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Bis(2,2′-bipyridine-κ^2N,N')(carbonato-κ^2O,O')cobalt(III) trifluoromethanesulfonate

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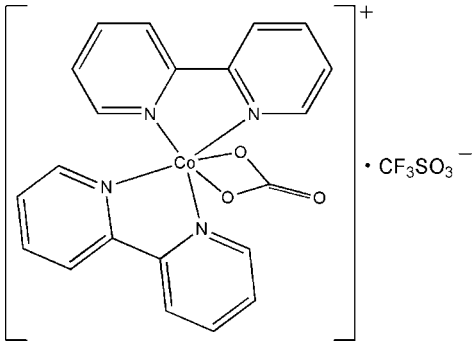
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.007 Å; R factor = 0.053; wR factor = 0.137; data-to-parameter ratio = 11.8.

In the title compound, $[Co(CO_3)(C_{10}H_8N_2)_2](CF_3SO_3)$, the Co^{III} ion is coordinated by four N atoms from two chelating 2,2′-bipyridine ligands and two O atoms from a bidentate chelating carbonate anion, and has a distorted octahedral environment. C—H···O hydrogen bonding is observed between bipyridine ligands and uncoordinated $(CF_3SO_3)^-$ anions and between bipyridine and carbonate ligands.

Related literature

For general background, see Belli *et al.* (2003); Leitner (1996); Yin & Moss (1999); Clark & Buckingham (1997); Catherine *et al.* (2003); Paul *et al.* (2005); Kim *et al.* (2004); Louise *et al.* (2001). For related structures, see Niederhoffer *et al.* (1982).



Experimental

Crystal data

$[Co(CO_3)(C_{10}H_8N_2)_2](CF_3O_3S)$
M_r = 580.38
Triclinic, $P\overline{1}$
a = 7.115 (3) Å
b = 11.054 (5) Å
c = 14.543 (6) Å
α = 95.668 (6)°
β = 94.203 (5)°
γ = 90.046 (6)°
V = 1135.1 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.92 mm^{-1}
T = 293 (2) K
0.25 × 0.12 × 0.10 mm

Data collection

Bruker APEX II CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.874, T_{max} = 0.921
6004 measured reflections
3928 independent reflections
2647 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.137
S = 1.05
3928 reflections
334 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O2	1.882 (3)	Co1—N2	1.940 (4)
Co1—O3	1.889 (3)	Co1—N3	1.929 (4)
Co1—N1	1.917 (4)	Co1—N4	1.922 (4)
O2—Co1—O3	69.39 (14)	N1—Co1—N3	97.16 (15)
O2—Co1—N1	87.40 (14)	N4—Co1—N3	83.45 (16)
O3—Co1—N1	91.32 (14)	O2—Co1—N2	96.67 (15)
O2—Co1—N4	92.14 (15)	O3—Co1—N2	165.10 (14)
O3—Co1—N4	89.29 (14)	N1—Co1—N2	82.56 (15)
N1—Co1—N4	179.06 (16)	N4—Co1—N2	96.68 (15)
O2—Co1—N3	167.98 (14)	N3—Co1—N2	94.95 (16)
O3—Co1—N3	99.30 (15)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···O5^{i}	0.93	2.39	3.266 (9)	157
C10—H10···O1^{ii}	0.93	2.30	3.137 (6)	149
C17—H17···O2^{iii}	0.93	2.32	3.155 (6)	148

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; 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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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2269).

