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trans-Dichlorobis{2-[2-(4-methoxyphenyl)-ethenyl]-5-methyl-1,3-benzoxazole-κN}cobalt(II)

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Key indicators

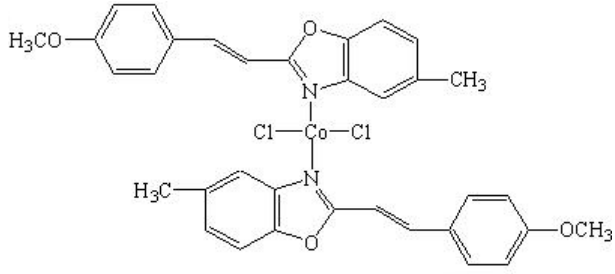
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.050
wR factor = 0.121
Data-to-parameter ratio = 16.9

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

The title complex, $[CoCl_2(C_{17}H_{15}NO_2)_2]$, has twofold rotation symmetry, and the geometry at the Co centre is a slightly distorted tetrahedron composed of two N atoms from two *trans*-2-[2-(4-methoxyphenyl)ethenyl]-5-methylbenzoxazole ligands and two Cl^- anions. The two organic ligands are arranged in reverse directions to give a head-to-tail structure. The two benzoxazole planes of these two ligands are almost perpendicular to each other, with a dihedral angle of 86.4 (4)°, while the corresponding angle for the two methoxyphenyl planes is 74.5 (4)°.

Comment

Photodimerization of 1,2-bisarylethenes under ultraviolet light is a classical method for the preparation of cyclobutane derivatives, and the photochemistry of *trans*-2-styryl-benzoxazole (BOEP) and its analogues has been extensively investigated in previous work by us (Zhuang & Zhang, 2003; Zhang *et al.*, 2002). It has also been found that BOEP derivatives are good candidates for coordination with transition metals *via* their N donors, and the resulting complexes exhibit excellent cytotoxic activity against CHO-K cells *in vitro* (Muir *et al.*, 1988). However, the crystal structures of such complexes have only rarely been reported (Liu *et al.*, 2002; Lozano *et al.*, 1998). In the present work, *trans*-2-[2-(4-methoxyphenyl)-ethenyl]-5-methylbenzoxazole (MeBOEP-OMe) has been synthesized and its complex with Co^{II}, (I), is reported here. The photochemical properties of coordinated MeBOEP-OMe are still under investigation.



(I)

The crystal structure of (I) is illustrated in Fig. 1. The molecule has crystallographic twofold rotation symmetry, and the geometry at the Co^{II} centre is a distorted tetrahedron composed of two N atoms from two MeBOEP-OMe ligands and two Cl^- anions. The dihedral angle between the Cl1—Co1—Cl1^{i} and N1—Co1—N1^{i} planes (symmetry codes in Table 1) is 87.1 (3)°. The two ligands are arranged in reverse directions to give a head-to-tail structure, rather than the

head-to-head structure observed in dichlorobis(*trans*-2-styrylbenzoxazole-κ^2N,N′)cobalt(II) (Liu *et al.*, 2002). The two benzoxazole planes of the two ligands are almost perpendicular to each other, subtending a dihedral angle of 86.4 (4)°, while the dihedral angle between the two methoxyphenyl planes is 74.5 (4)°. The dihedral angle between the benzoxazole and methoxyphenyl planes within the ligand is 7.3 (3)°, which is slightly larger than that between the benzothiazole and chlorophenyl planes in the $[Pt(CSB)Br_3]^-$ anion [CSB is 2-(2-chlorostyryl)benzothiazole; Muir *et al.*, 1990].

Experimental

The MeBOEP-OMe ligand was synthesized according to the method of Zhang *et al.* (2000). MeBOEP-OMe (2 mmol) in acetonitrile (10 ml) and $CoCl_2$ (1 mmol) in acetonitrile (10 ml) were mixed and stirred at room temperature for 30 min. The mixture was then filtered and the filtrate was allowed to evaporate slowly at ambient temperature to give single crystals of (I) suitable for X-ray analysis (m.p. 463–464 K).

Crystal data

$[CoCl_2(C_{17}H_{15}NO_2)_2]$	D_x = 1.360 Mg m^{-3}
M_r = 660.43	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 899 reflections
a = 15.172 (4) Å	θ = 2.3–21.8°
b = 12.218 (3) Å	μ = 0.74 mm^{-1}
c = 18.153 (5) Å	T = 293 (2) K
β = 106.603 (5)°	Prism, blue
V = 3225.0 (16) Å^3	0.22 × 0.18 × 0.14 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	3308 independent reflections
	1948 reflections with $I > 2\sigma(I)$
φ and ω scans	R_{int} = 0.048
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)	θ_{max} = 26.4°
	$h = -18 \rightarrow 7$
T_{min} = 0.852, T_{max} = 0.899	$k = -15 \rightarrow 15$
9098 measured reflections	$l = -22 \rightarrow 22$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0515P)^2 + 0.9349P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.050	
$wR(F^2)$ = 0.121	
S = 1.01	$(\Delta/\sigma)_{max} < 0.001$
3308 reflections	$\Delta\rho_{max}$ = 0.22 e Å^{-3}
196 parameters	$\Delta\rho_{min}$ = −0.24 e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Co1—N1	2.047 (2)	Co1—Cl1	2.2279 (10)
N1—Co1—N1^{i}	100.08 (14)	N1—Co1—Cl1	111.36 (7)
N1—Co1—Cl1^{i}	107.27 (7)	Cl1^{i}—Co1—Cl1	118.04 (6)

Symmetry code: (i) $1-x, y, \frac{3}{2}-z$.

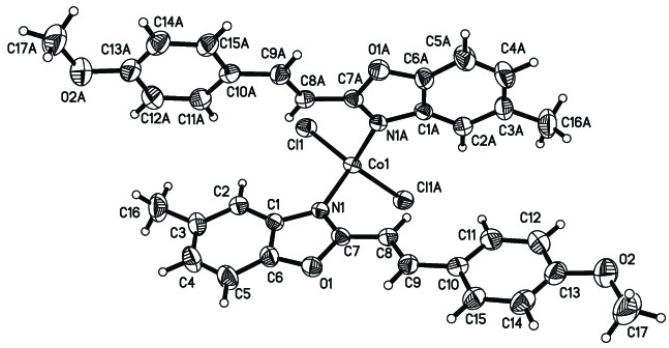


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids. The suffix A corresponds to symmetry code i in Table 1.

The H atoms were included in calculated positions and refined with riding-model constraints.

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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