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{*N*,*N*′-Bis[3-(2-nitrophenyl)allylidene]ethane-1,2-diamine-κ^2N,N'}dichlorocobalt(II)

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.007 Å
R factor = 0.066
wR factor = 0.176
Data-to-parameter ratio = 16.5

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

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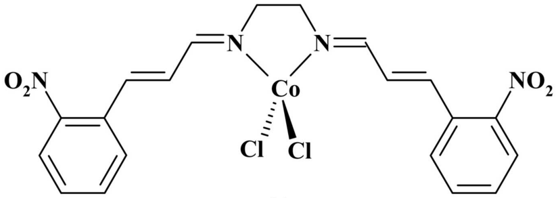
In the title complex, $[CoCl_2(C_{20}H_{18}N_4O_4)_2]$, the Co^{II} atom has a distorted tetrahedral coordination. The organic ligand is bidentate, coordinating the Co^{II} atom *via* two imine N atoms.

Comment

Transition metal complexes with Schiff base ligands have attracted substantial interest for many years (Yamada, 1999). These complexes play an important role in the study of coordination compounds related to catalysis and enzymatic reactions, magnetism and molecular architectures (Costamagna *et al.*, 1992). One aspect of transition-metal chemistry that makes it attractive in this context is the geometric, electronic and structural diversity that can be achieved by synthetic means. The title complex, (I), was prepared by the reaction of $CoCl_2$ with the bidentate ligand *N*,*N*′-bis[3-(2-nitrophenyl)allylidene]ethane-1,2-diamine (nca$_2$en).



(I)

The molecular structure of complex (I) and the atom-numbering scheme are shown in Fig. 1. The metal centre has a tetrahedral coordination which shows signficant distortion, mainly due to the presence of the five-membered chelate ring (Table 1): the endocyclic N1—Co1—N2 angle is much narrower than the ideal tetrahedral angle of 109.5°, whereas the opposite Cl1—Co1—Cl2 angle is much wider than the ideal tetrahedral angle. The Co1—Cl1 and Co1—Cl2 bond lengths are in good agreement with Co—Cl distances in other tetrahedral cobalt complexes, *e.g.* 2.229 (3) Å in Co(ethylenedimorpholine)Cl$_2$ (Scheidt *et al.*, 1969), and 2.2434 (8) and 2.2266 (8) Å in Co[*N*,*N*-bis(3,5-dimethylpyrazol-1-ylmethyl)-aminobenzene]Cl$_2$ (Blonk *et al.*, 1985).

The dimethylene group in the chelate ring of (I) is non-planar, the N1—C4—C5—N2 torsion angle being −48.4 (5). Each of the flanking azadiene fragments adopts a roughly planar *transoid* conformation, with torsion angles N1═C3—C2═C1 and N2═C6—C7═C8 of 174.6 (5) and 179.4 (5)°, respectively; their planes form a dihedral angle of 29.3 (5)° with each other.

π-Conjugation within the azadiene fragments is consistent with the observed pattern of C—C bond distances; the

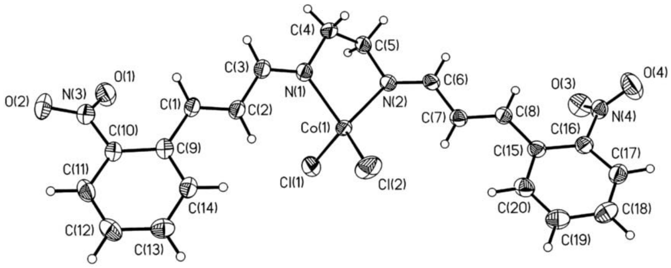


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

predominantly double C1═C2 and C7═C8 bonds are substantially shorter than the C2—C3 and C6—C7 bonds, which have a significant π-component; the latter bonds in their turn are much shorter than the single C4—C5 bond in the dimethylene bridge.

Experimental

Anhydrous $CoCl_2$ (12.9 mg, 0.1 mmol) was added to a solution of *N*,*N*′-bis[3-(2-nitrophenyl)allylidene]ethane-1,2-diamine (37.8 mg, 0.1 mmol) in CH_2Cl_2 (10 ml) and stirred at room temperature for 3 h under a nitrogen atmosphere. The reaction mixture was filtered and the volume of the solvent was reduced under vacuum to about 1 ml. The diffusion of diethyl ether vapour into the concentrated solution gave blue crystals of (I) suitable for X-ray study. The crystals were filtered off, washed with a mixture of diethyl ether and dichloromethane (9:1 *v*/*v*) and dried *in vacuo* (yield 80%). Analysis calculated for $C_{20}H_{18}Cl_2CoN_4O_4$: C 47.26, H 3.54, N 11.02%; found: C 47.25, H 3.55, N 11.01%.

Crystal data

$[CoCl_2(C_{20}H_{18}N_4O_4)]$
$M_r = 508.21$
Monoclinic, $P2_1/n$
$a = 7.8387$ (16) Å
$b = 16.048$ (3) Å
$c = 17.633$ (4) Å
$\beta = 100.27$ (3)°
$V = 2182.6$ (8) Å^3
$Z = 4$
$D_x = 1.547$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.07$ mm^{-1}
$T = 173$ (2) K
Prism, blue
0.20 × 0.15 × 0.10 mm

Data collection

Upgraded Syntex $P2_1$/Siemens $P3$ four-circle diffractometer
ω scans
Absorption correction: none
4931 measured reflections
4627 independent reflections
2974 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.059$
$\theta_{\rm max} = 27.0°$
2 standard reflections every 98 reflections intensity decay: 1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.066$
$wR(F^2) = 0.176$
$S = 1.01$
4627 reflections
280 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.096P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.001$
$\Delta\rho_{\rm max} = 0.58$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.63$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—N1	2.042 (4)	C2—C3	1.446 (6)
Co1—N2	2.022 (3)	C4—C5	1.528 (7)
Co1—Cl1	2.2335 (16)	C6—C7	1.434 (6)
Co1—Cl2	2.2233 (15)	C7—C8	1.337 (6)
C1—C2	1.344 (6)		
N2—Co1—N1	83.30 (14)	N2—Co1—Cl1	114.26 (12)
N2—Co1—Cl2	114.29 (12)	N1—Co1—Cl1	107.07 (12)
N1—Co1—Cl2	117.06 (12)	Cl2—Co1—Cl1	116.37 (6)

All H atoms were placed in calculated positions and refined using a riding-model approximation, with C—H = 0.95–0.99 Å and with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C).

Data collection: *P3*/*PC* (Siemens, 1989); cell refinement: *P3*/*PC*; data reduction: *P3*/*PC*; program(s) used to solve structure: *SHELXTL-Plus* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL-Plus*; molecular graphics: *SHELXTL-Plus*; software used to prepare material for publication: *SHELXTL-Plus*.

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Acta Cryst. (2006). E**62**, m1342–m1343 Dehghanpour *et al.* • $[CoCl_2(C_{20}H_{18}N_4O_4)]$ **m1343**