

cis-Bis(2,2'-bipyridyl)dicyanatocobalt(II)

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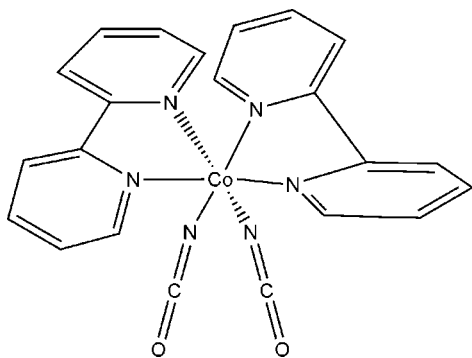
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.040; wR factor = 0.078; data-to-parameter ratio = 13.3.

In the title complex, $[\text{Co}(\text{NCO})_2(\text{C}_{10}\text{H}_8\text{N}_2)_2]$, the Co atom is coordinated by four N atoms from two 2,2'-bipyridyl ligands and two N atoms from two cyanate anions in a distorted octahedral geometry. The Co atom lies on a twofold rotation axis. The average Co—N bond length is 2.126 (7) Å. Weak intermolecular C—H...O interactions lead to the formation of a three-dimensional network.

Related literature

For the crystal structures of cobalt complexes with analogous ligands, see: Veidis *et al.* (1981); Tang *et al.* (2004). For related literature, see: Milani *et al.* (2003).



Experimental

Crystal data

$[\text{Co}(\text{NCO})_2(\text{C}_{10}\text{H}_8\text{N}_2)_2]$
 $M_r = 455.34$
 Orthorhombic, $Pbcn$
 $a = 14.148$ (12) Å
 $b = 9.774$ (8) Å
 $c = 15.253$ (13) Å

$V = 2109$ (3) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.84$ mm⁻¹
 $T = 298$ (2) K
 $0.30 \times 0.25 \times 0.06$ mm

Data collection

Bruker SMART 1000 diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.786$, $T_{\max} = 0.951$

10457 measured reflections
 1870 independent reflections
 1009 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.078$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.078$
 $S = 1.00$
 1870 reflections

141 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.25$ e Å⁻³
 $\Delta\rho_{\min} = -0.30$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Co1—N1	2.027 (3)	Co1—N3	2.176 (3)
Co1—N2	2.162 (3)		
N1 ⁱ —Co1—N1	97.0 (2)	N1—Co1—N3	93.59 (11)
N1 ⁱ —Co1—N2	166.18 (11)	N2—Co1—N3	75.22 (11)
N1—Co1—N2	90.76 (12)	N2 ⁱ —Co1—N3	97.44 (10)
N2—Co1—N2 ⁱ	84.07 (14)	N3—Co1—N3 ⁱ	170.29 (13)
N1 ⁱ —Co1—N3	92.83 (12)		

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C10—H10...O1 ⁱⁱ	0.93	2.50	3.236 (5)	137
C5—H5...O1 ⁱⁱⁱ	0.93	2.48	3.198 (5)	134

 Symmetry codes: (ii) $-x + \frac{1}{2}, -y + \frac{5}{2}, z + \frac{1}{2}$; (iii) $-x + 1, -y + 2, -z + 1$.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FI2060).

References

- Milani, B., Stabon, E., Zangrando, E., Mestroni, G., Sommazzi, A., Zannoni, C. (2003). *Inorg. Chim. Acta*, **349**, 209–216.
 Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
 Sheldrick, G. M. (2008). *Acta Cryst. A* **64**, 112–122.
 Siemens (1996). SMART and SAINT. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
 Tang, X. F., Ma, Y. S., Liang, F. P., Hu, R. X. & Yu, K. B. (2004). *Hua Xue Ying Yong Yu Yanjiu*, **16**, 459–462.
 Veidis, M. V., Dockum, B., Charron, F. F. & Reiff, W. M. (1981). *Inorg. Chim. Acta*, **53**, L197–L199.

supplementary materials

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***cis*-Bis(2,2'-bipyridyl)dicyanatocobalt(II)**

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Comment

Organometallic Co derivatives are applied as catalysts in polymerization reactions of polar olefins and for the elucidation of the hypothetical mechanism of these polymerization reactions (Milani *et al.*, 2003). In recent years the synthesis of the without bridge bonding mononucleate complex was used to find out the information to design the multidimensional structure complexes, so the homologic ligands complex [Co(2,2'-bipy)₂(N₃)₂].Cl.2H₂O was reported (Tang *et al.*, 2004). In this paper, Co(C₁₀H₈N₂)₂(NCO)₂ was synthesized by the reaction of CoCl₂.6H₂O, 2,2'-bipyridyl and NaOCN at room temperature and the structure of the resulting complex is presented here (Fig. 1).

