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Poly[[cyanatocobalt(II)]bis[μ-1,4-bis(1,2,4-triazol-1-ylmethyl)benzene]]

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Key indicators

Single-crystal X-ray study
T = 193 K
Mean σ(C–C) = 0.003 Å
R factor = 0.036
wR factor = 0.086
Data-to-parameter ratio = 13.1

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

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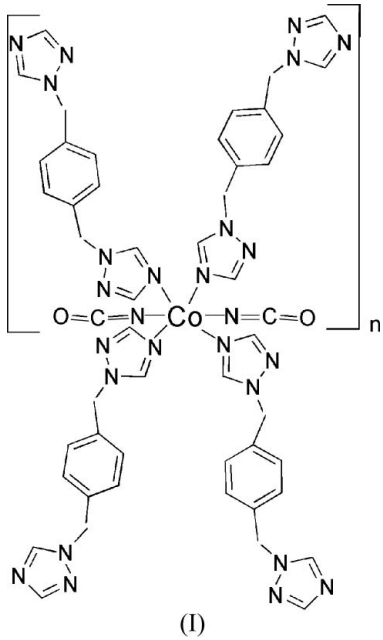
The coordination geometry of the Co^{II} atom in the title complex, $[Co(NCO)_2(C_{12}H_{12}N_6)_2]_n$ or $[Co(NCO)_2(bbtz)_2]_n$, where bbtz is 1,4-bis(1,2,4-triazol-1-methyl)benzene, is distorted octahedral, in which the Co^{II} atom lies on an inversion centre and is coordinated by four N atoms from the triazole rings of four symmetry-related bbtz ligands and two N atoms from two symmetry-related monodentate NCO^- ligands. The Co^{II} atoms are bridged by four bbtz ligands to form a two-dimensional (4,4)-network.

Comment

Recently, considerable attention has been paid to metal coordination polymers for their intriguing structures and potential applications as functional materials (Batten & Robson, 1998; Blake *et al.*, 1999; Kitagawa *et al.*, 2004). 1,2,4-Triazole and its derivatives are very interesting ligands because they combine the coordination geometry of both pyrazole and imidazole with regard to the arrangement of their three heteroatoms. Some novel coordination polymers with the flexible bis(triazole) ligands were synthesized (Haasnoot, 2000; Albada *et al.*, 2000; Zhao *et al.*, 2002; Meng *et al.*, 2004; Li *et al.*, 2005). In the present paper, we report the preparation and crystal structure of a new two-dimensional coordination polymer incorporating the 1,4-bis(1,2,4-triazol-1-ylmethyl)benzene (bbtz) ligand, $[Co(bbtz)_2(NCO)_2]_n$, (I).



(I)

As shown in Fig. 1, the Co^{II} atom of (I) occupies an inversion centre. The coordination geometry of the Co^{II} atom is

