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

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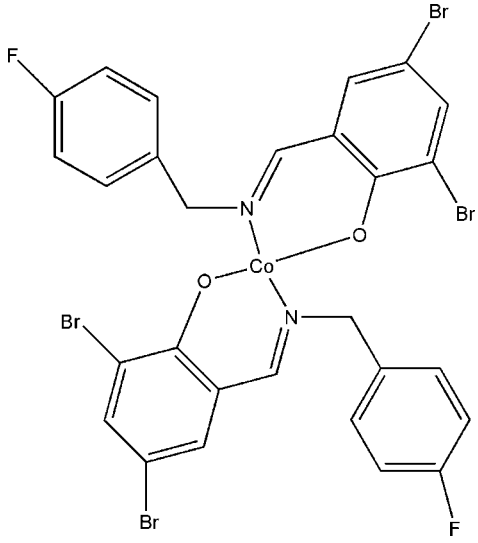
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.012 Å; R factor = 0.037; wR factor = 0.079; data-to-parameter ratio = 13.8.

The complete molecule of the title complex, $[Co(C_{14}H_9Br_2FNO)_2]$, is generated by crystallographic twofold symmetry, with the Co^{II} atom lying on the rotation axis. The coordination of the metal atom by the two *N*,*O*-bidentate ligands results in a squashed CoN_2O_2 tetrahedron. The six-membered chelate ring is an envelope, with the metal atom as the flap. The dihedral angle between the planes of the aromatic rings within each ligand is 84.1 (6)°.

Related literature

For a related structure, see: Jadeja & Shah (2007).



Experimental

Crystal data

$[Co(C_{14}H_9Br_2FNO)_2]$
M_r = 830.97
Monoclinic, $C2$
a = 14.6921 (14) Å
b = 9.7598 (3) Å
c = 13.1195 (13) Å
β = 133.608 (17)°
V = 1362.2 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 6.54 mm^{-1}
T = 293 K
0.33 × 0.21 × 0.12 mm

Data collection

Rigaku R-AXIS RAPID CCD diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.210, T_{max} = 0.456
5582 measured reflections
2437 independent reflections
2161 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.079
S = 1.02
2437 reflections
177 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}
Absolute structure: Flack (1983), 961 Friedel pairs
Flack parameter: −0.012 (14)

Table 1
Selected geometric parameters (Å, °).

Co1—O1	1.933 (4)	Co1—N1	2.023 (5)
O1—Co1—O1^{i}	143.6 (2)	O1^{i}—Co1—N1	104.12 (18)
O1—Co1—N1	92.90 (17)	N1—Co1—N1^{i}	123.7 (3)

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); 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: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6941).

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supporting information

Acta Cryst. (2012). E**68**, m1423 [doi:10.1107/S1600536812043929]

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

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S1. Experimental

Synthesis of the ligand 2-((*E*)-(4-fluorobenzylimino) methyl)-4,6-dibromophenol: 3,5-dibromo-2-hydroxybenzal dehyde and (4-fluorophenyl)methanamine (1:1) were dissolved in ethanol and the solution was refluxed for 2 h. After evaporation, a crude product was recrystallized twice from ethanol solution to give a yellow product.

1 mmol (0.77 g) of the ligand and 0.5 mmol (0.145 g) $Co(NO_3)_2$ were dissolved in ethanol and the solutions mixed and stirred for about 10 minutes. The slow vaporization of the solvent yielded after about 3 d dark red single blocks. Yield: 72.3%. Calcd. for $C_{28}H_{18}Br_4CoF_2N_2O_2$: C 40.37; H 2.42; O 3.84; N 3.36; Found: C 40.26; H 2.40; O 3.83; N 3.35%.

S2. Refinement

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms (C—H = 0.93%A) and U_{iso}(H) values equal to 1.2 U_{eq}(C).

