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Bis[1-(but-2-enyl)-5-nitro-1*H*-benzimidazole-κN^3]-dichlorocobalt(II)

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.004 Å
R factor = 0.043
wR factor = 0.114
Data-to-parameter ratio = 18.0

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

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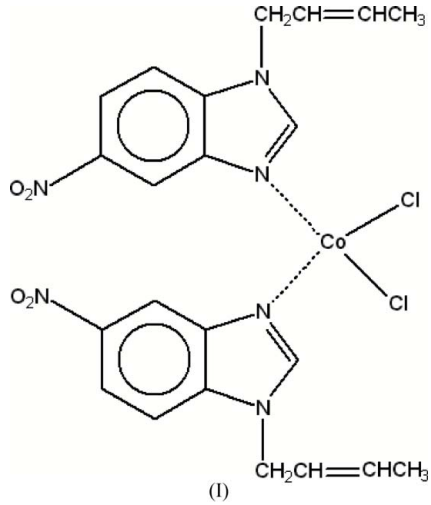
The title compound, $[CoCl_2(C_{11}H_{11}N_3O_2)_2]$, was synthesized from 1-(but-2-enyl)-5-nitrobenzimidazole and cobalt dichloride in ethanol. The Co^{II} atom has a distorted tetrahedral geometry, coordinated by two Cl atoms and two N atoms. The molecule is located on a twofold rotation axis, which passes through the Co atom. In the crystal structure, molecules are connected by intermolecular C—H···O hydrogen-bonding interactions.

Comment

Benzimidazole compounds show a variety of pharmacological activities, such as antifungal, antibacterial, antihelmintic, anti-allergic, antineoplastic, local analgesic, antihistaminic, hypotensive, vasodialator, spasmolytic and anti-ulcer activities (Küçükbay *et al.*, 1995, 1996, 2001; Küçükbay & Durmaz, 1997; Carlsson *et al.*, 2002). In general, heterocyclic compounds and their metal complexes display a wide range of biological activities as antitumor, antibacterial, antifungal and antiviral agents (Arjmand *et al.*, 2005). Metal complexes of biological important ligands are, however, sometimes more effective than the free ligand. Some ruthenium complexes of benzimidazole compounds also show effective catalytic activity for furan synthesis (Küçükbay *et al.*, 1996). The aim of this study was the synthesis and the crystal structure determination of a new benzimidazole cobalt complex and comparison of the results with previous studies (Türktekin *et al.*, 2004; Akkurt *et al.*, 2005).



(I)

The Co atom in the title compound, (I), is coordinated in a distorted tetrahedral manner by two Cl and two N atoms (Fig. 1 and Table 1). Bond lengths and angles around Co are

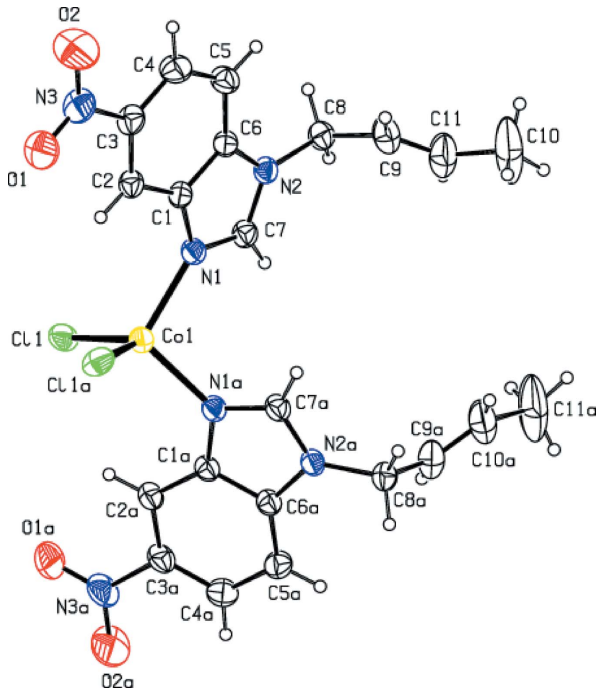


Figure 1
A plot of the title compound with the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level. [Symmetry code: (a) $-x, y, \frac{1}{2}-z$.]

comparable with the reported average values in the literature (Türktekin *et al.*, 2004; Pan & Xu, 2004; Castro *et al.*, 2002; Allen *et al.*, 1987). The molecule is located on a twofold rotation axis, which passes through the Co atom. The benzimidazole ring system is essentially planar, with a maximum deviation of 0.018 (2) Å for C1.