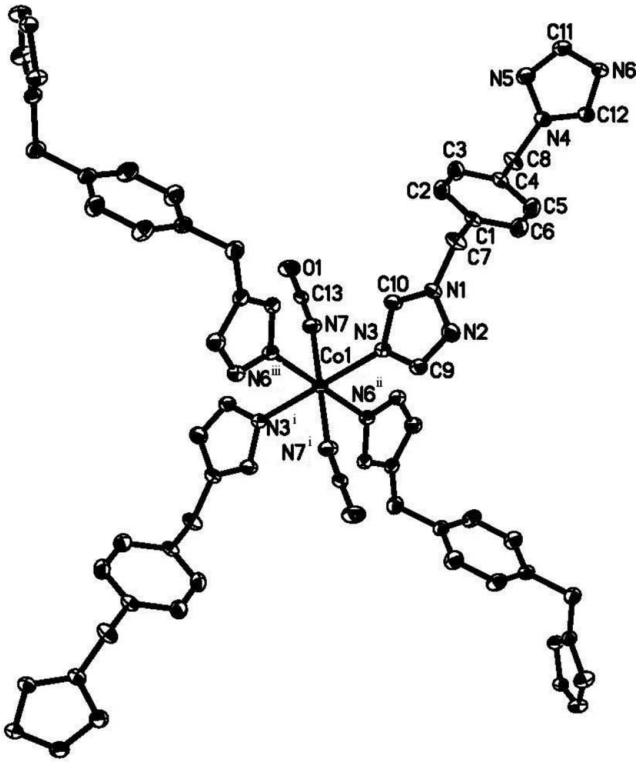


Figure 1
Part of the polymeric structure of (I), with displacement ellipsoids drawn at the 30% probability level. H atoms have been omitted for clarity. [Symmetry codes: (i) $-x$, $-y+1$, $-z+1$; (ii) $x-1$, $-y+\frac{3}{2}$, $z+\frac{1}{2}$; (iii) $-x+1$, $y-\frac{1}{2}$, $-z+\frac{1}{2}$.]

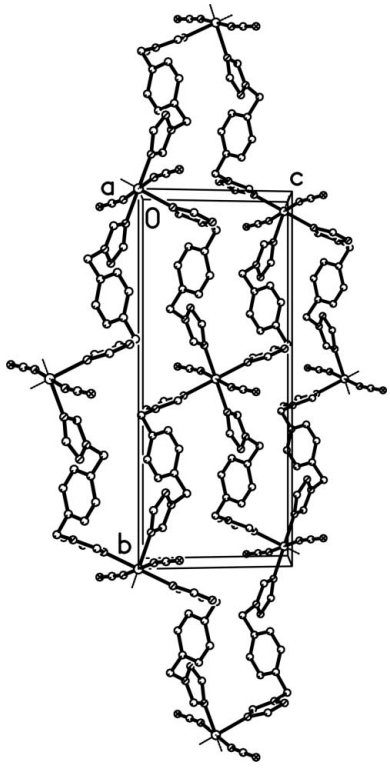


Figure 2
The two-dimensional (4,4)-network of (I). H atoms have been omitted.

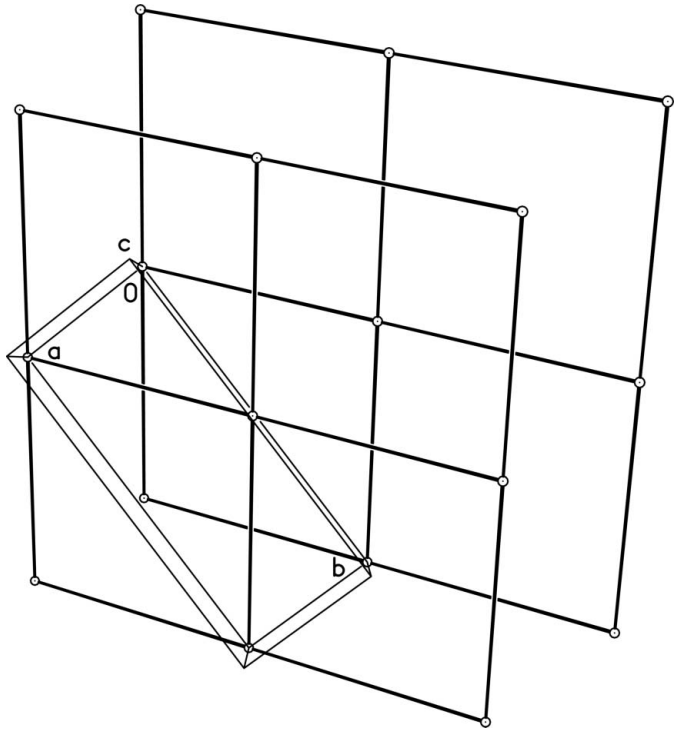


Figure 3
Schematic representation of the packing of the two-dimensional (4,4)-network of (I).

distorted octahedral, coordinated equatorially by four N atoms from the triazole rings of four symmetry-related bbtz ligands and axially by two N atoms from two symmetry-related cyanato ligands (Table 1). The *cis* N—Co—N bond angles are in the range 87.91 (7)–92.09 (7)°, close to 90°. The cyanato ligand is almost linear, in good agreement with the results usually obtained for monodentate cyanato complexes.

