Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Diisothiocyanatobis(2-methyl-1*H*-imidazole)-cobalt(II)

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Received 4 January 2005
Accepted 25 January 2005
Online 5 February 2005

Key indicators

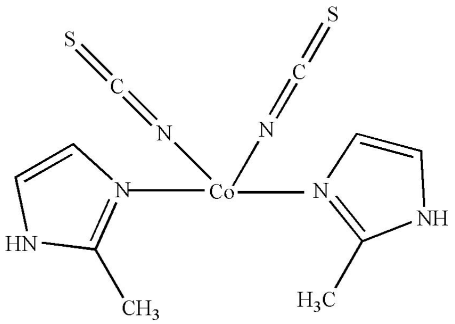
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.036
wR factor = 0.103
Data-to-parameter ratio = 13.8

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

In the title compound, $[Co(NCS)_2(C_4H_6N_2)_2]$, each cobalt(II) ion is coordinated by two N atoms from two 2-methyl-1*H*-imidazole ligands and two N atoms from two isothiocyanate groups. The Co atom lies on a mirror plane and adopts a slightly distorted tetrahedral coordination. The molecular structure and packing are stabilized by intramolecular and intermolecular hydrogen-bond interactions.

Comment

Imidazole is of considerable interest as a ligand in many biological systems in which it provides a potential binding site for metal ions (Brooks & Davidson, 1960). Imidazole itself is a unidentate ligand and forms complexes with metal ions through its tertiary N atoms. It has been reported that a large number of imidazole derivatives possess diverse pharmacological properties, including anti-inflammatory, antimalarial and antitumor activities (Eilbeck *et al.*, 1967; Davis & Smith, 1971). Furthermore, the isothiocyanate anion is a versatile inorganic ligand in the synthesis of coordination compounds. It appeared interesting to study the conditions of formation of thiocyanate-containing cobalt(II) complexes with imidazole derivatives and to investigate the influence of steric properties on the stoichiometry as well as on the structure of the resulting species (Maslejova *et al.*, 1997). In this paper, we report the crystal structure of the bis(2-methyl-1*H*-imidazole)bis(isothiocyanato)cobalt(II) complex, (I).



(I)

The coordination of the Co atom is nearly tetrahedral, with four N atoms, two from monodentate thiocyanate groups and the other two from two 2-methylimidazole ligands, building the CoN_4 chromophore. The N3—Co1—N1 angle [104.63 (9)°] shows the largest deviation from the ideal tetrahedral value. A mirror plane passes through the metal atom and the thiocyanate groups. The Co1—N3 and Co1—N4 distances are 1.953 (4) and 1.957 (4) Å, respectively, which agree with those observed in a similar structure reported previously (Maslejova *et al.*, 1997). The Co—N1 bond distance is 2.003 (2) Å, a value which is very close to that observed in other imidazole-containing cobalt(II) complexes with the metal atom in a tetrahedral environment (Gadet, 1971). The imidazole ring is planar as expected (the largest deviation from the mean plane is 0.015 Å for N2). The NCS groups are almost linear [179.1 (4) and 178.6 (4)° for N3—C5—S1 and N4—C6—S2, respectively], whereas a significant bending is displayed at the Co—N—C—S linkage [178.4 (4) and 173.1 (4)° for C5—N3—Co1 and C6—N4—Co1, respectively].

In the crystal structure, there are some stabilizing intramolecular and intermolecular hydrogen-bond interactions (Table 2).

Experimental

The title compound was prepared by the reaction of 2-methyl-1*H*-imidazole (0.82 g, 10 mmol) with $CoCl_2\cdot6H_2O$ (1.19 g, 5 mmol) and potassium thiocyanate (0.98 g, 10 mmol) by means of hydrothermal synthesis in a stainless steel reactor with a Teflon liner at 383 K for 24 h.

Crystal data

$[Co(NCS)_2(C_4H_6N_2)_2]$
$M_r = 339.33$
Orthorhombic, *Pnma*
$a = 8.4250$ (17) Å
$b = 12.577$ (3) Å
$c = 13.945$ (3) Å
$V = 1477.6$ (6) Å^3
$Z = 4$
$D_x = 1.525$ Mg m^{-3}

Mo *Kα* radiation
Cell parameters from 25 reflections
$\theta = 4$–14°
$\mu = 1.44$ mm^{-1}
$T = 293$ (2) K
Block, pink
0.35 × 0.25 × 0.25 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω scans
Absorption correction: none
2650 measured reflections
1354 independent reflections
1176 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.018$

$\theta_{\rm max} = 25.0°$
$h = 0 \rightarrow 10$
$k = 0 \rightarrow 14$
$l = -16 \rightarrow 16$
3 standard reflections every 100 reflections intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.103$
$S = 1.09$
1354 reflections
98 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0652P)^2 + 0.5535P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.43$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.71$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0047 (10)

Table 1
Selected geometric parameters (Å, °).

Co1—N3	1.953 (4)	S2—C6	1.624 (4)
Co1—N4	1.957 (4)	N3—C5	1.153 (6)
Co1—N1	2.003 (2)	N4—C6	1.157 (5)
S1—C5	1.612 (4)		
N3—Co1—N4	109.82 (17)	C4—N1—Co1	122.2 (2)
N3—Co1—N1	104.63 (9)	C5—N3—Co1	178.4 (4)
N4—Co1—N1	112.99 (8)	C6—N4—Co1	173.1 (4)
N1—Co1—N1$^{\rm i}$	111.10 (12)	N3—C5—S1	179.1 (4)
C2—N1—Co1	131.3 (2)	N4—C6—S2	178.6 (4)

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

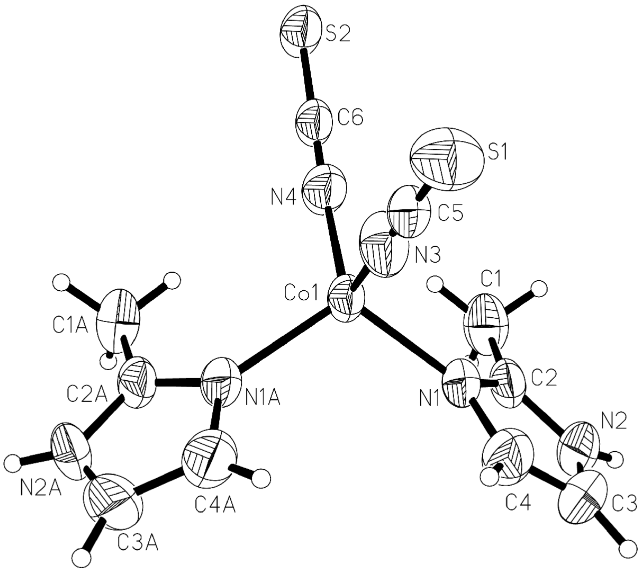


Figure 1
The structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···S2$^{\rm ii}$	0.86	2.67	3.460 (3)	154
C1—H1*A*···N4	0.96	2.53	3.412 (4)	153

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

H atoms were positioned geometrically and allowed to ride on their attached atoms, with C—H distances in the range 0.93–0.96 Å and with $U_{\rm iso} = 1.2$–$1.5U_{\rm eq}$(C,N).

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *NRCVAX* (Gabe *et al.*, 1989; program(s) used to solve structure: *SHELXTL/PC* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC*; software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors thank the Natural Science Foundation of Shandong Province (No. Y2002B06) and the Science Research Foundation of Qingdao University of Science and Technology (No. 03Z08).

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