As seen in Fig. 2, the structure is stabilized by C—H···O hydrogen-bonding interactions (Table 2).

Experimental

1-(But-2-enyl)-5-nitrobenzimidazole was synthesized from 5-nitrobenzimidazole, KOH and but-2-enyl bromide according to the literature procedure of Küçükbay *et al.* (2001). A mixture of 1-(but-2-enyl)-5-nitrobenzimidazole (0.5 g, 23.04 mmol) and cobalt dichloride (0.30 g, 23.04 mmol) in ethanol (20 ml) was heated under reflux for 4 h. All volatiles were removed *in vacuo* (0.02 mm Hg; 1 mm Hg = 133.322 Pa). The crude product was crystallized from an ethanol–propan-2-ol (3:1) mixture upon cooling to 243 K (yield 0.41 g, 63%; m.p. 494–495 K). Analysis calculated for $C_{22}H_{22}Cl_2CoN_6O_4$: C 46.81, H 3.90, N 14.89%; found: C 45.52, H 3.7, N 14.34%.

Crystal data

$[CoCl_2(C_{11}H_{11}N_3O_2)_2]$
$M_r = 564.29$
Monoclinic, $C2/c$
$a = 15.9533$ (11) Å
$b = 11.4385$ (6) Å
$c = 15.4545$ (10) Å
$\beta = 114.736$ (5)°
$V = 2561.4$ (3) Å^3
$Z = 4$
$D_x = 1.463$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.92$ mm^{-1}
$T = 296$ K
Prism, violet
0.62 × 0.47 × 0.38 mm

Data collection

Stoe IPDS-II diffractometer
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{min} = 0.600$, $T_{max} = 0.722$
21773 measured reflections
2882 independent reflections
2297 reflections with $I > 2\sigma(I)$
$R_{int} = 0.069$
$\theta_{max} = 27.9°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.114$
$S = 1.03$
2882 reflections
160 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0636P)^2 + 1.122P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.50$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0010 (4)

Table 1
Selected geometric parameters (Å, °).

Co1—Cl1	2.2680 (8)	N1—C7	1.318 (3)
Co1—N1	2.032 (2)	N2—C6	1.381 (3)
O1—N3	1.204 (4)	N2—C7	1.338 (3)
O2—N3	1.205 (7)	N2—C8	1.473 (3)
N1—C1	1.392 (3)	N3—C3	1.475 (4)
Cl1—Co1—N1	110.76 (6)	O1—N3—C3	119.9 (3)
Cl1—Co1—Cl1^{i}	114.43 (3)	O2—N3—C3	117.7 (3)
Cl1—Co1—N1^{i}	108.59 (6)	N1—C1—C2	130.3 (2)
N1—Co1—N1^{i}	103.14 (8)	N1—C1—C6	108.9 (2)
Co1—N1—C1	128.47 (15)	N3—C3—C2	117.0 (2)
Co1—N1—C7	126.44 (18)	N3—C3—C4	117.9 (3)
C1—N1—C7	104.9 (2)	N2—C6—C1	105.9 (2)
C6—N2—C7	106.77 (19)	N2—C6—C5	131.1 (2)
C6—N2—C8	126.6 (2)	N1—C7—N2	113.6 (2)
C7—N2—C8	126.6 (2)	N2—C8—C9	114.2 (2)
O1—N3—O2	122.4 (3)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···O2^{ii}	0.93	2.46	3.255 (5)	143
C8—H8B···O2^{ii}	0.97	2.48	3.302 (6)	142

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

All H atoms were positioned geometrically, with C—H = 0.93–0.97 Å, and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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