Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Dichlorobis(1*H*-benzimidazole-κN^3)cobalt(II)

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.004 Å
R factor = 0.037
wR factor = 0.097
Data-to-parameter ratio = 20.9

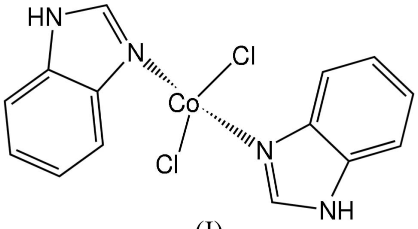
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 4 April 2005
Accepted 6 April 2005
Online 16 April 2005

The title compound, $[Co(C_7H_6N_2)_2Cl_2]$, is isostructural with the corresponding Zn complex. The metal centre is coordinated by two benzimidazole ligands and two Cl^- ions, with tetrahedral geometry.

Comment

Benzimidazole (Bz) is a classic example of a small organic molecule which has attracted considerable interest over several decades, in both the academic and industrial worlds, because of its numerous applications in several unrelated fields. First used as a fungicide in the mid 1960's, it was eventually replaced by more sophisticated molecules, due to a growing resistance phenomenon (*e.g.* Torres-Acosta *et al.*, 2003). In medicine, drugs based on Bz and derivatives have been patented, due to their antiviral and anthelmintic activity (*e.g.* Valdez *et al.*, 2002). In metallurgy, Bz has been used as a corrosion inhibitor (Khaled, 2003). Finally, coordination complexes of Bz derivatives with transition metals have been used in attempts to prepare structural and spectroscopic models of the active sites of some metalloenzymes (*e.g.* Sundberg & Martin, 1974; Hay *et al.*, 1998). Surprisingly, complexes with the very simple stoichiometry $[MBz_2X_2]$ (M is a transition metal, and X is Cl, Br or I) have been poorly studied by crystallography, probably because analytical and spectroscopic techniques allow the unambiguous determination of their formulae and coordination geometries. Single-crystal X-ray structures are available for $[CuBz_2Br_2]$ (Bukowska-Strzyzewska & Tosik, 1988, 1991), $[ZnBz_2Br_2]$ (Şahin *et al.*, 2002) and $[ZnBz_2Cl_2]$ (Şahin *et al.*, 2003). We now report the structure of $[CoBz_2Cl_2]$, (I).



(I)

The asymmetric unit of (I) contains one molecule in a general position. The metal centre presents a slightly distorted tetrahedral geometry (Fig. 1, Table 1), with the Co^{II} ion coordinated by two Bz molecules and two Cl^- anions. The oxidation state for the metal is in agreement with the magnetic moment measured for (I) at 298 K, μ = 4.41 BM. The very common mode of coordination of Bz, through the unprotonated atom N3, is confirmed by FT–IR spectroscopy: the stretching vibrations for the C═C and C═N bonds in free Bz,

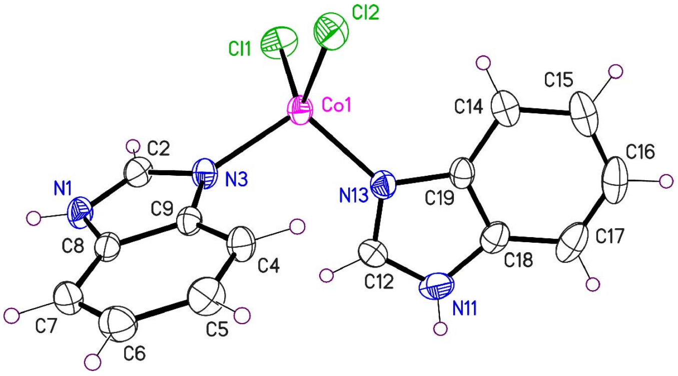


Figure 1
The structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

observed at 1619 and 1587 cm^{-1}, respectively, are shifted to 1621 and 1595 cm^{-1}, respectively, in (I).

The crystal structure of (I) is composed of a two-dimensional network of N—H···Cl hydrogen bonds of moderate strength (Fig. 2, Table 2), based on the vectors [100] and [010].

The crystal structures of (I) is identical, within experimental error, to that of [$ZnBz_2Cl_2$] (Şahin *et al.*, 2003). The decrease of 8.4 $Å^3$ observed for the cell volume when substituting Co^{II} by Zn^{II} is probably related to the radius contraction along the transition metal row. A fit carried out between (I) and [$ZnBz_2Cl_2$] (non-H atoms) gives an r.m.s deviation of 0.0184 Å. However, it should be mentioned that the fact that [$ZnBz_2Cl_2$] and [$CoBz_2Cl_2$] are found to be isostructural, even if not very surprising, should not be automatically assumed without a complete X-ray characterization. In some cases, Co^{II} and Zn^{II} complexes with equivalent formulae may generate different molecular and crystal structures (Galván-Tejada *et al.*, 2002). On the other hand, [$ZnBz_2Br_2$] is almost isostructural with [$ZnBz_2Cl_2$], but, unexpectedly, [$CuBz_2Br_2$] crystallizes in a monoclinic cell, with a significantly different coordination geometry (Bukowska-Strzyzewska & Tosik, 1988, 1991).