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supplementary materials

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Bis(2,2'-bipyridine-κ^2N,N')(carbonato-κ^2O,O')cobalt(III) trifluoromethanesulfonate

Y.-X. Lv, Y. Ling, H. Li and L. Zhang

Comment

Cobalt ions are found in many metalloenzymes (carbonic anhydrase, cobalt chelatase *etc*.) to play various functions at physiological conditions. Carbonic anhydrase (CA) is an important cobalt-containing metalloenzyme at active center and catalyzes the reversible hydration of carbon dioxide to bicarbonate to tune the physiological function of carbon dioxide (Belli *et al.*, 2003; Leitner, 1996; Yin & Moss, 1999). Therefore, a great deal of research has been performed on the chemical fixation and activation of carbon dioxide and on mimicking the function of CA (Clark & Buckingham, 1997; Catherine *et al.*, 2003; Paul *et al.*, 2005; Kim *et al.*, 2004; Louize *et al.*, 2001). A few of carbonate- and bicarbonate-cobalt complexes in bidentate chelate or tridentate bridge modes have been characterized by X-ray crystallography and reported. In order to further understand the feature of the species, we report in this paper the synthesis and crystal structural of the title compound.

The crystal structure of the title compound consists of Co^{III} complex cation and $(CF_3SO_3)^-$ counteranion, as shown in Fig. 1. In the cation, the central Co^{III} ion is six-coordinated in distroted octahedral coordiantion geometry. The equatorial plane is defined by two nitrogen atoms from two bipy ligands and two chelated oxygen atoms from a carbonate ion, while the other two nitrogen atoms from two bipy ligands occupy the axial positions. The average Co—N bond length is of 1.927 (4) Å (Table 1), which are similar to that found in *cis*-(carbonato)bis(2,2'-bipy)cobalt(III) nitrate pentahydrate (Niederhoffer *et al.*, 1982). The dihedral angles of 2,2'-bipy in the complex are 6.865 (3) and 3.294 (3)° between C15-ring and C16-ring and between C5-ring and C6-ring, respectively.

The C—H···O hydrogen bonding is observed between bipyridine ring and $(CF_3SO_3)^-$ anion and between bipyridine ring and carbonate anion (Table 2).

Experimental

To a mixture of $Co(CF_3SO_3)_2{\cdot}4H_2O$ (0.430 g, 1.0 mmol) and 2,2'-bipyridine (0.370 g, 2.0 mmol) in water-ethanol (1:1, 10 ml) was added dropwise an aqueous solution (4 ml, 0.5 *M*) of $NaHCO_3$. The solution was stirred at room temperature for 1 h and filtered. The clear solution was kept at room temperature to slowly evaporate for two weeks to obtain single crystals of the title compound. Anal. Calcd. for $C_{22}H_{16}CoF_3N_4O_6S$: C, 45.53; H, 2.78; N, 9.66%. Found: C, 45.49; H, 2.83; N, 9.66%.

Refinement

H atoms were placed in calculated positions with C—H = 0.93 Å and refined using a riding model with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

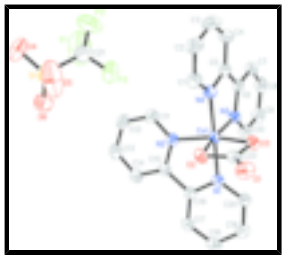


Fig. 1. The molecular structure of the title compound with 30% thermal ellipsoids.

Bis(2,2'-bipyridine-κ^2*N*,*N*')(carbonato-κ^2*O*,*O*')cobalt(III) trifluoromethanesulfonate

Crystal data

$[Co(CO_3)(C_{10}H_8N_2)_2](CF_3O_3S_1)$	$Z = 2$
$M_r = 580.38$	$F_{000} = 588$
Triclinic, $P\overline{1}$	$D_x = 1.698$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.115$ (3) Å	Cell parameters from 1120 reflections
$b = 11.054$ (5) Å	$\theta = 2.4$–22.1º
$c = 14.543$ (6) Å	$\mu = 0.92$ mm^{-1}
$\alpha = 95.668$ (6)º	$T = 293$ (2) K
$\beta = 94.203$ (5)º	BLOCK, red
$\gamma = 90.046$ (6)º	0.25 × 0.12 × 0.10 mm
$V = 1135.1$ (8) Å^3	

