Data collection: *DIF*4 (Stoe & Cie, 1992*a*). Cell refinement: *DIF*4. Data reduction: *REDU*4 (Stoe & Cie, 1992*b*). Program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*b*). Program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*). Molecular graphics: *XP* in *SHELXTL/PC* (Sheldrick, 1994) and *CAMERON* (Pearce *et al.*, 1993). Software used to prepare material for publication: *SHELXL*97.

The authors would like to thank Shin-Etsu Chemical Co. Ltd for granting study leave to MK, the EPSRC and Zeneca Specialties for funding (AB), and Dr Neil Feeder for assistance.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: CF1309). Services for accessing these data are described at the back of the journal.

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Acta Cryst. (1999). C**55**, 1262–1263

Dichlorobis(1-methyl-1*H*-benzimidazole-*N*³)-cobalt(II)

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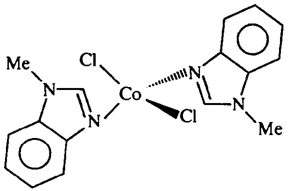
(*Received 13 July 1998; accepted 6 April 1999*)

Abstract

The metal atom in the title complex, $[CoCl_2(C_8H_8N_2)_2]$, has a slightly distorted tetrahedral coordination involving two Cl^- ions and two N atoms from the aromatic groups. The dihedral angle between the planes of the two 1-methylbenzimidazole ligands is 117.7 (7)°.

Comment

Benzimidazoles are an important class of compounds in biological systems and in coordination chemistry. This fused two-ring system occurs in many biologically active compounds, such as antinematodal and antitumor drugs. It also appears to bind to cobalt in vitamin B12. Metal complexes with benzimidazoles have been investigated in the search for new modes of biological activity (Allan *et al.*, 1981; Golič & Mirčeva, 1988). In order to investigate the role of the 1-alkyl substituent of benzimidazole in the coordinating behavior of this ligand, we have synthesized Co^{II} complexes of the type $CoX_2(L_2)$, where $X = Cl^-$ or NO_3^- and L = 1-methylbenzimidazole, 1,2-dimethylbenzimidazole, 1-isopropyl-2-methylbenzimidazole or 2-methyl-1-propenylbenzimidazole. In addition, the effect of the 1-alkyl group upon the donor and acceptor ability of benzimidazole is of special interest with regard to the electrochemical properties of the Co^{II} complexes. The title compound, (I), has been synthesized as a simple model for complexes with increased steric hindrance in the vicinity of the coordinating N atom of benzimidazole.



(I)

The X-ray crystallographic analysis of (I) revealed that the Co^{II} ion has a slightly distorted tetrahedral coordination, involving two Cl^- ions and two N atoms

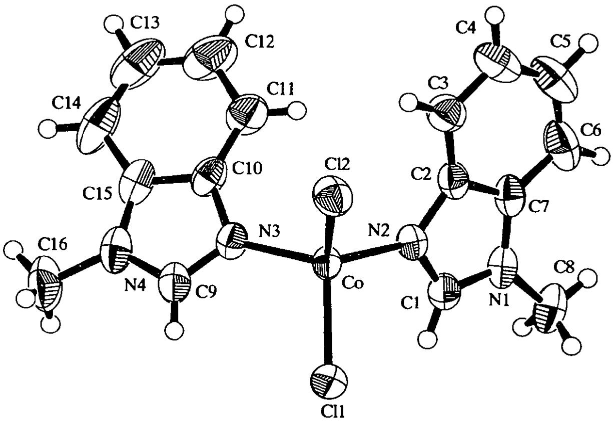


Fig. 1. An *ORTEP* (Johnson, 1965) representation of the title compound, showing the atom-numbering scheme and 50% probability displacement ellipsoids. H atoms are drawn as spheres of arbitrary radii.

from the two 1-methylbenzimidazole molecules. Both aromatic 1-methylbenzimidazcle groups are planar, with a mean deviation from the plane of 0.010 (9) Å for the plane formed by C1–C7, N1 and N2, and a mean deviation of 0.013 (6) Å for the plane formed by C9–C15, N3 and N4. The dihedral angle between these two planes is 117.7 (7)°. The Co—Cl and Co—N bond distances signify normal single bonds, and are comparable with those found in dichlorobis(quinoline-*N*)cobalt(II) (Golič & Mirčeva, 1988) and dichlorobis(2-methoxypyridine)cobalt(II) (Allan *et al.*, 1981). Because of the comparable crystal field splitting energies (CFSE) for the Co^{2+} ion (d^7) in both the octahedral and tetrahedral geometries, the adoption of either coordination is possible. In the current synthesis, no evidence was found for the presence of the octahedral complex.

