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Aquadithiocyanato(2,4,6-tri-2-pyridyl-1,3,5-triazine)cobalt(II)

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.011 Å
R factor = 0.050
wR factor = 0.144
Data-to-parameter ratio = 14.9

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

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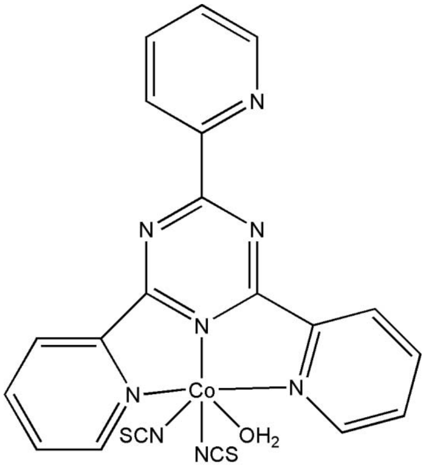
In the title compound, [Co(SCN)$_2$(C$_{18}$H$_{12}$N$_6$)(H$_2$O)], the Co^{II} atom shows a slightly distorted octahedral geometry and is hexacoordinated by five N atoms from a 2,4,6-tri-2-pyridyl-1,3,5-triazine ligand and thiocyanate ions and by one O atom of a water molecule.

Comment

There has been much interest in the use of triazine ligands, such as 2,4,6-tris-2-pyridyl-1,3,5-triazine (tptz), for the extraction and separation of metal ions and in establishing the nature of the extracted species (Majumder *et al.*, 2006). This particular ligand has three coordination sites (major, middle and minor) according to the number of donor N atoms (three, two and one, respectively). We report here a mononuclear complex which uses the major coordination site, namely [Co(SCN)$_2$(tptz)(H$_2$O)], (I), derived from the tptz ligand.



(I)

The title compound crystallized in the orthorhombic space group $Pna2_1$. The coordination environment of the central Co atom is shown in Fig. 1; it adopts a slightly distorted octahedral geometry in which N1, N2, N5 and N7 are in the equatorial plane and N8, O1 occupy the axial positions. The Co—N bond lengths from the N-donor sites of the tptz ligand span the range 2.062 (6)–2.214 (6) Å. They are therefore significantly longer than the Co—N bond lengths [2.008 (7) and 2.074 (7) Å] from the N-donor sites of the coordinating thiocyanate ions. The Co—O bond length is 2.162 (5) Å. In the octahedral coordination geometry of the Co atom, the N—Co—N bond angles range from 74.1 (2) to 167.0 (3)° in the equatorial plane, while Co—N8 and Co—O1 are almost perpendicular to this plane. The structure is therefore closely related to the other three structurally characterized cobalt

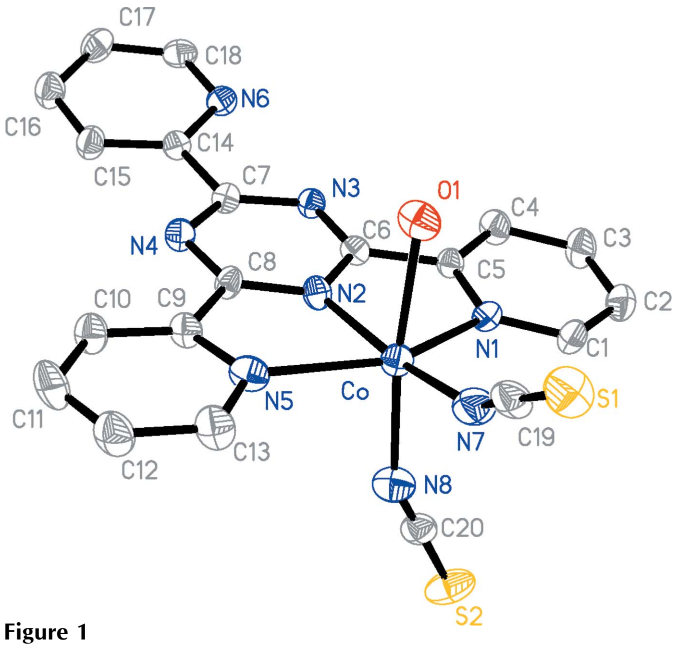


Figure 1
The molecular structure of the title complex, with displacement ellipsoids drawn at the 30% probability level. H atoms have been omitted for clarity.

