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trans-Bis[*N*-(4-bromophenyl)salicylaldiminato]cobalt(II)

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(*Received 11 October 1994; accepted 25 August 1995*)

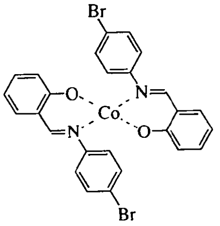
Abstract

In the title compound, *trans*-bis[2-(4-bromophenyliminomethyl)phenolato-*N*,*O*]cobalt(II), [Co($C_{13}H_9$BrNO)$_2$], the Co atom is situated on a twofold axis and the geometry around the metal centre can be described as distorted tetrahedral with a *trans* conformation. The Co—O and Co—N bond lengths are 1.891 (3) and 2.006 (4) Å, respectively.

Comment

Because of their preparative accessibility and structural variability a great number of Schiff base complexes of cobalt have been subject to extensive studies. Tetracoordinate Schiff base metal complexes may form *trans* and *cis* planar or tetrahedral structures. A strictly planar or slightly distorted *trans* configuration is characteristic for transition metal complexes of cobalt(II) with a CoN_2O_2 coordination sphere (Garnovskii, Nivorozhkin & Minkin, 1993). Structural and molecular properties of related Co^{II} complexes have been reported (Hennig, 1971; Panova, Vikulova & Popotov, 1980; Kogan, Kharabov, Osipov & Kochin, 1981).

In the course of a systematic investigation of the coordination spheres of Co^{II} in Schiff base complexes the structure of the title complex, (I), formed by the reaction of *N*-(4-bromophenyl)salicylaldimine with cobalt(II) acetate, was determined.



(I)

The Co atom lies on a twofold axis and is coordinated by two O and two N atoms. The distortion from idealized geometry is due to the O1—Co—N1 angle of 96.75 (4)°, which is smaller than the O1—Co—N1 angle of 111.59 (14)°. The Co—O and Co—N distances found in the structure agree with the values in other tetrahedral complexes.

The phenyl rings show small distortions from ideal geometry, with the C—C distances for the phenyl rings close to the expected value for aromatic rings [1.394 (5) Å; Sutton, 1965]. The bond lengths between the N1 and C1 atoms are typical of C═N double-bond lengths [1.287 (6) Å]. The bond lengths Br1—C11 of 1.892 (5), O1—C3 of 1.319 (5) and N1—C8 of 1.428 (6) Å are within expected ranges.

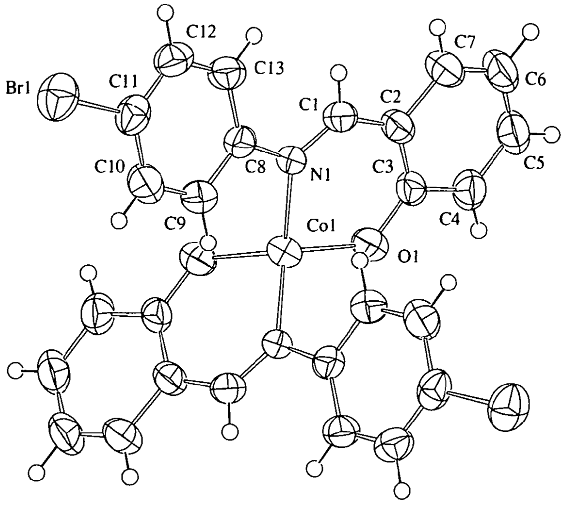


Fig. 1. *ORTEP* view (Johnson, 1965) of the molecular structure of the title compound. Displacement ellipsoids are plotted at the 50% probability level.

Experimental

0.5 mmol of [Co(AcO)$_2$].4H_2O in methanol was added to 1.0 mmol of *N*-(4-bromophenyl)salicylaldimine in acetonitrile with stirring and heating. The mixture was refluxed for 6 h. The red crystals that formed were washed twice with ethanol.