Experimental

The detailed synthesis of the title compound will be published elsewhere in due course. Slow evaporation of an ethanol solution of the compound at room temperature afforded deep-blue single crystals of X-ray quality.

Crystal data

$[CoCl_2(C_8H_8N_2)_2]$
$M_r = 394.17$
Monoclinic
$P2_1/c$
$a = 11.3231\ (7)$ Å
$b = 11.3446\ (7)$ Å
$c = 13.9047\ (9)$ Å
$\beta = 98.676\ (1)°$
$V = 1765.7\ (2)$ Å^3
$Z = 4$
$D_x = 1.48$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.7107$ Å
Cell parameters from 6387 reflections
$\theta = 1.59–27.11°$
$\mu = 1.28$ mm^{-1}
$T = 296\ (1)$ K
Prism
0.32 × 0.30 × 0.30 mm
Blue

Data collection

Bruker SMART CCD diffractometer
ω scans
Absorption correction: empirical *via* simulated ψ scans (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.59$, $T_{max} = 0.68$
9109 measured reflections
3633 independent reflections

2446 reflections with $I > 2.5\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 27.04°$
$h = 0 \rightarrow 14$
$k = -13 \rightarrow 14$
$l = -17 \rightarrow 16$
Intensity decay: none

Refinement

Refinement on F^2
$R(F) = 0.043$
$wR(F^2) = 0.070$
$S = 1.33$
2446 reflections
208 parameters
H-atom parameters not refined

$w = 1/[\sigma^2(F_o)]$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}
Extinction correction: none
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 1. *Selected geometric parameters (Å, °)*

Co—Cl1	2.2512 (8)	N2—C2	1.401 (4)
Co—Cl2	2.2393 (9)	C2—C3	1.388 (4)
Co—N2	2.017 (2)	C2—C7	1.394 (4)
Co—N3	2.008 (2)	C3—C4	1.387 (4)
N1—C1	1.341 (4)	C4—C5	1.395 (6)
N1—C7	1.379 (4)	C5—C6	1.361 (5)
N1—C8	1.462 (4)	C6—C7	1.390 (4)
N2—C1	1.323 (4)		
Cl1—Co—Cl2	116.40 (4)	N1—C1—N2	113.3 (3)
Cl1—Co—N2	104.62 (7)	N2—C2—C3	130.5 (3)
Cl1—Co—N3	105.59 (7)	N2—C2—C7	108.6 (3)
Cl2—Co—N2	110.27 (7)	C3—C2—C7	120.8 (3)
Cl2—Co—N3	106.90 (7)	C2—C3—C4	116.6 (3)
N2—Co—N3	113.2 (1)	C3—C4—C5	121.5 (3)
C1—N1—C7	107.1 (2)	C4—C5—C6	122.4 (3)
C1—N1—C8	126.2 (3)	C5—C6—C7	116.3 (3)
C7—N1—C8	126.8 (3)	N1—C7—C2	106.1 (3)
Co—N2—C1	123.5 (2)	N1—C7—C6	131.5 (3)
Co—N2—C2	131.5 (2)	C2—C7—C6	122.3 (3)
C1—N2—C2	104.9 (2)		

The H atoms were calculated and included in the structural model, but were fixed and not refined.

Data collection: *SMART* (Siemens, 1996). Cell refinement: *SAINT* (Siemens, 1996). Data reduction: *SAINT*. Program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1993). Program(s) used to refine structure: *TEXSAN* (Molecular Structure Corporation, 1992–1997). Software used to prepare material for publication: *TEXSAN*.

This work was supported by the NSF–EPSCoR (Grant No. OSR-9452893) and the DoE-EPSCoR (DE-FC02-91ER75674). We thank the National Institutes of Health for a grant in support of the purchase of a Bruker SMART CCD diffractometer (3S06GM08102-25S1/M1HREV).

Supplementary data for this paper are available from the IUCr electronic archives (Reference: BK1432). Services for accessing these data are described at the back of the journal.

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