Data collection

Bruker APEXII CCD area-detector diffractometer	3928 independent reflections
Radiation source: fine-focus sealed tube	2647 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.029$
$T = 293$(2) K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 1.8$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -8 \rightarrow 8$
$T_{min} = 0.874$, $T_{max} = 0.921$	$k = -6 \rightarrow 13$
6004 measured reflections	$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.053$	H-atom parameters constrained
$wR(F^2) = 0.137$	$w = 1/[\sigma^2(F_o^2) + (0.0368P)^2 + 1.2958P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.001$
3928 reflections	$\Delta\rho_{max} = 0.57$ e Å^{-3}
334 parameters	$\Delta\rho_{min} = -0.53$ e Å^{-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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.53111 (8)	0.76556 (6)	0.87210 (4)	0.0400 (2)
O1	0.9665 (5)	0.7961 (4)	1.0058 (2)	0.0663 (10)
O2	0.7420 (4)	0.6829 (3)	0.9198 (2)	0.0493 (8)
O3	0.7106 (4)	0.8768 (3)	0.9342 (2)	0.0458 (8)
N1	0.4185 (5)	0.7458 (3)	0.9855 (2)	0.0397 (9)
N2	0.3808 (5)	0.6222 (3)	0.8281 (2)	0.0432 (9)
N3	0.3506 (5)	0.8790 (3)	0.8257 (2)	0.0425 (9)
N4	0.6441 (5)	0.7825 (3)	0.7580 (3)	0.0456 (9)
C1	0.7991 (7)	0.7255 (5)	0.7293 (4)	0.0583 (13)
H1	0.8549	0.6672	0.7641	0.070*
C2	0.8765 (8)	0.7509 (6)	0.6505 (4)	0.0705 (16)
H2	0.9836	0.7100	0.6318	0.085*
C3	0.7959 (9)	0.8373 (6)	0.5987 (4)	0.0752 (18)
H3	0.8489	0.8563	0.5453	0.090*
C4	0.6367 (8)	0.8951 (5)	0.6266 (3)	0.0641 (15)
H4	0.5794	0.9532	0.5920	0.077*
C5	0.5618 (7)	0.8662 (4)	0.7070 (3)	0.0471 (12)
C6	0.3905 (6)	0.9196 (4)	0.7445 (3)	0.0454 (11)
C7	0.2779 (8)	1.0020 (5)	0.7022 (4)	0.0582 (13)
H7	0.3074	1.0288	0.6463	0.070*
C8	0.1204 (8)	1.0438 (5)	0.7445 (4)	0.0653 (15)
H8	0.0413	1.0990	0.7170	0.078*
C9	0.0802 (7)	1.0038 (5)	0.8275 (4)	0.0618 (14)
H9	−0.0250	1.0321	0.8572	0.074*
C10	0.1985 (6)	0.9213 (4)	0.8657 (3)	0.0505 (12)
H10	0.1713	0.8940	0.9218	0.061*

