

Chong Zhang,^a Hong-Qi Ai,^b
De-Zhi Sun^a and Seik Weng Ng^{c*}^aDepartment of Chemistry and Technology, Liaocheng University, Liaocheng 252059, People's Republic of China, ^bDepartment of Chemistry, Jinan University, Jinan 252059, People's Republic of China, and ^cDepartment of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

Correspondence e-mail: seikweng@um.edu.my

Key indicators

Single-crystal X-ray study
 $T = 295\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.006\text{ \AA}$
 R factor = 0.035
 wR factor = 0.095
Data-to-parameter ratio = 11.4For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.**catena-Poly[[[bis(1*H*-benzimidazole- κ N³)-cobalt(II)]-di- μ -azido] dihydrate]**

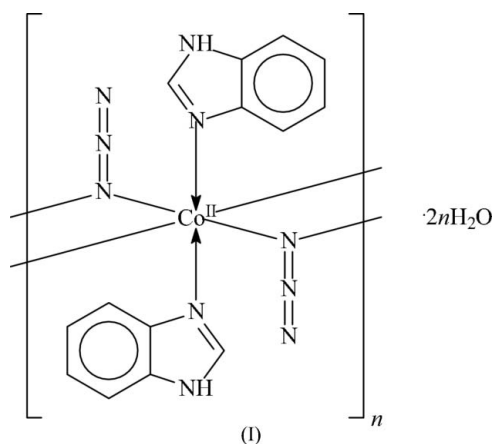
The crystal structure of the title compound, $\{[\text{Co}(\text{N}_3)_2(\text{C}_7\text{H}_6\text{N}_2)_2] \cdot 2\text{H}_2\text{O}\}_n$, consists of a di- μ -azido-bridged $[\text{Co}(\text{N}_3)_2]_n$ chain that propagates along the c axis of the orthorhombic unit cell, together with uncoordinated water molecules. Adjacent Co–N–Co–N rhombi are coplanar; the metal atom lies on a special position of $2/m$ site symmetry and the azide groups on special positions of site symmetry 2. The heterocycle lies on a mirror plane. The heterocycles are positioned above and below the rhombi so that the geometry of Co is an all-*trans* octahedral. The chain motif is consolidated by hydrogen bonding with the uncoordinated water molecules, which lie on mirror planes.

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Comment

The azide ($-\text{N}=\text{N}=\text{N}$) anion bridges two Co atoms through only one terminal N atom in a number of cobalt(II) azide adducts, e.g. the adducts with 1-methyl-2-(*p*-tolylazo)imidazole (Ray *et al.*, 2003), 2,2'-bithiazolanyl, 2,9-dimethyl-1,10-phenanthroline (Liu *et al.*, 2003) and 2,2'-bipyrimidine (de Munno *et al.*, 1996). The covalent Co–N bond distance is not statistically much different from that of the dative Co \leftarrow N bond in these examples; this feature is also noted in the adduct with benzimidazole, (I), which exists as a dihydrate (Fig. 1).



Two azide units, both functioning in a μ -bridging mode, link adjacent Co atoms into a linear chain; the chain is decorated with the donor heterocycle. The chains are consolidated into a three-dimensional network motif by hydrogen bonds (Table 2).

Experimental

Cobalt(II) nitrate hexahydrate (29 mg, 0.1 mmol), benzimidazole (24 mg, 0.2 mmol), sodium azide (13 mg, 0.2 mmol) and water (10 ml) were placed in a Teflon-lined stainless-steel Parr bomb. The bomb

was heated at 403 K for 24 h and then allowed to cool to room temperature; pink needle-shaped crystals were isolated in about 15% yield.

Crystal data

[Co(N₃)₂(C₇H₆N₂)₂].2H₂O
M_r = 415.30
 Orthorhombic, *Ibam*
a = 17.112 (2) Å
b = 15.361 (2) Å
c = 6.738 (1) Å
V = 1771.1 (4) Å³
Z = 4
D_x = 1.557 Mg m⁻³
 Mo *K*α radiation
 μ = 1.00 mm⁻¹
T = 295 (2) K
 Needle, pink
 0.16 × 0.12 × 0.08 mm

Data collection

Bruker SMART area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.856, *T_{max}* = 0.924
 4780 measured reflections
 993 independent reflections
 702 reflections with *I* > 2σ(*I*)
R_{int} = 0.058
 θ_{max} = 26.4°

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.035
wR(*F*²) = 0.095
S = 1.03
 993 reflections
 87 parameters
 H atoms treated by a mixture of independent and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.045P)^2 + 1.8594P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} = 0.001$
 $\Delta\rho_{max} = 0.26 \text{ e \AA}^{-3}$
 $\Delta\rho_{min} = -0.51 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Co1—N1	2.193 (2)	Co1—N4	2.098 (3)
N1—Co1—N1 ⁱ	79.7 (1)	N1—Co1—N4	88.3 (1)
N1—Co1—N1 ⁱⁱⁱ	100.4 (1)	N1—Co1—N4 ⁱⁱ	91.7 (1)

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

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N5—H5 <i>n</i> ...O1 <i>w</i>	0.85 (1)	1.94 (1)	2.777 (5)	171 (5)
O1 <i>w</i> —H1 <i>o</i> ...N3 ^{iv}	0.84 (1)	2.24 (2)	2.983 (4)	148 (4)

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

The amino and water H atoms were located in a difference Fourier map, and were refined with a distance restraint of N—H = O—H = 0.85 (1) Å. The C-bound H atoms were placed in calculated positions [C—H = 0.93 Å and *U*_{iso}(H) = 1.2*U*_{eq}(C)], and were included in the refinement in the riding-model approximation.

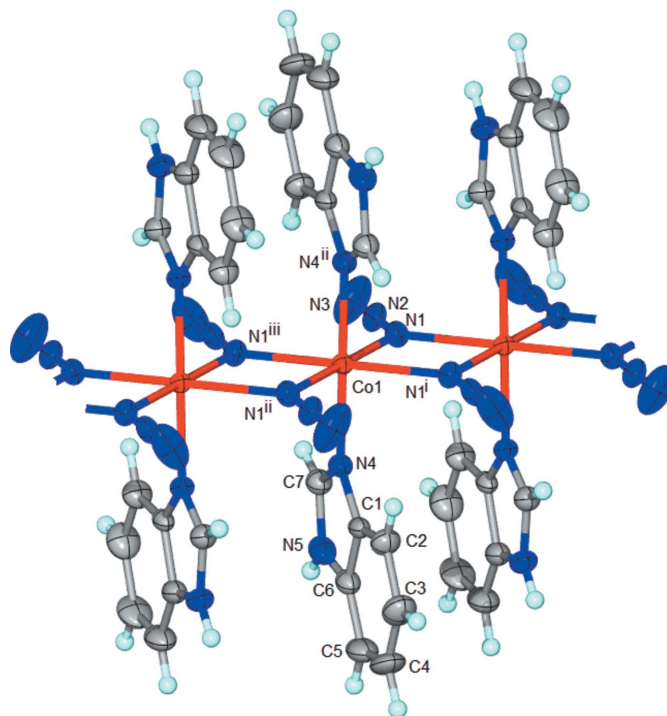


Figure 1

Part of a polymeric chain of the title compound. Displacement ellipsoids are drawn at the 50% probability level and H atoms are drawn as spheres of arbitrary radii. Uncoordinated water molecules have been omitted for clarity. Symmetry codes are as given in Table 1.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINTE* (Bruker, 1998); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *SHELXL97*.

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