Crystal data

$[Co(C_{13}H_9BrNO)_2]$
$M_r = 609.18$
Monoclinic
$C2/c$
$a = 21.839\ (9)$ Å
$b = 8.995\ (5)$ Å
$c = 11.823\ (5)$ Å
$\beta = 95.91\ (4)°$
$V = 2310.2\ (2)$ Å^3
$Z = 4$
$D_x = 1.751$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71069$ Å
Cell parameters from 24 reflections
$\theta = 7.26–19.05°$
$\mu = 4.229$ mm^{-1}
$T = 298\ (2)$ K
Prism
0.20 × 0.15 × 0.05 mm
Red

Data collection

Stoe Stadi4 four-circle diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North, Phillips & Mathews, 1968)
$T_{min} = 0.59$, $T_{max} = 0.99$
3385 measured reflections
1604 independent reflections

1210 observed reflections $[I > 2\sigma(I)]$
$R_{int} = 0.0341$
$\theta_{max} = 23.02°$
$h = -24 \rightarrow 24$
$k = 0 \rightarrow 9$
$l = -13 \rightarrow 13$
3 standard reflections frequency: 120 min intensity decay: 0.9%

Refinement

Refinement on F^2
$R(F) = 0.0334$
$wR(F^2) = 0.0924$
$S = 1.057$
1603 reflections
150 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0420P)^2 + 3.6412P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.366$ e Å^{-3}
$\Delta\rho_{min} = -0.321$ e Å^{-3}
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2)*

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
Co	0	0.51515 (10)	1/4	0.0484 (3)
Br1	−0.15744 (3)	1.07167 (7)	−0.10946 (5)	0.0717 (2)
N1	0.0262 (2)	0.6253 (4)	0.1155 (3)	0.0406 (9)
O1	0.07476 (14)	0.4118 (4)	0.2873 (3)	0.0542 (9)
C1	0.0776 (2)	0.5921 (5)	0.0775 (4)	0.048 (1)
C2	0.1242 (2)	0.4912 (5)	0.1241 (4)	0.047 (1)
C3	0.1219 (2)	0.4070 (5)	0.2259 (4)	0.046 (1)
C4	0.1711 (2)	0.3130 (6)	0.2608 (4)	0.056 (1)
C5	0.2211 (2)	0.2993 (7)	0.1986 (5)	0.065 (2)
C6	0.2235 (2)	0.3826 (7)	0.0995 (5)	0.071 (2)
C7	0.1767 (2)	0.4750 (6)	0.0645 (5)	0.061 (1)
C8	−0.0137 (2)	0.7336 (5)	0.0588 (4)	0.044 (1)
C9	−0.0602 (2)	0.7914 (6)	0.1193 (4)	0.055 (1)
C10	−0.1021 (2)	0.8928 (6)	0.0698 (5)	0.060 (1)
C11	−0.0979 (2)	0.9379 (5)	−0.0408 (4)	0.053 (1)
C12	−0.0518 (2)	0.8844 (5)	−0.1008 (4)	0.053 (1)
C13	−0.0101 (2)	0.7835 (5)	−0.0513 (4)	0.050 (1)

Table 2. *Selected geometric parameters (Å, °)*

Co—O1	1.891 (3)	C4—C5	1.383 (7)
Co—N1	2.006 (4)	C5—C6	1.396 (8)
Br1—C11	1.892 (5)	C6—C7	1.348 (8)
N1—C1	1.287 (6)	C8—C13	1.387 (6)
N1—C8	1.428 (6)	C8—C9	1.401 (7)
O1—C3	1.319 (5)	C9—C10	1.379 (7)
C1—C2	1.431 (7)	C10—C11	1.380 (7)
C2—C7	1.414 (6)	C11—C12	1.377 (7)
C2—C3	1.427 (7)	C12—C13	1.374 (7)
C3—C4	1.396 (6)		
O1^i—Co—O1	121.1 (2)	N1—C1—C2	128.6 (4)
O1—Co—N1^i	111.59 (14)	O1—C3—C4	118.6 (4)
O1—Co—N1	96.75 (14)	O1—C3—C2	122.9 (4)
N1^i—Co—N1	120.8 (2)	C13—C8—N1	124.8 (4)
C1—N1—C8	120.4 (4)	C9—C8—N1	116.9 (4)
C1—N1—Co1	119.5 (3)	C12—C11—Br1	120.5 (4)
C8—N1—Co1	119.9 (3)	C10—C11—Br1	119.0 (4)
C3—O1—Co1	126.3 (3)		

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

All the phenyl rings were refined without constraints. Values of the distances and angles in the rings show no significant differences from those of an ideal benzene ring. H atoms were positioned geometrically.

Data collection: *DIF*4 (Stoe & Cie, 1991*a*). Cell refinement: *DIF*4. Data reduction: *REDU*4 (Stoe & Cie, 1991*b*). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *Xtal*3.2 (Hall, Flack & Stewart, 1992). Software used to prepare material for publication: *SHELXL*93.

AE is grateful to the Scientific and Technical Research Council of Turkey (TUBITAK) and the Deutsche Forschungsgemeinschaft (DFG) for support.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: AB1229). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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