The Co atom lies on a special position (Wyckoff position 4c, site symmetry 2). It is formed by coordination of two 2,2'-bipyridyls ligands and two cyanate anions. The coordination geometry of the central Co atom is distorted octahedral with four N atoms from two 2,2'-bipyridyls and two N atoms from two cyanate anions. The equatorial plane consists of N1, N2, N3 and N3ⁱ with an average bond length of 2.135 (3) Å. The apical positions are occupied by a cyanate anion and a N atom from a 2,2'-bipyridyl with the bond length 2.027 (3) Å and 2.162 (3) Å, respectively. The distances Co—N(2,2'-bipyridyl) in the title complex are significantly longer (2.176 (3) Å and 2.162 (3) Å) than those in the comparable bond length (1.950 (3) Å and 1.954 (3) Å, Tang *et al.* (2004)). The complexes arrange into a three-dimensional network *via* weak intermolecular C—H⋯O interactions (H⋯O distances: 2.499 (3) Å and 2.481 (4) Å; C⋯O distances: 3.417 (5) Å and 3.084 (7) Å).

Experimental

CoCl₂.6H₂O (0.0476 g 0.2 mmol) was dissolved in 10 ml MeOH, the solution was then added to an aqueous solution of 2,2'-bipyridyl (0.0316 g 0.2 mmol). The reaction mixture was stirred for 10 minutes until the solution color became red. NaOCN (0.0130 g 0.2 mmol) was added to the reaction mixture. The mixture was filtered and red single crystals were obtained by slow evaporation of the mother liquid for three weeks at room temperature. Elemental analysis for C₂₂H₁₆CoN₆S₂ calculated: C 58.03, H 3.54, N 18.45%; found: C 58.23, H 3.23, N 18.30%.

Refinement

All H atoms were placed geometrically and treated as riding on their parent atoms with C—H 0.93 Å (2,2'-bipyridyl) [*U*_{iso}(H) = 1.2*U*_{eq}(C)].

Figures

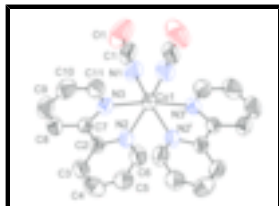


Fig. 1. The crystal structure of the title compound showing the atomic numbering and 30% probability displacement ellipsoids. H atoms have been omitted for clarity. The second ligand is generated by $i: -x+1, y, -z+3/2$.

(I)

Crystal data

$[\text{Co}(\text{NCO})_2(\text{C}_{10}\text{H}_8\text{N}_2)_2]$

$M_r = 455.34$

Orthorhombic, $Pbcn$

Hall symbol: $-P2n2ab$

$a = 14.148$ (12) Å

$b = 9.774$ (8) Å

$c = 15.253$ (13) Å

$V = 2109$ (3) Å³

$Z = 4$

$F_{000} = 932$

$D_x = 1.434$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 1484 reflections

$\theta = 2.5$ – 20.8°

$\mu = 0.85$ mm⁻¹

$T = 298$ (2) K

Plate, red

$0.30 \times 0.25 \times 0.06$ mm

Data collection

Bruker Smart 1000
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298$ (2) K

φ & ω scans

Absorption correction: multi-scan
[SADABS; Sheldrick, 1996]

$T_{\min} = 0.786$, $T_{\max} = 0.951$

10457 measured reflections

1870 independent reflections

1009 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.078$

$\theta_{\max} = 25.0^\circ$

$\theta_{\min} = 2.5^\circ$

$h = -16 \rightarrow 14$

$k = -11 \rightarrow 9$

$l = -18 \rightarrow 17$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.039$

