. Comment

The Lewis base adducts of the 3,5-dibromosalicylidene compounds derived from the condensation of 3,5-dibromosalicylaldehyde with various primary amines are of interest, forming complexes with a large number of transition metals (Chen *et al.*, 2007; Qiu *et al.*, 2007; Maneiro *et al.*, 2001; Bermejo *et al.*, 1996). Recently, mononuclear zinc(II) and nickel(II) compounds of Schiff base ligands derived from the condensation of 3,5-dibromosalicylaldehyde with cyclopropylamine have been structurally characterized (Li & Wang, 2007; Yuan *et al.*, 2007). As an extension of this work, the crystal structure of the title Co^{II} complex, $[C_{20}H_{20}Br_4CoN_2O_2]$ (I), is reported here.

In (I), the Co^{II} atoms have distorted tetrahedral coordination environments with two bidentate Schiff base ligands, derived from the condensation of 3,5-dibromosalicylaldehyde and *n*-propylamine, acting as chelates through their phenolate O and azomethine N atoms [Co—N 1.989 (3) Å; Co—O 1.924 (2) Å; bond-angle range 94.53 (10)–125.40 (15)°] (Fig. 1). The Co atoms lie on two-fold rotation axes. The C7═N1 bond length of 1.274 (4) Å is somewhat shorter than 1.284 (2) Å observed in the previously reported compound of a Schiff base ligand derived from the condensation of salicylaldehyde with *n*-propylamine (Li *et al.*, 2008). The angle between the two O1—Co1—N1 planes of the molecule is equal to 84.13°. All bond lengths are within normal ranges (Allen *et al.*, 1987). In the crystal structure, the molecules are linked *via* weak intermolecular C—H···O hydrogen bonds and there are also short inversion-related inermolecular Br···Br contacts [3.4263 (6) Å] (Fig. 2).

S2. Experimental

3,5-Dibromosalicylaldehyde (560 mg, 2 mmol) and *n*-propylamine (118 mg, 2 mmol) were dissolved in methanol (25 ml). The mixture was stirred for 30 min 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 20 min at room temperature to give a red solution and then filtered. The filtrate was kept in air for 5 d, forming red blocky crystals. The crystals were isolated, washed three times with distilled water and dried in a vacuum desiccator containing anhydrous $CaCl_2$ (yield 68%). Analysis calculated for $C_{20}H_{20}Br_4CoN_2O_2$: C 34.37, H 2.88, N 4.01%; found: C 34.17, H 2.90, N 3.99%. IR (KBr, cm^{-1}): 3447, 3062, 2966, 2877, 2359, 1619, 1577, 1504, 1434, 1407, 1307, 1212, 1161, 1095, 1040, 865, 838, 749, 705, 604, 466.

S3. Refinement

All the H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93–0.97 Å, and with U_{iso}(H) = 1.2U_{eq}(carrier) or 1.5U_{eq}(methyl groups).

