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cis-Bis[(1*H*-benzimidazol-2-yl)methanol-κ^2N,O]-bis(thiocyanato-κN)cobalt(II)

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Key indicators

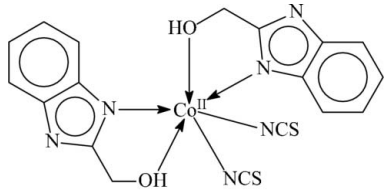
Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.004 Å
R factor = 0.037
wR factor = 0.101
Data-to-parameter ratio = 15.1

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

The title complex, $[Co(NCS)_2(C_8H_8N_2O)_2]$, possesses crystallographically imposed twofold symmetry. The Co^{II} atom is coordinated by four N atoms and two O atoms in a distorted octahedral geometry. The crystal packing is stabilized by weak intermolecular O—H···S and N—H···S hydrogen bonds.

Comment

2-Hydroxymethylbenzimidazole, an organic compound with a known crystal structure (Aubry *et al.*, 1995), affords, with transition metal salts such as cobalt(II) halides, adducts having a 1:3 metal to ligand stoichiometry. In solution, the ligand is able to chelate to cobalt (Rzepka & Surga, 1993). Cobalt(II) thiocyanate forms a 1:2 adduct (Artemenko & Slyusarenko, 1971), with the three-dimensional structure revealed in the present study of the title compound, (I).



(I)

In (I), the ligand chelates through the hydroxy O and imino N atoms, resulting in a *cis*-N_4O_2Co octahedral geometry (Table 1) at the metal center (Fig. 1), like that observed in copper (Hamilton *et al.*, 1979) and nickel (Alagna *et al.*, 1984) adducts. The complex has twofold crystallographic symmetry. The crystal packing in (I) is stabilized by weak intermolecular O—H···S and N—H···S hydrogen bonds (Table 2).

Experimental

(1*H*-Benzimidazol-2-yl)methanol was purchased from a chemical supplier. This reagent (0.15 g, 1 mmol), cobalt(II) nitrate hexahydrate (0.15 g, 0.5 mmol) and ammonium thiocyanate (0.08 g, 1 mmol) were dissolved in water (10 ml) that was kept at about 333 K. Red platelets separated from the solution after two weeks.

Crystal data

$[Co(NCS)_2(C_8H_8N_2O)_2]$
M_r = 471.42
Monoclinic, *C*2/*c*
a = 15.318 (1) Å
b = 8.3847 (7) Å
c = 16.140 (1) Å
β = 109.771 (1)°
V = 1950.7 (3) Å^3
Z = 4
D_x = 1.605 Mg m^{-3}
Mo *K*α radiation
μ = 1.12 mm^{-1}
T = 173 (2) K
Plate, red
0.44 × 0.24 × 0.07 mm

Data collection

Bruker SMART area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.638, T_{max} = 0.926
4847 measured reflections
2115 independent reflections
1586 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 27.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.101
S = 1.04
2115 reflections
140 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.058P)^2 + 0.7176P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O1	2.268 (2)	Co1—N3	2.049 (2)
Co1—N1	2.077 (2)		
O1—Co1—O1^{i}	89.6 (1)	N1—Co1—N1^{i}	158.7 (1)
O1—Co1—N1	74.9 (1)	N1—Co1—N3	94.6 (1)
O1—Co1—N1^{i}	89.9 (1)	N1—Co1—N3^{i}	99.3 (1)
O1—Co1—N3	86.2 (1)	N3—Co1—N3^{i}	98.6 (1)
O1—Co1—N3^{i}	172.8 (1)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···S1^{ii}	0.86 (3)	2.35 (3)	3.199 (2)	176 (3)
N2—H2···S1^{iii}	0.86 (3)	2.54 (3)	3.360 (2)	161 (3)

Symmetry codes: (ii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (iii) $-x+\frac{3}{2}, -y+\frac{3}{2}, -z+1$.

The C-bound H atoms were placed in calculated positions (C—H = 0.95–0.99 Å) and included in the refinement in the riding-model approximation, with U_{iso}(H) = 1.2U_{eq}(C). The amino and hydroxy H atoms were located in a difference Fourier map and refined isotropically with distance restraints of O(N)—H = 0.85 (1) Å.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

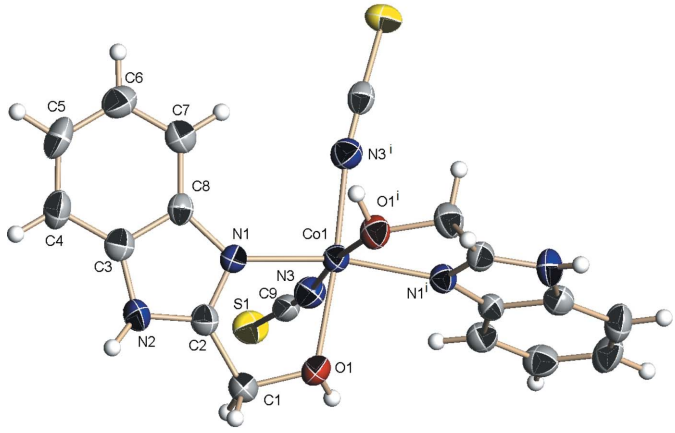


Figure 1
The molecular structure, showing displacement ellipsoids drawn at the 75% probabilty level and the atom labelling. [Symmetry code: (i) $1+x, -y, z-\frac{1}{2}$.]

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References

Alagna, L., Hasnain, S. S., Piggott, B. & Williams, D. J. (1984). *Biochem. J.* **220**, 591–595.
Artemenko, M. V. & Slyusarenko, K. F. (1971). *Ukr. Khim. Zhur.* **37**, 753–758. (In Russian.)
Aubry, A., Brembilla, A., Faivre, V. & Lochon, P. (1995). *Acta Cryst.* C**51**, 115–116.
Bruker (1999). *SAINT* (Version 6.45A) and *SMART* (Version 6.45A). Bruker AXS Inc, Madison, Wisconsin, USA.
Hamilton, G. J., Ferraro, J. R. & Sinn, E. (1979). *J. Chem. Soc. Dalton Trans.* pp. 515–519.
Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Rzepka, M. & Surga, W. (1993). *Pol. J. Chem.* **67**, 2121–2132.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.