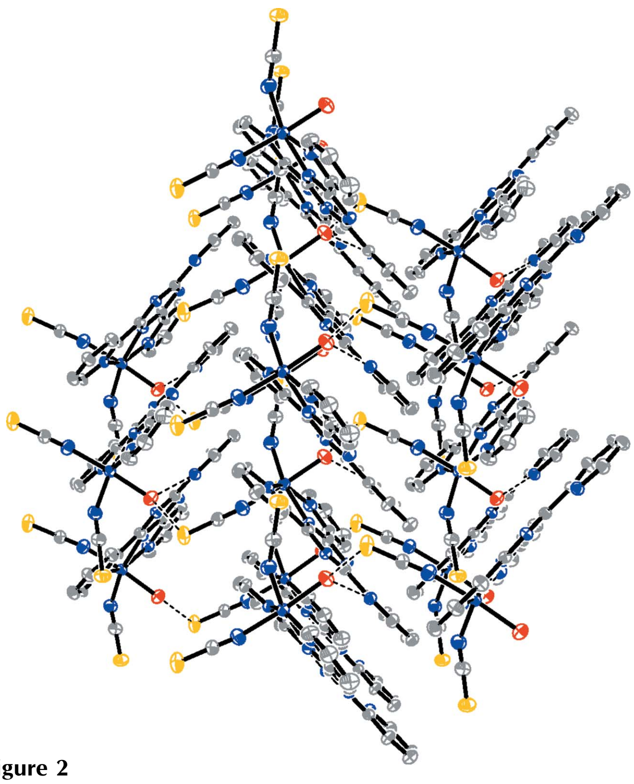


Figure 2
The packing of the title compound. Dashed lines indicate hydrogen bonds. H atoms have been omitted.

complexes with the same tptz ligand (also mononuclear complexes; Majumder *et al.*, 2005, 2006; Holbrey *et al.*, 2006).

A packing diagram is shown in Fig. 2. The water ligand links two neighboring molecular units by O—H···N hydrogen bonds with the pyridine substituent which is not coordinated to the central Co atom. In additon, the thiocyanate ion is connected to the water ligand by an O—H···S interaction, forming a three-dimensional network.

Experimental

A solution of tptz (0.5 mmol) in CH_3OH (10 ml) was added to a solution of $Co(ClO_4)_2 \cdot 6H_2O$ (0.5 mmol) in water (5 ml). The solution was stirred for a few minutes at room temperature. An aqueous solution (10 ml) of KCNS (1 mmol) was then added dropwise to this solution with constant stirring. The deep-red solution was filtered off and the filtrate was kept at room temperature. After 4 d, red block-shaped crystals suitable for X-ray diffraction were obtained from the filtrate (yield 72%). Analysis calculated for $C_{20}H_{14}CoN_8OS_2$: C 47.53, H 2.79, N 22.17%; found: C 47.53, H 2.81, N 22.16%.

Crystal data

$[Co(SCN)_2(C_{18}H_{12}N_6)(H_2O)]$
$M_r = 505.44$
Orthorhombic, $Pna2_1$
$a = 9.342\ (6)$ Å
$b = 15.701\ (9)$ Å
$c = 14.822\ (9)$ Å
$V = 2174\ (2)$ Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 1.01$ mm^{-1}
$T = 294\ (2)$ K
$0.20 \times 0.12 \times 0.10$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.576$, $T_{max} = 0.904$
11052 measured reflections
4334 independent reflections
2488 reflections with $I > 2\sigma(I)$
$R_{int} = 0.075$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.144$
$S = 1.07$
4334 reflections
290 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max} = 0.75$ e Å^{-3}
$\Delta\rho_{min} = -0.88$ e Å^{-3}
Absolute structure: Flack (1983), 2009 Friedel pairs
Flack parameter: −0.01 (3)

H atoms were included in calculated positions (C—H = 0.93 and O—H = 0.85 Å) and refined with $U_{iso}(H) = 1.2U_{eq}$(parent atom).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; 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

Bruker (1998). *SMART-NT*, *SAINT-NT* and *SHELXTL-NT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Holbrey, J. D., Vigour, K. B., Reichert, W. M. & Rogers, R. D. (2006). *J. Chem. Crystallogr.* **36**, 799–804.
Majumder, A., Choudhury, C. R., Mitra, S., Marschner, C. & Baumgartner, J. (2005). *Z. Naturforsch. Teil B*, **60**, 99–105.
Majumder, A., Gramlich, V., Rosair, G. M., Batten, S. R., Masuda, J. D., El Fallah, M. S., Ribas, J., Sutter, J.-P., Desplanches, C. & Mitra, S. (2006). *Cryst. Growth Des.* **6**, 2355–2368.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

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