C11	0.3564 (7)	0.5689 (5)	0.7410 (3)	0.0563 (13)
H11	0.4067	0.6063	0.6937	0.068*
C12	0.2604 (8)	0.4618 (5)	0.7194 (4)	0.0678 (16)
H12	0.2447	0.4275	0.6582	0.081*
C13	0.1873 (7)	0.4052 (5)	0.7887 (4)	0.0644 (15)
H13	0.1231	0.3316	0.7752	0.077*
C14	0.2100 (7)	0.4589 (5)	0.8791 (4)	0.0544 (13)
H14	0.1615	0.4219	0.9271	0.065*
C15	0.3056 (6)	0.5680 (4)	0.8965 (3)	0.0410 (11)
C16	0.3330 (6)	0.6378 (4)	0.9882 (3)	0.0390 (10)
C17	0.2752 (6)	0.6004 (4)	1.0690 (3)	0.0469 (11)
H17	0.2198	0.5242	1.0695	0.056*
C18	0.3008 (7)	0.6775 (5)	1.1488 (3)	0.0539 (13)
H18	0.2643	0.6540	1.2046	0.065*
C19	0.3809 (7)	0.7896 (5)	1.1453 (3)	0.0551 (13)
H19	0.3952	0.8441	1.1984	0.066*
C20	0.4394 (6)	0.8207 (5)	1.0638 (3)	0.0481 (12)
H20	0.4956	0.8964	1.0624	0.058*
C21	0.3001 (11)	0.6267 (7)	0.4529 (5)	0.087 (2)
C22	0.8195 (7)	0.7871 (5)	0.9570 (3)	0.0483 (12)
S1	0.2292 (3)	0.77396 (14)	0.42698 (10)	0.0751 (5)
F1	0.4729 (8)	0.6320 (6)	0.4945 (5)	0.194 (3)
F2	0.1955 (10)	0.5801 (5)	0.5083 (4)	0.174 (3)
F3	0.3080 (8)	0.5490 (4)	0.3809 (3)	0.1387 (18)
O4	0.2291 (6)	0.8439 (5)	0.5120 (3)	0.1022 (15)
O5	0.0497 (10)	0.7494 (5)	0.3834 (5)	0.189 (4)
O6	0.3662 (13)	0.8078 (5)	0.3710 (4)	0.197 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0416 (4)	0.0350 (4)	0.0438 (4)	0.0002 (3)	0.0041 (3)	0.0059 (3)
O1	0.047 (2)	0.087 (3)	0.065 (2)	0.0043 (19)	−0.0060 (18)	0.011 (2)
O2	0.0482 (18)	0.0407 (19)	0.060 (2)	0.0047 (15)	0.0050 (15)	0.0114 (16)
O3	0.0435 (17)	0.0426 (19)	0.0517 (18)	−0.0034 (15)	0.0007 (14)	0.0080 (15)
N1	0.037 (2)	0.038 (2)	0.044 (2)	0.0002 (17)	0.0006 (16)	0.0049 (18)
N2	0.044 (2)	0.041 (2)	0.044 (2)	−0.0018 (18)	0.0034 (17)	0.0033 (18)
N3	0.042 (2)	0.042 (2)	0.044 (2)	−0.0042 (18)	0.0030 (17)	0.0085 (18)
N4	0.047 (2)	0.040 (2)	0.050 (2)	0.0001 (19)	0.0070 (18)	0.0054 (19)
C1	0.055 (3)	0.058 (3)	0.062 (3)	0.011 (3)	0.016 (3)	0.001 (3)
C2	0.065 (4)	0.083 (4)	0.064 (4)	−0.002 (3)	0.027 (3)	−0.004 (3)
C3	0.072 (4)	0.103 (5)	0.052 (3)	−0.010 (4)	0.022 (3)	0.006 (3)
C4	0.074 (4)	0.071 (4)	0.049 (3)	−0.008 (3)	0.007 (3)	0.013 (3)
C5	0.053 (3)	0.045 (3)	0.042 (3)	−0.014 (2)	0.003 (2)	0.000 (2)
C6	0.051 (3)	0.038 (3)	0.046 (3)	−0.006 (2)	−0.005 (2)	0.005 (2)
C7	0.074 (4)	0.047 (3)	0.052 (3)	0.000 (3)	−0.005 (3)	0.009 (3)
C8	0.072 (4)	0.047 (3)	0.073 (4)	0.009 (3)	−0.022 (3)	0.005 (3)
C9	0.053 (3)	0.060 (4)	0.070 (4)	0.010 (3)	−0.003 (3)	0.000 (3)