$wR(F^2) = 0.078$

$S = 1.00$

1870 reflections

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0386P)^2 + 2.2714P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.25$ e Å⁻³

141 parameters

$$\Delta\rho_{\min} = -0.30 \text{ e } \text{\AA}^{-3}$$

Primary atom site location: structure-invariant direct methods

Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.5000	1.02936 (6)	0.7500	0.0514 (2)
N1	0.45099 (19)	1.1668 (3)	0.6615 (2)	0.0780 (10)
N2	0.42837 (17)	0.8651 (2)	0.68223 (17)	0.0525 (7)
N3	0.36432 (16)	1.0105 (3)	0.81603 (17)	0.0538 (7)
O1	0.4129 (2)	1.3351 (3)	0.5593 (2)	0.1331 (13)
C1	0.4337 (2)	1.2469 (5)	0.6118 (3)	0.0737 (12)
C2	0.3390 (2)	0.8363 (3)	0.7088 (2)	0.0501 (8)
C3	0.2898 (2)	0.7277 (4)	0.6735 (2)	0.0655 (10)
H3	0.2289	0.7081	0.6927	0.079*
C4	0.3309 (3)	0.6491 (4)	0.6103 (3)	0.0802 (12)
H4	0.2983	0.5754	0.5863	0.096*
C5	0.4205 (3)	0.6794 (4)	0.5821 (2)	0.0738 (11)
H5	0.4496	0.6275	0.5388	0.089*
C6	0.4657 (2)	0.7879 (4)	0.6196 (2)	0.0669 (10)
H6	0.5263	0.8090	0.6002	0.080*
C7	0.3019 (2)	0.9245 (3)	0.7788 (2)	0.0511 (9)
C8	0.2077 (2)	0.9216 (3)	0.8059 (3)	0.0676 (10)
H8	0.1645	0.8642	0.7784	0.081*
C9	0.1797 (3)	1.0036 (4)	0.8731 (3)	0.0808 (13)
H9	0.1172	1.0020	0.8921	0.097*
C10	0.2434 (3)	1.0881 (4)	0.9122 (2)	0.0804 (12)
H10	0.2256	1.1444	0.9585	0.096*
C11	0.3354 (2)	1.0883 (3)	0.8814 (2)	0.0685 (10)
H11	0.3790	1.1460	0.9082	0.082*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0391 (3)	0.0536 (4)	0.0615 (4)	0.000	0.0011 (3)	0.000

supplementary materials

N1	0.064 (2)	0.078 (2)	0.092 (3)	0.0116 (17)	0.0007 (18)	0.0301 (19)
N2	0.0402 (15)	0.0601 (19)	0.0573 (19)	0.0020 (13)	0.0000 (14)	-0.0038 (14)
N3	0.0457 (15)	0.0555 (19)	0.0603 (19)	0.0050 (14)	0.0027 (14)	-0.0032 (14)
O1	0.115 (2)	0.152 (3)	0.133 (3)	0.055 (2)	0.025 (2)	0.070 (2)
C1	0.052 (2)	0.090 (4)	0.079 (3)	0.020 (2)	0.018 (2)	0.012 (2)
C2	0.0385 (19)	0.056 (2)	0.056 (2)	-0.0010 (17)	-0.0047 (17)	0.0121 (17)
C3	0.051 (2)	0.070 (3)	0.076 (3)	-0.011 (2)	-0.0061 (19)	0.004 (2)
C4	0.087 (3)	0.077 (3)	0.077 (3)	-0.020 (2)	-0.011 (2)	-0.012 (2)
C5	0.074 (3)	0.074 (3)	0.072 (3)	0.001 (2)	0.001 (2)	-0.019 (2)
C6	0.053 (2)	0.079 (3)	0.069 (3)	-0.0057 (19)	-0.0008 (19)	-0.009 (2)
C7	0.0420 (19)	0.047 (2)	0.064 (3)	0.0030 (16)	0.0052 (16)	0.0113 (16)
C8	0.046 (2)	0.071 (3)	0.086 (3)	-0.0028 (18)	0.009 (2)	0.010 (2)
C9	0.053 (2)	0.092 (4)	0.097 (3)	0.012 (2)	0.028 (2)	0.016 (3)
C10	0.079 (3)	0.077 (3)	0.086 (3)	0.014 (2)	0.033 (3)	0.002 (2)
C11	0.062 (2)	0.066 (3)	0.078 (3)	0.0021 (19)	0.013 (2)	-0.009 (2)

