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trans-Bis[4-(4-methoxyphenyl)-3,5-di-2-pyridyl-4*H*-1,2,4-triazole-κN^1]dithiocyanatocobalt(II)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.057
wR factor = 0.186
Data-to-parameter ratio = 15.3

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

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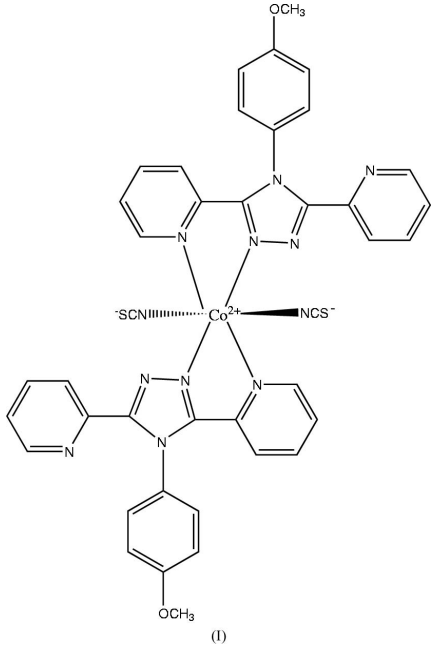
In the title centrosymmetric mononuclear cobalt(II) compound, $[Co(NCS)_2(C_{19}H_{15}N_5O)_2]$, the central Co^{II} atom is coordinated by four N atoms from two 4-(4-methoxyphenyl)-3,5-di-2-pyridyl-4*H*-1,2,4-triazole ligands and two N atoms from two thiocyanate counter-ions. The coordination geometry is slightly distorted octahedral.

Comment

Substituted 1,2,4-triazoles have been actively studied as bridging ligands, coordinating through their adjacent N atoms between transition metal(II) ions, since these complexes have interesting structures and magnetic properties (Antolini *et al.*, 1990, 1991; Bencini *et al.*, 1987; Lavrenova *et al.*, 1995). Recently, we have reported the crystal structures of nickel(II) and copper(II) complexes with the ligand 4-(4-methoxyphenyl)-3,5-di-2-pyridyl-4*H*-1,2,4-triazole (MDPT) (Shao *et al.*, 2004; Zhang *et al.*, 2005). As an extension of our work, we report here the crystal structure of a new cobalt(II) complex, (I), with the MDPT ligand.



(I)

Compound (I) consists of a centrosymmetric mononuclear cobalt(II) complex (Fig. 1), the central Co atom lying on a crystallographic inversion centre. It is six-coordinated by four N atoms from two MDPT ligands and by centrosymmetrically related N atoms from two thiocyanate anions, forming a slightly distorted octahedral environment. The Co—N distances range from 2.098 (3) to 2.147 (3) Å, *i.e.* normal values. The three *trans* angles at the Co^{II} atom are exactly 180°

by virtue of the crystallographic symmetry (Table 1), and the other angles subtended at the Co^{II} atom vary from 76.02 (9) to 103.98 (9)°. The MDPT molecule acts as a bidentate ligand. In the ligand, the dihedral angles between the triazole ring and the pyridine rings are 11.7 (2) and 40.7 (1)°.

Experimental

$Co(CH_3COO)_2{\cdot}4H_2O$, MDPT and KSCN in a molar ratio 1:2:1 were dissolved in ethanol with stirring. After allowing the resulting clear colourless solution to stand at room temperature in air for 30 d, large brown crystals were formed on slow evaporation of the solvent. The crystals were isolated and washed twice with ethanol and dried in a vacuum desiccator using $CaCl_2$ (yield 46%). Analysis found: C 57.63, H 3.68, N 20.12%; calculated for $C_{40}H_{30}CoN_{12}O_2S_2$: C 57.62, H 3.63, N 20.16%.

Crystal data

$[Co(NCS)_2(C_{19}H_{15}N_5O)_2]$
M_r = 833.81
Triclinic, $P\overline{1}$
a = 8.6247 (8) Å
b = 8.8862 (9) Å
c = 12.7604 (12) Å
α = 78.810 (2)°
β = 89.371 (2)°
γ = 81.935 (2)°
V = 949.75 (16) Å^3
Z = 1
D_x = 1.458 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2041 reflections
θ = 4.6–28.4°
μ = 0.62 mm^{-1}
T = 298 (2) K
Block, brown
0.31 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.832, T_{max} = 0.897
5626 measured reflections
3974 independent reflections
3589 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 27.0°
$h = -10 \rightarrow 11$
$k = -11 \rightarrow 11$
$l = -16 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.186
S = 1.21
3974 reflections
260 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1084P)^2 + 0.1232P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.011
$\Delta\rho_{max}$ = 0.76 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—N6	2.098 (3)	Co1—N1	2.147 (3)
Co1—N2	2.124 (2)		
N6^i—Co1—N6	180	N2—Co1—N1^i	103.98 (9)
N6—Co1—N2^i	84.93 (11)	N6—Co1—N1	91.88 (10)
N6—Co1—N2	95.07 (11)	N2—Co1—N1	76.02 (9)
N2^i—Co1—N2	180	N1^i—Co1—N1	180
N6—Co1—N1^i	88.12 (10)		

Symmetry code: (i) $2-x, -y, -z$.

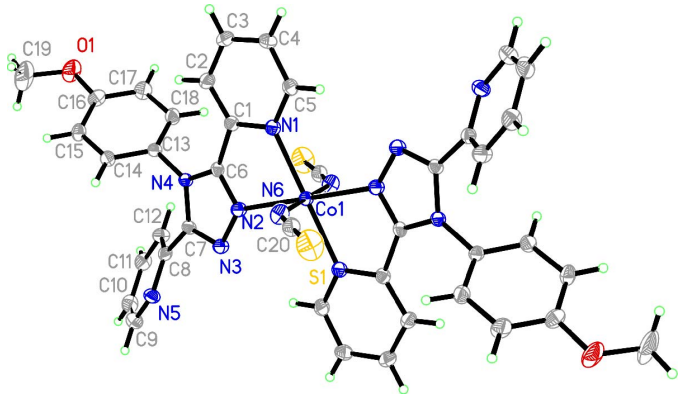


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. Unlabelled atoms are related to labelled atoms by $(2-x, -y, -z)$.

H atoms were positioned geometrically and constrained to ride on their parent atoms, with C—H distances of 0.93 or 0.96 Å, and with U_{iso}(H) values of 1.2 or 1.5 (for methyl) times U_{eq}(carrier atom).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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