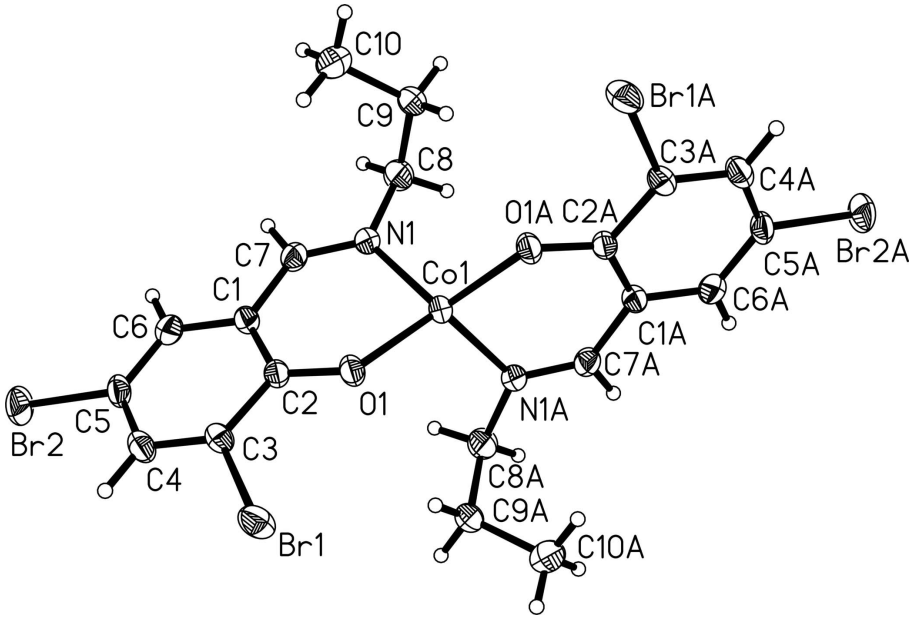

Figure 1

The structure and atom-numbering scheme of the title compound (I), showing 30% probability displacement ellipsoids. The complex has two-fold rotational symmetry, the atoms labeled with the suffix A are related to the primary atoms by the symmetry code -*x*, *y*, -*z* + 3/2.

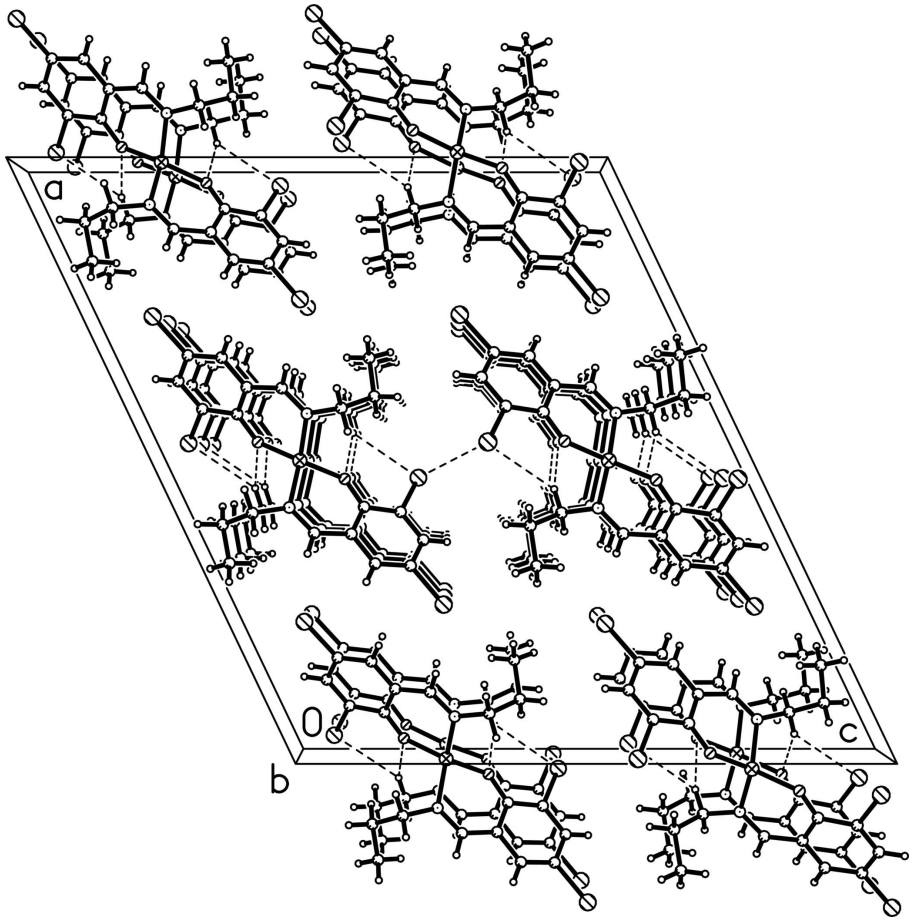

Figure 2

The crystal packing of the title compound (I) viewed along the *b* axis, linked *via* intermolecular C—H···O hydrogen bonds (dashed lines).