Geometric parameters (Å, °)

Co1—N1 ⁱ	2.027 (3)	C3—H3	0.9300
Co1—N1	2.027 (3)	C4—C5	1.371 (4)
Co1—N2	2.162 (3)	C4—H4	0.9300
Co1—N2 ⁱ	2.162 (3)	C5—C6	1.364 (4)
Co1—N3	2.176 (3)	C5—H5	0.9300
Co1—N3 ⁱ	2.176 (3)	C6—H6	0.9300
N1—C1	1.117 (4)	C7—C8	1.396 (4)
N2—C6	1.327 (4)	C8—C9	1.360 (4)
N2—C2	1.358 (3)	C8—H8	0.9300
N3—C11	1.319 (4)	C9—C10	1.361 (5)
N3—C7	1.345 (3)	C9—H9	0.9300
O1—C1	1.213 (4)	C10—C11	1.384 (4)
C2—C3	1.378 (4)	C10—H10	0.9300
C2—C7	1.469 (4)	C11—H11	0.9300
C3—C4	1.363 (4)		
N1 ⁱ —Co1—N1	97.0 (2)	C4—C3—H3	120.2
N1 ⁱ —Co1—N2	166.18 (11)	C2—C3—H3	120.2
N1—Co1—N2	90.76 (12)	C3—C4—C5	119.6 (4)
N1 ⁱ —Co1—N2 ⁱ	90.76 (12)	C3—C4—H4	120.2
N1—Co1—N2 ⁱ	166.18 (11)	C5—C4—H4	120.2
N2—Co1—N2 ⁱ	84.07 (14)	C6—C5—C4	118.1 (4)
N1 ⁱ —Co1—N3	92.83 (12)	C6—C5—H5	121.0
N1—Co1—N3	93.59 (11)	C4—C5—H5	121.0
N2—Co1—N3	75.22 (11)	N2—C6—C5	123.8 (3)
N2 ⁱ —Co1—N3	97.44 (10)	N2—C6—H6	118.1
N1 ⁱ —Co1—N3 ⁱ	93.59 (11)	C5—C6—H6	118.1
N1—Co1—N3 ⁱ	92.83 (12)	N3—C7—C8	121.0 (3)
N2—Co1—N3 ⁱ	97.44 (10)	N3—C7—C2	116.1 (3)

N2 ⁱ —Co1—N3 ⁱ	75.22 (11)	C8—C7—C2	123.0 (3)
N3—Co1—N3 ⁱ	170.29 (13)	C9—C8—C7	119.3 (3)
C1—N1—Co1	172.6 (3)	C9—C8—H8	120.3
C6—N2—C2	117.9 (3)	C7—C8—H8	120.3
C6—N2—Co1	125.4 (2)	C8—C9—C10	119.7 (3)
C2—N2—Co1	116.6 (2)	C8—C9—H9	120.2
C11—N3—C7	118.4 (3)	C10—C9—H9	120.2
C11—N3—Co1	125.1 (2)	C9—C10—C11	118.4 (4)
C7—N3—Co1	115.9 (2)	C9—C10—H10	120.8
N1—C1—O1	178.3 (5)	C11—C10—H10	120.8
N2—C2—C3	120.9 (3)	N3—C11—C10	123.2 (3)
N2—C2—C7	115.3 (3)	N3—C11—H11	118.4
C3—C2—C7	123.7 (3)	C10—C11—H11	118.4
C4—C3—C2	119.6 (3)		

Symmetry codes: (i) $-x+1, y, -z+3/2$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C10—H10 \cdots O1 ⁱⁱ	0.93	2.50	3.236 (5)	137
C5—H5 \cdots O1 ⁱⁱⁱ	0.93	2.48	3.198 (5)	134

Symmetry codes: (ii) $-x+1/2, -y+5/2, z+1/2$; (iii) $-x+1, -y+2, -z+1$.

Fig. 1

