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Dichlorobis(*trans*-2-styrylbenzoxazole-κ^2N,N')-cobalt(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.011 Å
R factor = 0.052
wR factor = 0.216
Data-to-parameter ratio = 13.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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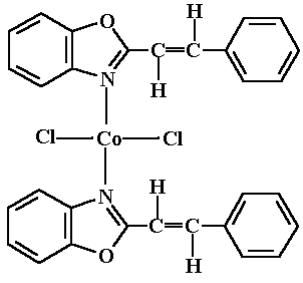
The title complex, $[CoCl_2(C_{15}H_{11}NO)_2]$, crystallizes in the monoclinic system in space group $P2_1/c$. The Co atom is four-coordinated by two Cl^- anions and two N atoms of two *trans*-2-styrylbenzoxazole ligands. The coordination sphere displays a slightly distorted tetrahedral geometry. The coordination angles lie in the range 100.5 (2)–113.7 (2)°. The dihedral angles between the benzoxazolyl and phenyl planes are 6.7 (5) and 25.0 (8)° for the two ligands.

Comment

Derivatives of *trans*-2-styrylbenzoxazole (BOEP) are used extensively as optical whitening agents and laser dyes (Rehák *et al.*, 1985), as well as bacteriostats and tranquilizers (Zhou & Zhao, 1990). Most studies on these compounds have focused on the synthesis and photo-properties (Zhou & Zhao, 1990; Zhang *et al.*, 2000). However, studies on the coordination with transition metals are still rare. It is reported that two platinum(II) complexes, *viz*. $NEt_4[PtBr_3$(2-hydroxystyrylbenzothiazole)] and $NEt_4[PtBr_3$(BOEP)], show excellent cytotoxic activity against CHO-K cells *in vitro* (Muir *et al.*, 1988) and U937 human histiocytic lymphoma cells (Lozano *et al.*, 1998), respectively. We report herein the crystal structure of the cobalt(II) complex $CoCl_2(BOEP)_2$, (I).



(I)

The title compound is a neutral complex. The Co^{II} cation is coordinated by two Cl^- anions and two N atoms from the benzoxazolyl groups of two BOEP ligands. The dihedral angle between the N1/Co1/N2 and Cl1/Co1/Cl2 planes is 86.7 (2)°, which shows that the Co cation is situated in a slightly distorted tetrahedral coordination geometry. According to a reported X-ray structure, three *trans*-1,2-bis(4-pyridyl)ethylene ligands are coordinated to one Co^{II} cation in a monodentate mode to form a T-shaped complex (Jung *et al.*, 1998). However, the steric effect of the N atom of the benzoxazolyl group is too large to give a high coordination number for the Co center, resulting in the title complex with two Cl^- anions and two BOEP ligands.

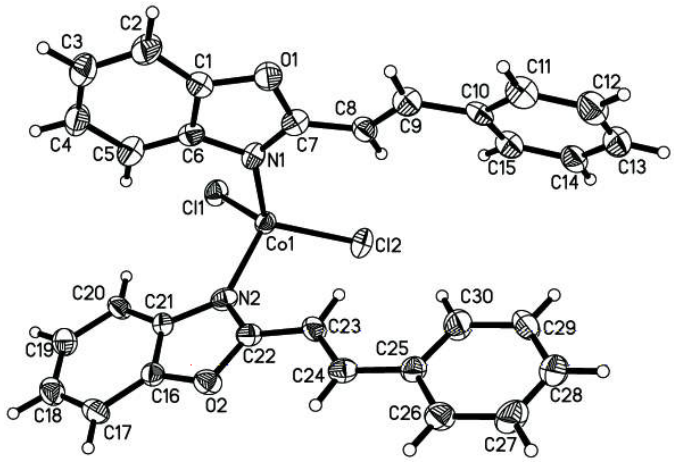


Figure 1
The molecular structure of the title compound, with displacement ellipsoids at the 50% probability level. H atoms are shown as small spheres of arbitrary radii.

The Co1—Cl1 and Co1—Cl2 bond distances are 2.206 (2) and 2.217 (3) Å, and those of Co1—N1 and Co1—N2 are 2.028 (5) and 2.050 (5) Å, respectively; these are similar to the corresponding Co—Cl (2.230 Å) and Co—N (2.023 Å) distances in $CoCl_2$(PPP), where PPP is 2,2′-(2,5-diphenyl-3,4-pyrroldiyl)dipyridine (Viossat *et al.*, 1994). The angles C6—N1—C7 and C21—N2—C22 are 105.6 (5) and 104.8 (5)°, respectively, near to the value of 104.5 (3)° in 2-(2-chloro-5-nitrostyryl)benzoxazole (Muir *et al.*, 1992).