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Crystal data

$[Co(C_{10}H_{10}Br_2NO)_2]$
$M_r = 698.91$
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
$a = 24.3684\ (10)$ Å
$b = 4.8555\ (2)$ Å
$c = 21.8132\ (10)$ Å
$\beta = 115.523\ (4)°$
$V = 2329.08\ (19)$ Å^3
$Z = 4$
$F(000) = 1348$
$D_x = 1.993$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1806 reflections
$\theta = 3.3–25.5°$
$\mu = 7.62$ mm^{-1}
$T = 296$ K
Block, red
0.32 × 0.22 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.097$, $T_{max} = 0.218$
6076 measured reflections
2270 independent reflections

1657 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 26.0°$, $\theta_{min} = 1.9°$
$h = -29 \rightarrow 21$
$k = -5 \rightarrow 5$
$l = -26 \rightarrow 26$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.065$
$S = 1.00$
2270 reflections
133 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
$w = 1/[\sigma^2(F_o^2) + (0.0251P)^2 + 0.88P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.41$ e Å^{-3}
$\Delta\rho_{min} = -0.50$ e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.0000	0.31955 (14)	0.7500	0.03770 (18)
Br1	0.028614 (18)	0.79002 (8)	0.569909 (19)	0.05211 (14)
Br2	0.232643 (17)	0.11525 (10)	0.62503 (2)	0.06655 (17)
N1	0.07574 (11)	0.1053 (6)	0.80081 (13)	0.0385 (7)
O1	0.03028 (9)	0.5013 (5)	0.69236 (11)	0.0413 (6)
C1	0.11919 (14)	0.2181 (7)	0.72164 (16)	0.0369 (8)
C2	0.07618 (13)	0.4180 (7)	0.68171 (16)	0.0341 (8)
C3	0.08482 (14)	0.5258 (7)	0.62579 (16)	0.0368 (8)
C4	0.13048 (15)	0.4419 (8)	0.60975 (18)	0.0440 (9)
H4	0.1343	0.5164	0.5725	0.053*
C5	0.17107 (15)	0.2444 (8)	0.64965 (19)	0.0437 (9)
C6	0.16661 (15)	0.1351 (8)	0.70498 (18)	0.0468 (9)
H6	0.1949	0.0056	0.7318	0.056*
C7	0.11686 (14)	0.0829 (7)	0.77979 (17)	0.0415 (9)
H7	0.1491	−0.0336	0.8046	0.050*
C8	0.08417 (17)	−0.0483 (8)	0.86238 (18)	0.0516 (10)
H8A	0.1148	−0.1894	0.8712	0.062*
H8B	0.0464	−0.1385	0.8552	0.062*
C9	0.10364 (16)	0.1417 (9)	0.92354 (18)	0.0559 (11)
H9A	0.0750	0.2931	0.9127	0.067*
H9B	0.1023	0.0408	0.9612	0.067*
C10	0.16709 (18)	0.2569 (10)	0.9451 (2)	0.0746 (14)

H10A	0.1958	0.1081	0.9567	0.112*
H10B	0.1772	0.3744	0.9838	0.112*
H10C	0.1685	0.3610	0.9083	0.112*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0308 (3)	0.0523 (4)	0.0343 (4)	0.000	0.0181 (3)	0.000
Br1	0.0656 (3)	0.0533 (3)	0.0443 (2)	0.0123 (2)	0.03017 (19)	0.01239 (19)
Br2	0.0498 (2)	0.0945 (4)	0.0726 (3)	0.0031 (2)	0.0427 (2)	−0.0139 (3)
N1	0.0333 (15)	0.0490 (19)	0.0339 (16)	−0.0022 (14)	0.0150 (12)	0.0031 (14)
O1	0.0377 (12)	0.0517 (16)	0.0424 (13)	0.0080 (11)	0.0247 (11)	0.0090 (12)
C1	0.0351 (18)	0.044 (2)	0.0357 (19)	−0.0021 (16)	0.0191 (15)	−0.0042 (16)
C2	0.0324 (17)	0.038 (2)	0.0349 (19)	−0.0042 (16)	0.0176 (15)	−0.0035 (16)
C3	0.0448 (19)	0.035 (2)	0.0363 (19)	−0.0020 (16)	0.0230 (16)	−0.0034 (16)
C4	0.050 (2)	0.050 (2)	0.042 (2)	−0.0075 (19)	0.0297 (18)	−0.0053 (18)
C5	0.0372 (19)	0.056 (3)	0.049 (2)	−0.0048 (18)	0.0285 (17)	−0.0104 (19)
C6	0.0334 (19)	0.061 (3)	0.045 (2)	0.0065 (18)	0.0156 (16)	0.0001 (19)
C7	0.0323 (18)	0.049 (2)	0.042 (2)	0.0064 (16)	0.0147 (16)	0.0080 (17)
C8	0.050 (2)	0.060 (3)	0.047 (2)	−0.003 (2)	0.0231 (18)	0.015 (2)
C9	0.046 (2)	0.088 (3)	0.037 (2)	−0.006 (2)	0.0215 (17)	0.010 (2)
C10	0.053 (3)	0.112 (4)	0.051 (3)	−0.016 (3)	0.015 (2)	0.002 (3)