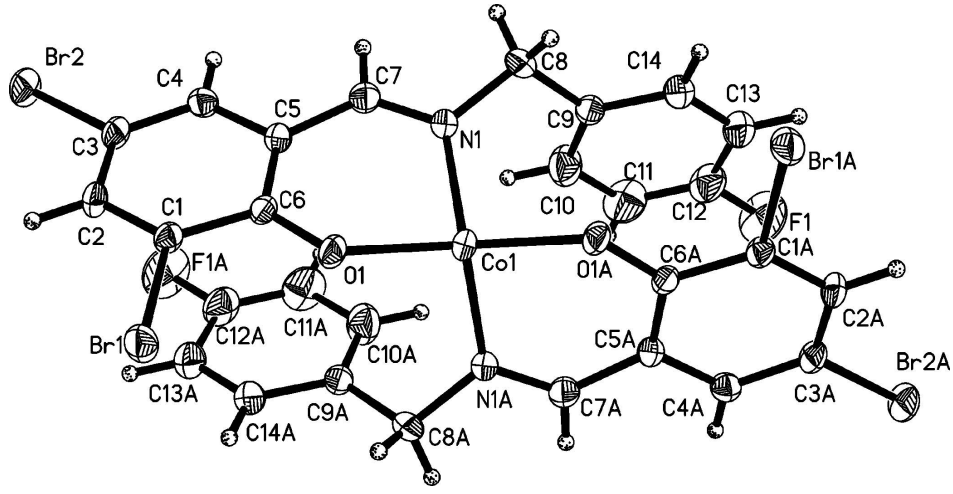

Figure 1

The molecular structure of the title complex, showing 30% probability displacement ellipsoids. Atoms with label suffix A are generated by (2–x, –y, 2–z).

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Crystal data

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M_r = 830.97	b = 9.7598 (3) Å
Monoclinic, *C*2	c = 13.1195 (13) Å
Hall symbol: C 2y	β = 133.608 (17)°

V = 1362.2 (4) Å^3
Z = 2
F(000) = 802
D_x = 2.026 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
θ = 2.8–26.4°
μ = 6.54 mm^{-1}
T = 293 K
Block, red
0.33 × 0.21 × 0.12 mm

Data collection

Rigaku R-AXIS RAPID CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.210, T_{max} = 0.456
5582 measured reflections
2437 independent reflections
2161 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 26.4°, θ_{min} = 2.8°
h = −16→18
k = −12→11
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.079
S = 1.02
2437 reflections
177 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0352P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}
Absolute structure: Flack (1983), 961 Friedel pairs
Absolute structure parameter: −0.012 (14)

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}
Br1	1.04553 (6)	0.62756 (5)	1.37969 (7)	0.04722 (19)
Br2	0.66469 (6)	0.25233 (7)	1.20378 (7)	0.0518 (2)
Co1	1.0000	0.46517 (11)	1.0000	0.0378 (3)
F1	1.0441 (5)	0.0042 (6)	0.6661 (7)	0.108 (2)
O1	0.9762 (3)	0.5270 (4)	1.1203 (4)	0.0377 (9)
N1	0.8324 (4)	0.3673 (5)	0.8675 (5)	0.0380 (11)
C1	0.9177 (5)	0.5015 (5)	1.2457 (6)	0.0317 (12)
C2	0.8477 (5)	0.4400 (6)	1.2682 (6)	0.0354 (13)
H2	0.8609	0.4636	1.3462	0.043*
C3	0.7584 (5)	0.3434 (6)	1.1736 (6)	0.0372 (14)