Fig. 1 shows that each BOEP ligand retains a *trans* configuration. The two benzoxazolyl planes of the two ligands are almost perpendicular to each other, subtending a dihedral angle of 87.3°. The BOEP ligands in the complex are non-planar. The dihedral angles between the benzoxazolyl and phenyl planes in the two ligands are 25.0 (8) and 6.7 (5)°. The latter is the same [6.7(2)°] as between the benzothiazolyl and chlorophenyl planes in the $[Pt(CSB)Br_3]^-$ anion, where CSB is 2-(2-chlorostyryl)benzothiazole (Muir *et al.*, 1990). With regard to the unexpected significant difference between the planarity of the two BOEP ligands, it is presumed that this difference is attributed principally to packing forces. From the packing diagram, viewed along the *a* axis (Fig. 2), it can be seen that there are no π-stacking interactions between aromatic rings of the ligand molecules.

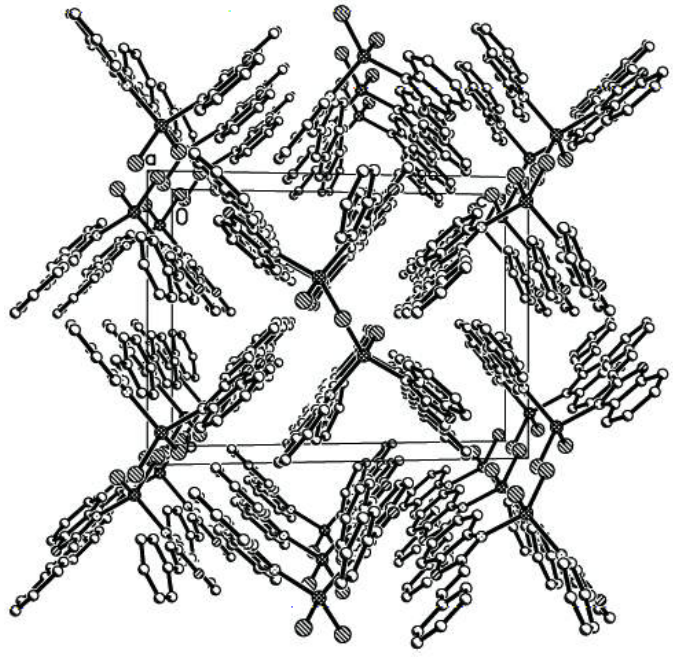


Figure 2
A packing diagram, viewed along the *a* axis.

Experimental

The ligand *trans*-2-styrylbenzoxazole (BOEP) was synthesized according to the literature (Zhang *et al.*, 2000). BOEP (2 mmol) and $CoCl_2$ (1 mmol) were added to 20 ml of acetonitrile. The reaction mixture was stirred at room temperature for 30 min. The blue precipitate was filtered off and dissolved in 60 ml of hot acetonitrile. A single crystal of the title compound, suitable for X-ray analysis, was grown by slow evaporation of the solvent (m.p. 521–523 K). IR (KBr): 1635 (*vs*), 1519 (*s*), 1457 (*s*), 1373 (*s*), 1245(*s*), 1175 (*m*), 1011 (*m*), 977 (*s*), 762 (*s*), 738 (*s*), 711 (*m*), 685 (*m*) cm^{-1}.

Crystal data

$[CoCl_2(C_{15}H_{11}NO)_2]$	D_x = 1.443 Mg m^{-3}
M_r = 572.33	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 2651 reflections
a = 14.607 (18) Å	θ = 2.3–24.5°
b = 11.679 (15) Å	μ = 0.89 mm^{-1}
c = 16.20 (2) Å	T = 293 (2) K
β = 107.57 (2)°	Prism, blue
V = 2635 (6) $Å^3$	0.30 × 0.25 × 0.20 mm
Z = 4	

Data collection

Bruker CCD area-detector diffractometer	4581 independent reflections
φ and ω scans	2522 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)	R_{int} = 0.071
T_{min} = 0.777, T_{max} = 0.843	θ_{max} = 25.0°
9394 measured reflections	$h = -14 \rightarrow 17$
	$k = -13 \rightarrow 13$
	$l = -19 \rightarrow 8$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.052	$w = 1/[\sigma^2(F_o^2) + (0.1325P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.216	$(\Delta/\sigma)_{max} < 0.001$
S = 0.96	$\Delta\rho_{max}$ = 0.60 e $Å^{-3}$
4581 reflections	$\Delta\rho_{min}$ = −0.82 e $Å^{-3}$
334 parameters	

Table 1
Selected geometric parameters (Å, °).

Co1—N1	2.028 (5)	N1—C7	1.311 (8)
Co1—N2	2.050 (5)	N1—C6	1.410 (8)
Co1—Cl1	2.206 (2)	N2—C22	1.317 (7)
Co1—Cl2	2.217 (3)	N2—C21	1.417 (8)
N1—Co1—N2	100.5 (2)	N2—Co1—Cl2	109.81 (16)
N1—Co1—Cl1	107.38 (16)	Cl1—Co1—Cl2	112.45 (10)
N2—Co1—Cl1	112.44 (17)	C7—N1—C6	105.6 (5)
N1—Co1—Cl2	113.74 (17)	C22—N2—C21	104.8 (5)

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1997) and *SHELXTL* (Bruker, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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