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[1,2-Bis(benzimidazol-2-yl)ethane]diisothiocyanatocobalt(II)

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.003 Å
R factor = 0.030
wR factor = 0.066
Data-to-parameter ratio = 13.7

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

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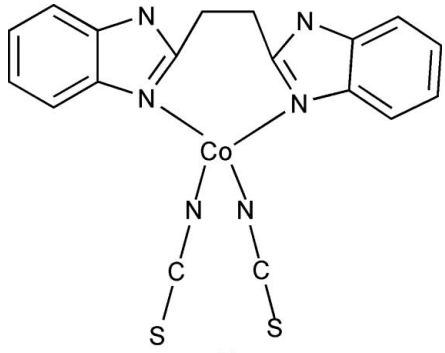
The coordination geometry of the Co^{II} atom in the title complex, $[Co(NCS)_2(C_{16}H_{14}N_4)]$ or $[Co(NCS)_2(dbz)]$, where dbz is bis(benzimidazol-2-yl)ethane, is distorted tetrahedral; the Co^{II} atom is coordinated by two N atoms from one dbz molecule and two N atoms from two monodentate NCS^- anions.

Comment

A series of transition metal coordination compounds with various bis(benzimidazol-2-yl)alkanes have been synthesized and structurally characterized (Albada *et al.*, 1999, 2000; Riggio *et al.*, 2001). In the present work, we report the synthesis and crystal structure of a new bis(benzimidazole-2-yl)ethane (dbz) cobalt(II) coordination compound, $[Co(NCS)_2(dbz)]$, (I).



(I)

As shown in Fig. 1, the coordination geometry of the cobalt(II) atom is distorted tetrahedral; the four coordination sites are occupied by two N atoms from one dbz molecule and two N atoms from two NCS^- anions (Table 1). The N—Co—N bond angles are in the range 105.88 (8)–116.50 (8)°. The isothiocyanato ions are almost linear, in good agreement with the results usually obtained for *N*-monodentate NCS^- complexes. The dbz ligand shows a *gauche* conformation, with a C7—C15—C16—C14 torsion angle of 88.4 (2)°. The dihedral angle between the two benzimidazole ring systems is 20.14 (8)°.

In the crystal structure of (I), there are weak N—H···S hydrogen-bonding interactions involving the dbz ligand and adjacent NCS^- anions (Table 2, Fig. 2). The crystal structure is further stabilized by π–π stacking interactions occurring between centrosymmetrically related molecules [$Cg1\cdots Cg1^{i}$ = 3.754 (3) Å; $Cg2\cdots Cg2^{ii}$ = 3.804 (4) Å; *Cg*1 and *Cg*2 are the centroids of the N1/N2/C1–C7 and N3/N4/C8–C14 benzim-

idazole ring systems; symmetry codes: (i) $-x, 1-y, -z$; (ii) $-x, -y, 1-z$].

Experimental

An H_2O/MeOH solution (20 ml, 1:1 *v*/*v*) of $Co(NO_3)_2{\cdot}6H_2O$ (0.50 mmol) and KNCS (1.0 mmol) was added to one leg of an H-shaped tube, and an H_2O/MeOH solution (20 ml, 1:1 *v*/*v*) of dbz (0.5 mmol) was added to the other leg of the tube. After several weeks, well shaped blue single crystals were obtained. Found: C, 49.31; H, 3.14; N,19.08%. Calcd. For $C_{18}H_{14}CoN_6S_2$: C, 49.43; H, 3.23; N, 19.22%.