C4	0.7374 (5)	0.3097 (6)	1.0577 (6)	0.0358 (13)
H4	0.6756	0.2459	0.9939	0.043*
C5	0.8088 (5)	0.3712 (6)	1.0336 (6)	0.0323 (12)
C6	0.9041 (5)	0.4673 (5)	1.1321 (6)	0.0294 (12)
C7	0.7747 (5)	0.3358 (6)	0.9051 (6)	0.0395 (14)
H7	0.7020	0.2837	0.8416	0.047*
C8	0.7686 (5)	0.3365 (7)	0.7212 (6)	0.0437 (15)
H8A	0.7490	0.4220	0.6718	0.052*
H8B	0.6898	0.2904	0.6748	0.052*
C9	0.8460 (5)	0.2477 (7)	0.7099 (6)	0.0373 (13)
C10	0.9141 (7)	0.1382 (8)	0.7983 (8)	0.0622 (19)
H10	0.9152	0.1193	0.8686	0.075*
C11	0.9810 (8)	0.0557 (8)	0.7835 (11)	0.076 (3)
H11	1.0272	−0.0183	0.8435	0.092*
C12	0.9781 (7)	0.0843 (8)	0.6809 (9)	0.063 (2)
C13	0.9111 (6)	0.1905 (8)	0.5902 (8)	0.0566 (18)
H13	0.9091	0.2069	0.5189	0.068*
C14	0.8456 (5)	0.2737 (7)	0.6069 (7)	0.0431 (15)
H14	0.8008	0.3483	0.5474	0.052*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0476 (3)	0.0584 (4)	0.0421 (4)	−0.0195 (3)	0.0334 (3)	−0.0154 (3)
Br2	0.0528 (4)	0.0658 (4)	0.0576 (5)	−0.0160 (3)	0.0460 (4)	−0.0025 (3)
Co1	0.0322 (6)	0.0575 (7)	0.0337 (6)	0.000	0.0265 (5)	0.000
F1	0.113 (4)	0.110 (4)	0.138 (5)	0.045 (4)	0.101 (4)	0.006 (4)
O1	0.035 (2)	0.049 (2)	0.041 (2)	−0.0131 (18)	0.031 (2)	−0.0094 (18)
N1	0.031 (2)	0.056 (3)	0.030 (3)	0.002 (2)	0.022 (2)	−0.001 (2)
C1	0.031 (3)	0.034 (3)	0.035 (3)	−0.008 (2)	0.025 (3)	−0.005 (2)
C2	0.043 (3)	0.040 (3)	0.041 (4)	−0.003 (3)	0.035 (3)	−0.001 (3)
C3	0.036 (3)	0.045 (3)	0.042 (4)	−0.008 (3)	0.032 (3)	−0.002 (3)
C4	0.033 (3)	0.039 (3)	0.033 (3)	−0.005 (3)	0.022 (3)	−0.003 (3)
C5	0.032 (3)	0.038 (3)	0.031 (3)	−0.001 (3)	0.023 (3)	0.002 (2)
C6	0.028 (3)	0.033 (3)	0.032 (3)	0.004 (2)	0.022 (3)	0.006 (2)
C7	0.034 (3)	0.048 (3)	0.036 (4)	−0.009 (3)	0.024 (3)	−0.009 (3)
C8	0.034 (3)	0.063 (4)	0.026 (3)	0.002 (3)	0.018 (3)	−0.003 (3)
C9	0.033 (3)	0.046 (3)	0.033 (3)	−0.010 (3)	0.023 (3)	−0.011 (3)
C10	0.071 (5)	0.066 (5)	0.067 (5)	0.008 (4)	0.055 (4)	0.015 (4)
C11	0.079 (5)	0.059 (5)	0.099 (8)	0.029 (4)	0.065 (6)	0.024 (5)
C12	0.061 (5)	0.069 (5)	0.072 (6)	0.005 (4)	0.051 (5)	−0.011 (4)
C13	0.053 (4)	0.076 (5)	0.050 (4)	−0.002 (4)	0.039 (4)	−0.008 (4)
C14	0.043 (3)	0.049 (4)	0.040 (4)	0.001 (3)	0.030 (3)	−0.002 (3)

Geometric parameters (Å, º)

Br1—C1	1.891 (5)	C5—C6	1.419 (7)
Br2—C3	1.896 (5)	C5—C7	1.430 (8)

Co1—O1	1.933 (4)	C7—H7	0.9300
Co1—O1^{i}	1.933 (4)	C8—C9	1.515 (8)
Co1—N1	2.023 (5)	C8—H8A	0.9700
Co1—N1^{i}	2.023 (5)	C8—H8B	0.9700
F1—C12	1.359 (8)	C9—C14	1.371 (8)
O1—C6	1.308 (6)	C9—C10	1.374 (10)
N1—C7	1.279 (7)	C10—C11	1.383 (11)
N1—C8	1.474 (8)	C10—H10	0.9300
C1—C2	1.387 (8)	C11—C12	1.346 (12)
C1—C6	1.400 (7)	C11—H11	0.9300
C2—C3	1.380 (8)	C12—C13	1.358 (10)
C2—H2	0.9300	C13—C14	1.388 (8)
C3—C4	1.367 (8)	C13—H13	0.9300
C4—C5	1.420 (7)	C14—H14	0.9300
C4—H4	0.9300		