C10	0.047 (3)	0.052 (3)	0.053 (3)	0.003 (2)	0.001 (2)	0.005 (2)
C11	0.064 (3)	0.055 (3)	0.048 (3)	−0.006 (3)	0.004 (2)	−0.002 (3)
C12	0.076 (4)	0.066 (4)	0.057 (3)	−0.018 (3)	0.001 (3)	−0.012 (3)
C13	0.062 (3)	0.051 (3)	0.077 (4)	−0.014 (3)	−0.003 (3)	−0.002 (3)
C14	0.053 (3)	0.046 (3)	0.065 (3)	−0.008 (2)	0.005 (2)	0.008 (3)
C15	0.035 (2)	0.037 (3)	0.052 (3)	0.002 (2)	0.002 (2)	0.009 (2)
C16	0.031 (2)	0.039 (3)	0.048 (3)	0.0063 (19)	−0.0009 (19)	0.008 (2)
C17	0.048 (3)	0.041 (3)	0.054 (3)	−0.001 (2)	0.007 (2)	0.013 (2)
C18	0.051 (3)	0.066 (4)	0.048 (3)	0.004 (3)	0.011 (2)	0.017 (3)
C19	0.054 (3)	0.065 (4)	0.045 (3)	−0.002 (3)	0.004 (2)	−0.002 (3)
C20	0.049 (3)	0.049 (3)	0.046 (3)	−0.004 (2)	0.004 (2)	0.003 (2)
C21	0.108 (6)	0.083 (5)	0.073 (4)	0.016 (4)	0.014 (4)	0.010 (4)
C22	0.046 (3)	0.057 (3)	0.045 (3)	0.002 (3)	0.010 (2)	0.014 (2)
S1	0.1093 (13)	0.0584 (10)	0.0538 (8)	−0.0008 (9)	−0.0114 (8)	0.0005 (7)
F1	0.145 (5)	0.146 (5)	0.273 (8)	0.056 (4)	−0.081 (5)	0.002 (5)
F2	0.258 (7)	0.129 (4)	0.163 (5)	0.031 (4)	0.107 (5)	0.078 (4)
F3	0.222 (5)	0.069 (3)	0.125 (4)	0.021 (3)	0.047 (4)	−0.015 (3)
O4	0.097 (3)	0.107 (4)	0.091 (3)	0.011 (3)	0.000 (2)	−0.042 (3)
O5	0.210 (7)	0.094 (4)	0.230 (7)	0.015 (4)	−0.175 (6)	−0.009 (4)
O6	0.374 (11)	0.085 (4)	0.153 (5)	−0.046 (5)	0.164 (7)	0.005 (4)

Geometric parameters (Å, °)

Co1—O2	1.882 (3)	C8—C9	1.376 (7)
Co1—O3	1.889 (3)	C8—H8	0.9300
Co1—N1	1.917 (4)	C9—C10	1.371 (7)
Co1—N2	1.940 (4)	C9—H9	0.9300
Co1—N3	1.929 (4)	C10—H10	0.9300
Co1—N4	1.922 (4)	C11—C12	1.364 (7)
O1—C22	1.218 (5)	C11—H11	0.9300
O2—C22	1.325 (6)	C12—C13	1.370 (7)
O3—C22	1.312 (6)	C12—H12	0.9300
N1—C20	1.338 (5)	C13—C14	1.387 (7)
N1—C16	1.345 (5)	C13—H13	0.9300
N2—C11	1.343 (6)	C14—C15	1.377 (6)
N2—C15	1.352 (5)	C14—H14	0.9300
N3—C10	1.330 (6)	C15—C16	1.473 (6)
N3—C6	1.352 (5)	C16—C17	1.374 (6)
N4—C1	1.343 (6)	C17—C18	1.372 (7)
N4—C5	1.350 (6)	C17—H17	0.9300
C1—C2	1.360 (7)	C18—C19	1.371 (7)
C1—H1	0.9300	C18—H18	0.9300
C2—C3	1.374 (8)	C19—C20	1.360 (6)
C2—H2	0.9300	C19—H19	0.9300
C3—C4	1.369 (8)	C20—H20	0.9300
C3—H3	0.9300	C21—F2	1.280 (7)
C4—C5	1.384 (6)	C21—F3	1.291 (7)
C4—H4	0.9300	C21—F1	1.329 (8)
C5—C6	1.473 (7)	C21—S1	1.773 (7)