Experimental

Benzimidazole (0.118 g, 1.0 mmol) was dissolved at 308 K in ethanol (20 ml) and this solution was added dropwise, with stirring, to $CoCl_2 \cdot 6H_2O$ (0.119 g, 0.5 mmol) dissolved in ethanol (10 ml) at 308 K. The mixture was refluxed for 2 h and then cooled to 298 K. Slow evaporation afforded blue crystals of (I) after 3 weeks; these were separated and used for X-ray diffraction without further treatment.

Crystal data

[$Co(C_7H_6N_2)_2Cl_2$]
$M_r = 366.11$
Triclinic, $P\bar{1}$
$a = 7.4713$ (12) Å
$b = 7.7792$ (7) Å
$c = 13.3329$ (12) Å
$\alpha = 85.785$ (6)°
$\beta = 86.057$ (9)°
$\gamma = 82.954$ (9)°
$V = 765.59$ (16) $Å^3$
$Z = 2$
$D_x = 1.588$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 70 reflections
$\theta = 3.9$–13.8°
$\mu = 1.47$ mm^{-1}
$T = 296$ (2) K
Thick plate, blue
0.36 × 0.26 × 0.12 mm

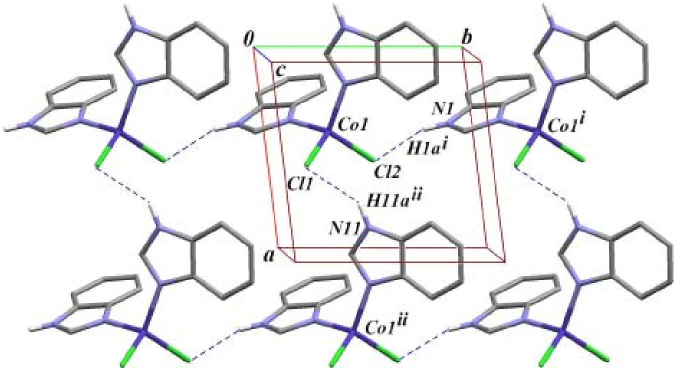


Figure 2
Part of the crystal structure of (I), showing the hydrogen-bonding scheme (dashed lines). For clarity, H atoms not participating in the hydrogen bonding have been omitted [symmetry codes: (i) *x*, 1 + *y*, *z*; (ii) 1 + *x*, *y*, *z*].

Data collection

Bruker P4 diffractometer
$2\theta/\omega$ scans
Absorption correction: ψ scan (*XSCANS*; Siemens, 1996)
$T_{min} = 0.698$, $T_{max} = 0.839$
6679 measured reflections
3983 independent reflections
3318 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$
$\theta_{max} = 28.8°$
$h = -10 \rightarrow 5$
$k = -10 \rightarrow 10$
$l = -18 \rightarrow 18$
3 standard reflections every 97 reflections intensity decay: 0.5%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.097$
$S = 1.05$
3983 reflections
191 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0473P)^2 + 0.2331P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.44$ e $Å^{-3}$
$\Delta\rho_{min} = -0.34$ e $Å^{-3}$
Extinction correction: *SHELXTL-Plus* (Sheldrick, 1998)
Extinction coefficient: 0.0057 (17)

Table 1
Selected geometric parameters (Å, °).

Co1—N13	2.0034 (18)	Co1—Cl1	2.2406 (7)
Co1—N3	2.0105 (16)	Co1—Cl2	2.2544 (6)
N13—Co1—N3	106.21 (7)	N13—Co1—Cl2	111.21 (6)
N13—Co1—Cl1	109.05 (5)	N3—Co1—Cl2	107.64 (5)
N3—Co1—Cl1	110.62 (5)	Cl1—Co1—Cl2	111.96 (3)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···$Cl2^i$	0.86	2.60	3.2712 (18)	136
N11—H11*A*···$Cl1^{ii}$	0.86	2.50	3.258 (2)	147

Symmetry codes: (i) *x*, *y* − 1, *z*; (ii) *x* − 1, *y*, *z*.

H atoms were placed in idealized positions and treated as riding atoms, with N—H and C—H distances constrained to 0.86 and 0.93 Å, respectively, and with $U_{iso}(H) = 1.2U_{eq}$(parent atom).

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Data collection: *XSCANS* (Siemens, 1996); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXTL-Plus* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL-Plus*; molecular graphics: *SHELXTL-Plus* and *MERCURY* (Bruno *et al.*, 2002); software used to prepare material for publication: *SHELXTL-Plus*.

The authors thank DGAPA-UNAM (grant No. 41128-Q) for financial support.

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