Dichlorobis{2-[(triphenylmethyl)amino]pyridyl}-cobalt(II)

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In the title compound, $[CoCl_2(C_{24}H_{20}N_2)_2]$, Co^{II} is coordinated in an approximately tetrahedral geometry by two Cl atoms and two N atoms of the pyridine rings from two 2-[(triphenylmethyl)imino]pyridyl ligands.

Comment

Transition metal complexes have attracted interest because of their useful properties, such as microporosity, molecular magnetism or linear optical behavior. The title compound, (I) (Fig. 1), is a Co^{II} complex of the N-donor ligand 2-[N-(triphenylmethyl)imino]pyridyl. The complex exhibits approximate C_2 point symmetry, and the Co^{II} atom is coordinated in a slightly distorted tetrahedral geometry by atoms Cl1, Cl2, N1 and N2 (Table 1). The dihedral angle between the two pyridyl rings directly coordinated to Co^{II} is 109.8 (1)°. The formation of a four-coordinate complex, rather than a possible six-coordinate one, is attributed to the large volume of the 2-[N-(triphenylmethyl)imino]pyridyl ligand.

(I)
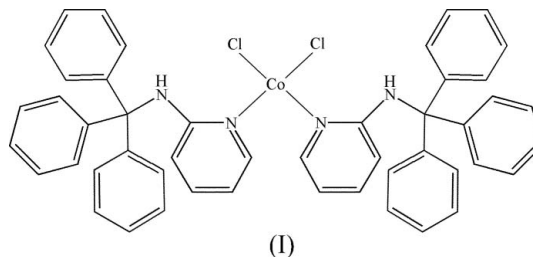
Experimental

In a 100 ml round-bottomed flask, 2-[N-(triphenyl)imino]pyridine (0.672 g, 2 mmol) was dissolved in THF (20 ml), and then $CoCl_2$
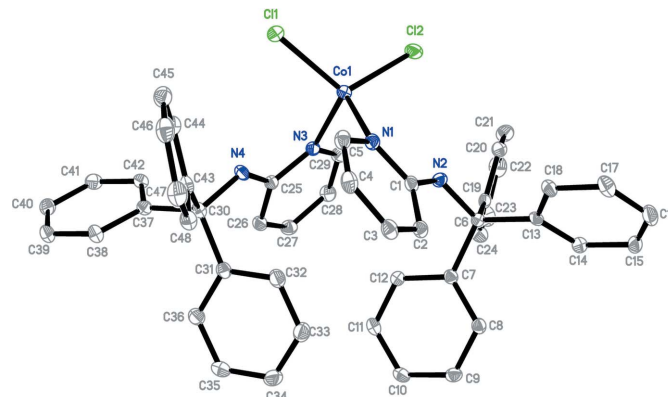
Figure 1
Molecular structure of (I), showing displacement ellipsoids at the 30% probability level. H atoms have been omitted.

metal-organic papers

(0.13 g, 1 mmol) was added to the solution. The solution was refluxed for 6 h and then stirred overnight. The THF was removed under vacuum and the residue was dissolved in CH_2Cl_2 (20 ml). The filtrate was layered with hexane (20 ml), and blue crystals were obtained after one week. All manipulations were carried out under an atmosphere of Ar gas.

Crystal data

$[CoCl_2(C_{24}H_{20}N_2)_2]$
$M_r = 802.67$
Monoclinic, $P2_1/n$
$a = 9.920 (2)$ Å
$b = 22.620 (5)$ Å
$c = 17.460 (4)$ Å
$\beta = 97.36 (3)°$
$V = 3885.6 (15)$ Å^3

$Z = 4$
$D_x = 1.372$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.62$ mm^{-1}
$T = 150 (2)$ K
Block, blue
$0.35 \times 0.34 \times 0.30$ mm

Data collection

Bruker APEXII CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{min} = 0.812$, $T_{max} = 0.836$

25600 measured reflections
6823 independent reflections
5433 reflections with $I > 2\sigma(I)$
$R_{int} = 0.081$
$\theta_{max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.098$
$S = 1.02$
6823 reflections
496 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.039P)^2 + 2.5598P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.69$ e Å^{-3}
$\Delta\rho_{min} = -0.52$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—Cl1	2.2415 (8)	Co1—N1	2.054 (2)
Co1—Cl2	2.2394 (8)	Co1—N3	2.0510 (18)
Cl1—Co1—Cl2	114.53 (3)	Cl2—Co1—N1	110.63 (6)
Cl1—Co1—N1	110.26 (6)	Cl2—Co1—N3	109.08 (6)
Cl1—Co1—N3	109.41 (6)	N1—Co1—N3	102.21 (8)

All H atoms were placed in calculated positions and allowed to ride during subsequent refinement, with C—H = 0.95 Å, N—H = 0.88 Å, and $U_{iso}(H) = 1.2U_{eq}(C,N)$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

References

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