C6—C7	1.375 (7)	S1—O6	1.389 (6)
C7—C8	1.375 (7)	S1—O4	1.392 (4)
C7—H7	0.9300	S1—O5	1.398 (5)
O2—Co1—O3	69.39 (14)	C9—C8—H8	120.1
O2—Co1—N1	87.40 (14)	C10—C9—C8	118.6 (5)
O3—Co1—N1	91.32 (14)	C10—C9—H9	120.7
O2—Co1—N4	92.14 (15)	C8—C9—H9	120.7
O3—Co1—N4	89.29 (14)	N3—C10—C9	122.5 (5)
N1—Co1—N4	179.06 (16)	N3—C10—H10	118.7
O2—Co1—N3	167.98 (14)	C9—C10—H10	118.7
O3—Co1—N3	99.30 (15)	N2—C11—C12	122.4 (5)
N1—Co1—N3	97.16 (15)	N2—C11—H11	118.8
N4—Co1—N3	83.45 (16)	C12—C11—H11	118.8
O2—Co1—N2	96.67 (15)	C11—C12—C13	119.3 (5)
O3—Co1—N2	165.10 (14)	C11—C12—H12	120.4
N1—Co1—N2	82.56 (15)	C13—C12—H12	120.4
N4—Co1—N2	96.68 (15)	C12—C13—C14	119.4 (5)
N3—Co1—N2	94.95 (16)	C12—C13—H13	120.3
C22—O2—Co1	90.7 (3)	C14—C13—H13	120.3
C22—O3—Co1	90.8 (3)	C15—C14—C13	118.7 (5)
C20—N1—C16	118.2 (4)	C15—C14—H14	120.6
C20—N1—Co1	126.3 (3)	C13—C14—H14	120.6
C16—N1—Co1	114.8 (3)	N2—C15—C14	121.6 (4)
C11—N2—C15	118.6 (4)	N2—C15—C16	113.8 (4)
C11—N2—Co1	127.5 (3)	C14—C15—C16	124.6 (4)
C15—N2—Co1	113.7 (3)	N1—C16—C17	122.2 (4)
C10—N3—C6	118.6 (4)	N1—C16—C15	113.0 (4)
C10—N3—Co1	127.1 (3)	C17—C16—C15	124.8 (4)
C6—N3—Co1	114.3 (3)	C18—C17—C16	118.7 (4)
C1—N4—C5	119.2 (4)	C18—C17—H17	120.7
C1—N4—Co1	126.2 (3)	C16—C17—H17	120.7
C5—N4—Co1	114.4 (3)	C19—C18—C17	119.1 (4)
N4—C1—C2	121.7 (5)	C19—C18—H18	120.4
N4—C1—H1	119.2	C17—C18—H18	120.4
C2—C1—H1	119.2	C20—C19—C18	119.6 (5)
C1—C2—C3	119.7 (5)	C20—C19—H19	120.2
C1—C2—H2	120.2	C18—C19—H19	120.2
C3—C2—H2	120.2	N1—C20—C19	122.1 (4)
C4—C3—C2	119.3 (5)	N1—C20—H20	118.9
C4—C3—H3	120.4	C19—C20—H20	118.9
C2—C3—H3	120.4	F2—C21—F3	107.2 (7)
C3—C4—C5	119.2 (6)	F2—C21—F1	106.1 (7)
C3—C4—H4	120.4	F3—C21—F1	105.7 (7)
C5—C4—H4	120.4	F2—C21—S1	113.5 (5)
N4—C5—C4	120.9 (5)	F3—C21—S1	114.1 (5)
N4—C5—C6	114.0 (4)	F1—C21—S1	109.7 (6)
C4—C5—C6	125.1 (5)	O1—C22—O3	126.4 (5)
N3—C6—C7	122.0 (5)	O1—C22—O2	124.7 (5)
N3—C6—C5	113.6 (4)	O3—C22—O2	109.0 (4)

