Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[bis(thiocyanato-κN)cobalt(II)]-di-μ-2-aminobenzonitrile-$\kappa^2 N,N'$]

Lesego J. Moitsheki,* Susan A. Bourne and Luigi R. Nassimbeni

Department of Chemistry, University of Cape Town, Rondebosch 7701, South Africa

Correspondence e-mail: mlesego@science.uct.ac.za

Key indicators

Single-crystal X-ray study
T = 113 K
Mean σ(C–C) = 0.003 Å
R factor = 0.027
wR factor = 0.068
Data-to-parameter ratio = 13.5

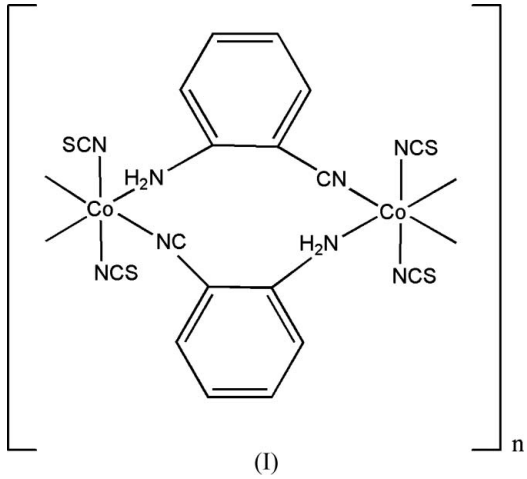
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 12 October 2005
Accepted 9 November 2005
Online 16 November 2005

Reaction of $Co(NCS)_2$ and 2-aminobenzonitrile (ABN) produces the title one-dimensional polymer, $[Co(NCS)_2(ABN)_2]_n$, where ABN is 2-aminobenzonitrile ($C_7H_6N_2$). Octahedrally coordinated Co^{II} ions are bridged by the ABN molecules, which are coordinated to the central metal *via* the N donors of the cyano and nitrile groups.

Comment

Coordination polymers constructed from transition metals have recently attracted a great deal of attention (Eddaoudi *et al.*, 2001; Vujovic *et al.*, 2003, 2004; Noro *et al.*, 2005; Ye *et al.*, 2005). Polymers of Ni^{II} and Cd^{II} with 2-aminobenzonitrile (ABN) isomers investigated by Vujovic *et al.* (2004) possess different kinds of bonding networks. In addition to hydrogen-bonded networks, the ABN isomers also form one-, two- and three-dimensional polymeric networks as a result of different coordination preferences, such as coordination to the metal centre using either amine or cyanide N atoms, or in a bridging fashion (using both N donors). Here, we report the title self-assembled one-dimensional coordination polymer of $Co(NCS)_2$ and 2-aminobenzonitrile, (I).



(I)

Compound (I) forms a double strand when viewed along [010]. The polymer chains run parallel to [001] (Fig. 1). The Co^{II} ion possesses octahedral symmetry, with angles between adjacent ligands ranging from 86.26 to 93.74°. The ABN ligands are located *trans* to one another, as are the NCS^- ligands. Furthermore, the ABN ligands occupy equatorial positions while the NCS^- ligands are in axial positions. The metal centres are linked by the ABN molecules, which act as bidentate ligands by coordination through N donors at both ends.

Expected bond lengths (Allen *et al.*, 1987) for Co—N and C—C are 1.97 and 1.40 Å, respectively. The C11—C12 bond length [1.441 (3) Å] is longer than expected, owing to coordination of the cyano group to the central metal. Likewise, the Co—N bond lengths are slightly elongated.

There are no conventional hydrogen bonds. A weak N5—H5*A*···S4 hydrogen-bonding interaction occurs, with a donor–acceptor distance of 3.67 (2) Å. The geminal atom H5*B* is not involved in non-bonding interactions, presumably because the N5—H5*B*···S4 angle is unfavourable.

Experimental

2-Aminobenzonitrile (23.63 mg, 0.20 mmol) was dissolved in methanol (5 ml) and added to a methanolic solution (5 ml) of $Co(NCS)_2$ (0.20 *M*). The mixture was heated to 338 K for about 15 min and then cooled to room temperature. Brown needles of (I) formed by slow evaporation within two weeks.