Geometric parameters (Å, º)

Co1—O1^{i}	1.924 (2)	C4—C5	1.383 (5)
Co1—O1	1.924 (2)	C4—H4	0.9300
Co1—N1^{i}	1.989 (3)	C5—C6	1.365 (5)
Co1—N1	1.989 (3)	C6—H6	0.9300
Br1—C3	1.889 (3)	C7—H7	0.9300
Br2—C5	1.905 (3)	C8—C9	1.520 (5)
N1—C7	1.274 (4)	C8—H8A	0.9700
N1—C8	1.471 (4)	C8—H8B	0.9700
O1—C2	1.301 (3)	C9—C10	1.516 (5)
C1—C6	1.411 (5)	C9—H9A	0.9700
C1—C2	1.419 (4)	C9—H9B	0.9700
C1—C7	1.451 (4)	C10—H10A	0.9600
C2—C3	1.424 (4)	C10—H10B	0.9600
C3—C4	1.365 (4)	C10—H10C	0.9600
O1^{i}—Co1—O1	125.40 (15)	C5—C6—C1	120.2 (3)
O1^{i}—Co1—N1^{i}	94.53 (10)	C5—C6—H6	119.9
O1—Co1—N1^{i}	113.63 (10)	C1—C6—H6	119.9
O1^{i}—Co1—N1	113.64 (10)	N1—C7—C1	127.5 (3)
O1—Co1—N1	94.53 (10)	N1—C7—H7	116.2
N1^{i}—Co1—N1	116.90 (16)	C1—C7—H7	116.2
C7—N1—C8	117.6 (3)	N1—C8—C9	111.2 (3)
C7—N1—Co1	122.0 (2)	N1—C8—H8A	109.4

C8—N1—Co1	120.3 (2)	C9—C8—H8A	109.4
C2—O1—Co1	125.1 (2)	N1—C8—H8B	109.4
C6—C1—C2	120.5 (3)	C9—C8—H8B	109.4
C6—C1—C7	116.1 (3)	H8A—C8—H8B	108.0
C2—C1—C7	123.3 (3)	C10—C9—C8	112.8 (3)
O1—C2—C1	124.6 (3)	C10—C9—H9A	109.0
O1—C2—C3	119.6 (3)	C8—C9—H9A	109.0
C1—C2—C3	115.8 (3)	C10—C9—H9B	109.0
C4—C3—C2	123.2 (3)	C8—C9—H9B	109.0
C4—C3—Br1	118.8 (3)	H9A—C9—H9B	107.8
C2—C3—Br1	117.9 (2)	C9—C10—H10A	109.5
C3—C4—C5	119.1 (3)	C9—C10—H10B	109.5
C3—C4—H4	120.4	H10A—C10—H10B	109.5
C5—C4—H4	120.4	C9—C10—H10C	109.5
C6—C5—C4	121.2 (3)	H10A—C10—H10C	109.5
C6—C5—Br2	119.6 (3)	H10B—C10—H10C	109.5
C4—C5—Br2	119.2 (3)		

Symmetry code: (i) $-x$, y, $-z+3/2$.