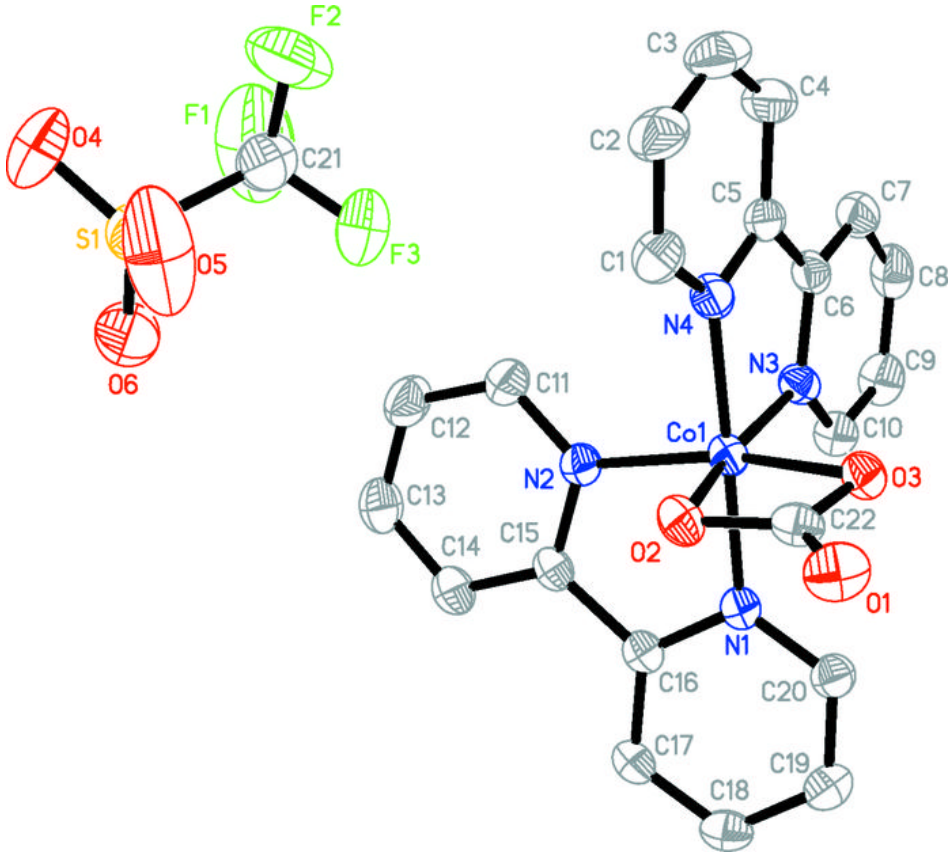
C7—C6—C5	124.4 (5)	O6—S1—O4	114.1 (4)
C6—C7—C8	118.4 (5)	O6—S1—O5	116.3 (5)
C6—C7—H7	120.8	O4—S1—O5	114.1 (4)
C8—C7—H7	120.8	O6—S1—C21	103.3 (4)
C7—C8—C9	119.9 (5)	O4—S1—C21	105.7 (3)
C7—C8—H8	120.1	O5—S1—C21	101.1 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···O5^{i}	0.93	2.39	3.266 (9)	157
C10—H10···O1^{ii}	0.93	2.30	3.137 (6)	149
C17—H17···O2^{iii}	0.93	2.32	3.155 (6)	148

Symmetry codes: (i) −*x*, −*y*+2, −*z*+1; (ii) *x*−1, *y*, *z*; (iii) −*x*+1, −*y*+1, −*z*+2.

Fig. 1


F2
F1
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C21
S1
O5
F3
O6
C3
C4
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C5
C7
C1
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C6
N3
C9
C11
C12
Co1
C10
N2
O3
C13
C22
C15
C14
O2
O1
N1
C16
C20
C17
C19
C18