Crystal data

$[Cu(NCS)_2(C_7H_6N_2)_2]$	D_x = 1.602 Mg m^{-3}
M_r = 411.37	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 13748 reflections
a = 22.088 (4) Å	θ = 1.0–26.0°
b = 7.5560 (15) Å	μ = 1.26 mm^{-1}
c = 11.152 (2) Å	T = 113 (2) K
β = 113.56 (3)°	Needle, brown
V = 1706.1 (7) Å^3	0.18 × 0.10 × 0.08 mm
Z = 4	

Data collection

Nonius KappaCCD area-detector diffractometer	1676 independent reflections
	1432 reflections with $I > 2\sigma(I)$
ω and φ scans	R_{int} = 0.057
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)	θ_{max} = 26.0°
	$h = -27 \rightarrow 26$
T_{min} = 0.805, T_{max} = 0.906	$k = -9 \rightarrow 9$
10161 measured reflections	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0344P)^2 + 0.4652P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.027	
$wR(F^2)$ = 0.068	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.06	$\Delta\rho_{max}$ = 0.33 e Å^{-3}
1676 reflections	$\Delta\rho_{min}$ = −0.49 e Å^{-3}
124 parameters	Extinction correction: *SHELXL97* (Sheldrick, 1997)
H atoms treated by a mixture of independent and constrained refinement	Extinction coefficient: 0.0019 (4)

N-bound atoms H5*A* and H5*B* were located in a difference map and refined isotropically. The remaining H atoms were positioned geometrically, with C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997) and *X-SEED* (Barbour, 2001); molecular graphics: *POV-RAY* (Persistence of Vision Development Team, 1999); software used to prepare material for publication: *SHELXL97*.

We thank the National Research Fund (grant No. FA2004032500017), the University of Cape Town Research Committee and the CSIR (LJM) for financial support.

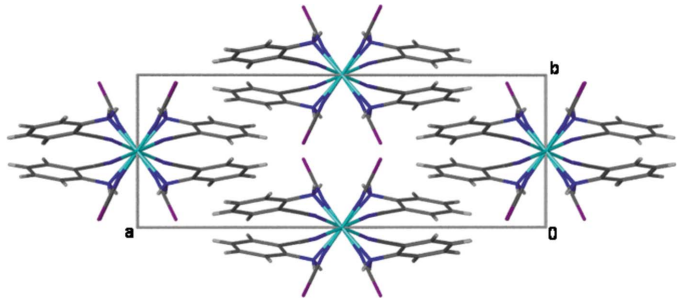


Figure 1
The molecular packing of (I), showing chains running parallel to [001].

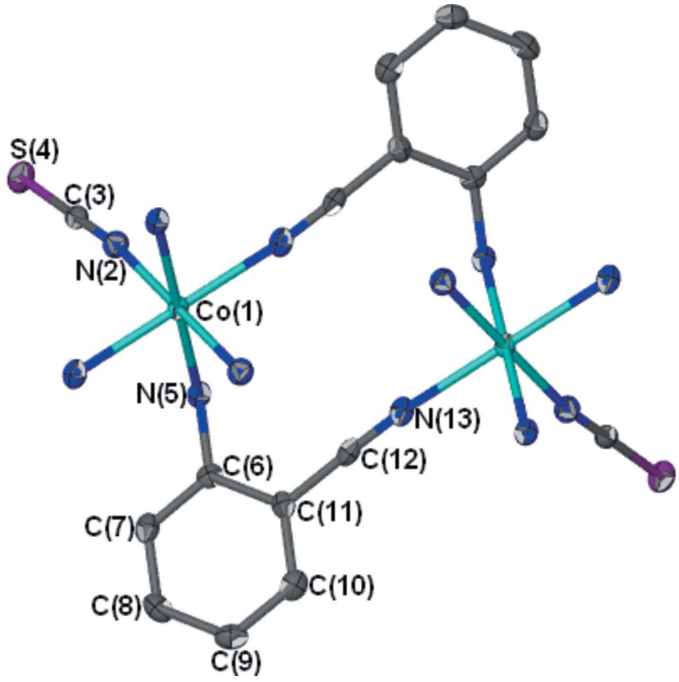


Figure 2
A plot of (I), showing the atomic numbering scheme. Displacement ellipsoids are shown at the 70% probability level and H atoms have been omitted for clarity.

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Eddaoudi, M., Kim, J., Wachter, J. B., Chae, H. K., O'Keeffe, M. & Yaghi, O. M. (2001). *J. Am. Chem. Soc.* **123**, 4368–4369.
Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Noro, S., Kitangwa, S., Nakaruma, T. & Wada, T. (2005). *Inorg. Chem.* **44**, 3960–3971.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Persistence of Vision Development Team (1999). *POV-RAY*. Version 3.1e.watcom.win32. URL: http://www.povray.org/
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (2001). *SADABS*. Bruker AXS Inc. Madison, Wisconsin, USA.
Vujovic, D., Raubenheimer, H. G. & Nassimbeni, L. R. (2003). *Dalton Trans.* pp. 631–637.
Vujovic, D., Raubenheimer, H. G. & Nassimbeni, L. R. (2004). *Eur. J. Inorg. Chem.* pp. 2943–2949.
Ye, L. & Wu, Y. (2005). *Acta Cryst.* E**61**, m1894–m1896.