Crystal data

$[Co(NCS)_2(C_{16}H_{14}N_4)]$	$V = 915.8\ (3)$ Å^3
$M_r = 437.40$	$Z = 2$
Triclinic, $P\overline{1}$	$D_x = 1.586$ Mg m^{-3}
$a = 9.4393\ (19)$ Å	Mo $K\alpha$ radiation
$b = 9.4588\ (19)$ Å	$\mu = 1.18$ mm^{-1}
$c = 11.552\ (2)$ Å	$T = 173\ (2)$ K
$\alpha = 96.323\ (3)^\circ$	Block, blue
$\beta = 94.908\ (3)^\circ$	0.23 × 0.22 × 0.15 mm
$\gamma = 115.407\ (3)^\circ$	

Data collection

Rigaku Mercury CCD diffractometer	9000 measured reflections
	3332 independent reflections
ω scans	2940 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (Jacobson, 1998)	$R_{int} = 0.060$
	$\theta_{max} = 25.4^\circ$
$T_{min} = 0.773$, $T_{max} = 0.843$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0237P)^2 + 0.5317P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.030$	
$wR(F^2) = 0.066$	
$S = 1.07$	$(\Delta/\sigma)_{max} = 0.001$
3332 reflections	$\Delta\rho_{max} = 0.32$ e Å^{-3}
244 parameters	$\Delta\rho_{min} = -0.25$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Co1—N6	1.946 (2)	Co1—N3	1.9952 (17)
Co1—N5	1.947 (2)	Co1—N1	2.0005 (18)
N6—Co1—N5	111.91 (8)	N3—Co1—N1	106.64 (7)
N6—Co1—N3	116.50 (8)	C17—N5—Co1	177.20 (18)
N5—Co1—N3	106.84 (8)	C18—N6—Co1	174.42 (19)
N6—Co1—N1	105.88 (8)	N5—C17—S1	178.4 (2)
N5—Co1—N1	108.75 (8)	N6—C18—S2	179.0 (2)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*B*···S2^{i}	0.88	2.64	3.4572 (19)	155
N4—H4*B*···S1^{ii}	0.88	2.57	3.3387 (18)	146

Symmetry codes: (i) $x-1, y, z$; (ii) $x-1, y-1, z$.

H atom were placed in idealized positions and refined as riding, with C—H = 0.95–0.99 Å, N—H = 0.88 Å, and with U_{iso}(H) = $1.2U_{eq}$(C,N).

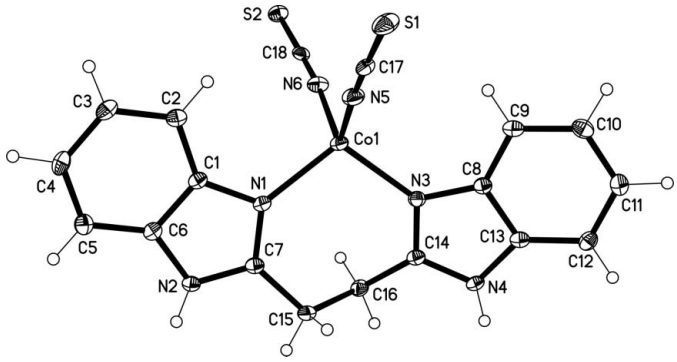


Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level.

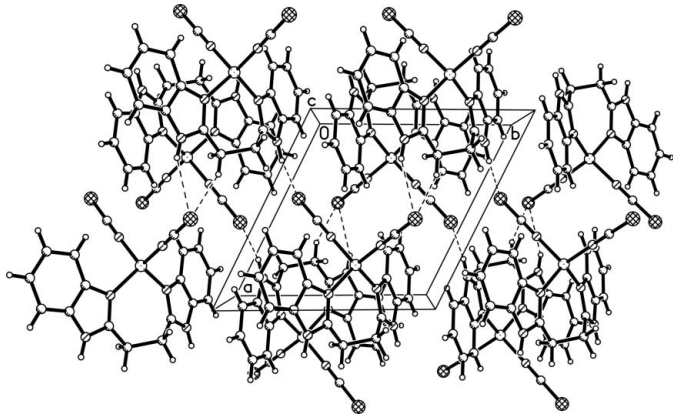


Figure 2
Packing diagram of (I), viewed along the *c* axis, showing the intermolecular hydrogen interactions as dashed lines.

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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