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

The coordination geometry of the Co\textsuperscript{II} atom in the title complex, [Co\textsubscript{2}(C\textsubscript{10}H\textsubscript{14}N\textsubscript{4})\textsubscript{2}] or [Co(NCS)\textsubscript{2}(dbz)], where dbz is bis(benzimidazol-2-yl)ethane, is distorted tetrahedral; the Co\textsuperscript{II} atom is coordinated by two N atoms from one dbz molecule and two N atoms from two monodentate NCS\textsuperscript{-} anions.

Comment

A series of transition metal coordination compounds with various bis(benzimidazol-2-yl)alkanes have been synthesized and structurally characterized (Albada \textit{et al.}, 1999, 2000; Riggio \textit{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)\textsubscript{2}(dbz)], (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\textsuperscript{-} anions (Table 1). The N—Co—N bond angles are in the range 105.88 (8)—116.50 (8)\degree. The isothiocyanato ions are almost linear, in good agreement with the results usually obtained for N-monodentate NCS\textsuperscript{-} complexes. The dbz ligand shows a gauche conformation, with a C7—C15—C16—C14 torsion angle of 88.4 (2)\degree. The dihedral angle between the two benzimidazole ring systems is 20.14 (8)\degree.

In the crystal structure of (I), there are weak N—H···S hydrogen-bonding interactions involving the dbz ligand and adjacent NCS\textsuperscript{-} anions (Table 2, Fig. 2). The crystal structure is further stabilized by \(\pi\)—\(\pi\) stacking interactions occurring between centrosymmetrically related molecules [\(Cg1\cdot\cdot\cdotCg1' = 3.754 (3)\) \AA; \(Cg2\cdot\cdot\cdotCg2'' = 3.804 (4)\) \AA; \(Cg1\) and \(Cg2\) 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$_2$O/MeOH solution (20 ml, 1:1 v/v) of Co(NO$_3$)$_2$·6H$_2$O (0.50 mmol) and KNCS (1.0 mmol) was added to one leg of an H-shaped tube, and an H$_2$O/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$_6$S$_2$: 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$^3$

$Z = 2$

$D_x = 1.586$ Mg m$^{-3}$

$\mu = 1.18$ mm$^{-1}$

$T = 173$ (2) K

Block, blue

$D_m = 1.586$ Mg m$^{-3}$

$V = 915.8$ (3) Å$^3$

$Z = 2$

$D_r = 1.18$ mm$^{-1}$

$T = 173$ (2) K

Table 1

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</table>

**Data collection**

Rigaku Mercury CCD

diffractometer

$\omega$ scans

Absorption correction: multi-scan

(Jacobson, 1998)

$T_{min} = 0.773$, $T_{max} = 0.843$

9000 measured reflections

3332 independent reflections

2940 reflections with $I > 2\sigma(I)$

$R_{int} = 0.060$

$\theta_{max} = 25.4$

$\Delta\sigma_{max} = 0.001$

$\Delta\rho_{max} = 0.32$ e Å$^{-3}$

$\Delta\rho_{min} = -0.25$ e Å$^{-3}$

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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**References**