O1—Co1—O1^{i}	143.6 (2)	N1—C7—C5	127.6 (5)
O1—Co1—N1	92.90 (17)	N1—C7—H7	116.2
O1^{i}—Co1—N1	104.12 (18)	C5—C7—H7	116.2
O1—Co1—N1^{i}	104.12 (18)	N1—C8—C9	113.4 (5)
O1^{i}—Co1—N1^{i}	92.90 (17)	N1—C8—H8A	108.9
N1—Co1—N1^{i}	123.7 (3)	C9—C8—H8A	108.9
C6—O1—Co1	125.1 (3)	N1—C8—H8B	108.9
C7—N1—C8	117.3 (5)	C9—C8—H8B	108.9
C7—N1—Co1	121.3 (4)	H8A—C8—H8B	107.7
C8—N1—Co1	121.3 (4)	C14—C9—C10	118.7 (6)
C2—C1—C6	122.7 (5)	C14—C9—C8	119.8 (6)
C2—C1—Br1	119.3 (4)	C10—C9—C8	121.5 (6)
C6—C1—Br1	117.8 (4)	C9—C10—C11	120.6 (7)
C3—C2—C1	119.3 (5)	C9—C10—H10	119.7
C3—C2—H2	120.4	C11—C10—H10	119.7
C1—C2—H2	120.4	C12—C11—C10	119.0 (7)
C4—C3—C2	120.6 (5)	C12—C11—H11	120.5
C4—C3—Br2	118.7 (4)	C10—C11—H11	120.5
C2—C3—Br2	120.6 (4)	C11—C12—C13	122.6 (7)
C3—C4—C5	120.8 (5)	C11—C12—F1	119.4 (8)
C3—C4—H4	119.6	C13—C12—F1	118.1 (8)
C5—C4—H4	119.6	C12—C13—C14	118.1 (7)
C6—C5—C4	119.5 (5)	C12—C13—H13	121.0
C6—C5—C7	123.8 (5)	C14—C13—H13	121.0
C4—C5—C7	116.6 (5)	C9—C14—C13	121.1 (6)
O1—C6—C1	119.1 (5)	C9—C14—H14	119.5
O1—C6—C5	123.9 (5)	C13—C14—H14	119.5
C1—C6—C5	117.0 (5)		

O1^{i}—Co1—O1—C6	143.4 (4)	C4—C5—C6—O1	178.6 (5)
N1—Co1—O1—C6	24.7 (4)	C7—C5—C6—O1	−4.6 (8)
N1^{i}—Co1—O1—C6	−101.1 (4)	C4—C5—C6—C1	−3.2 (7)

O1—Co1—N1—C7	−18.8 (5)	C7—C5—C6—C1	173.6 (5)
O1^{i}—Co1—N1—C7	−166.3 (5)	C8—N1—C7—C5	−171.0 (6)
N1^{i}—Co1—N1—C7	90.3 (5)	Co1—N1—C7—C5	5.6 (9)
O1—Co1—N1—C8	157.8 (4)	C6—C5—C7—N1	10.5 (10)
O1^{i}—Co1—N1—C8	10.2 (5)	C4—C5—C7—N1	−172.7 (6)
N1^{i}—Co1—N1—C8	−93.1 (4)	C7—N1—C8—C9	−124.3 (6)
C6—C1—C2—C3	−1.7 (9)	Co1—N1—C8—C9	59.1 (7)
Br1—C1—C2—C3	−177.1 (4)	N1—C8—C9—C14	−140.6 (6)
C1—C2—C3—C4	−0.9 (9)	N1—C8—C9—C10	41.5 (8)
C1—C2—C3—Br2	177.8 (4)	C14—C9—C10—C11	0.0 (10)
C2—C3—C4—C5	1.3 (9)	C8—C9—C10—C11	178.0 (7)
Br2—C3—C4—C5	−177.4 (4)	C9—C10—C11—C12	−0.2 (13)
C3—C4—C5—C6	0.8 (8)	C10—C11—C12—C13	−0.6 (13)
C3—C4—C5—C7	−176.2 (5)	C10—C11—C12—F1	179.6 (7)
Co1—O1—C6—C1	164.8 (4)	C11—C12—C13—C14	1.4 (11)
Co1—O1—C6—C5	−17.0 (7)	F1—C12—C13—C14	−178.8 (6)
C2—C1—C6—O1	−178.0 (5)	C10—C9—C14—C13	0.9 (9)
Br1—C1—C6—O1	−2.5 (7)	C8—C9—C14—C13	−177.1 (6)
C2—C1—C6—C5	3.7 (8)	C12—C13—C14—C9	−1.5 (9)
Br1—C1—C6—C5	179.2 (4)		

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