The methyl C atom of bbtz can freely rotate to adjust itself to the coordination environment, so bbtz can exhibit both *trans–gauche* and *gauche–gauche* conformations (Li *et al.*, 2005). The bbtz ligands exhibit the *trans–gauche* conformation in (I). The three rings (two triazole rings and one benzene ring) of one bbtz ligand are not coplanar. The dihedral angle between the two triazole planes is 58.35 (9)°. The dihedral angles between the benzene plane and the N1–N3/C9/C10 and N4–N6/C11/C12 triazole planes are 68.80 (9) and 66.17 (7)°, respectively.

As illustrated in Fig. 2, each bbtz ligand in (I) coordinates to Co^{II} atoms through its two triazole N atoms, thus acting as a bridging bidentate ligand to form a two-dimensional neutral (4,4)-network. The networks contain almost square grids (52-membered rings), with a Co^{II} atom at each corner and a bbtz ligand at each edge connecting two Co^{II} atoms. As a consequence of the symmetry of the crystal structure, the edge lengths are equal with the value of 14.4450 (14) Å. The diagonal lengths of the approximate square are 20.627 (2) and 20.228 (2) Å; the corner angles are 88.9 (1) and 91.1 (1)°.

The square-grid sheets are stacked in an offset fashion parallel to the *c* direction. The offset half-cell superpositions

of each pair of adjacent networks divides the voids into smaller rectangles whereby the cyanate anions of one sheet project into the holes of the next sheet. In the superposition structure, the sheets are arranged in the sequence ···A—B—A—B··· (Fig. 3).

Experimental

An H_2O/MeOH solution (20 ml, 1:1 *v*/*v*) of $Co(NO_3)_2{\cdot}6H_2O$ (0.146 g, 0.50 mmol) and KNCO (0.162 g, 1.00 mmol) was added to one leg of an H-shaped tube, and an H_2O/MeOH solution (20 ml, 1:1 *v*/*v*) of bbtz (0.240 g, 1.00 mmol) was added to the other leg of the tube. After several weeks, red single crystals were obtained as blocks. Found: C 49.95, H 3.81, N 31.40%; calculated for $C_{26}H_{24}CoN_{14}O_2$: C 50.08, H 3.88, N 31.46%.

Crystal data

$[Co(NCO)_2(C_{12}H_{12}N_6)_2]$
M_r = 623.52
Monoclinic, $P2_1/c$
a = 8.4172 (14) Å
b = 20.228 (3) Å
c = 8.4801 (12) Å
β = 104.225 (4)°
V = 1399.6 (4) Å^3
Z = 2
D_x = 1.480 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.67 mm^{-1}
T = 193 (2) K
Block, red
0.31 × 0.21 × 0.19 mm

Data collection

Rigaku Mercury CCD diffractometer
ω scans
Absorption correction: multi-scan (Jacobson, 1998)
T_{min} = 0.820, T_{max} = 0.884
13731 measured reflections
2566 independent reflections
2317 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 25.4°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.086
S = 1.04
2566 reflections
196 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0384P)^2 + 0.782P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—N7	2.0884 (19)	Co1—N3	2.1691 (16)
Co1—N6^{ii}	2.1660 (17)		
N7—Co1—N6^{ii}	90.43 (7)	C13—N7—Co1	168.89 (17)
N7—Co1—N3	87.91 (7)	N7—C13—O1	178.5 (2)
N6^{ii}—Co1—N3	89.52 (6)		

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

H atoms were placed in idealized positions and refined as riding, with C—H distances of 0.95 (triazole and benzene) and 0.99 Å (CH_2), and with $U_{iso}(H) = 1.2U_{eq}(C)$.

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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