Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis(pyridine-κN)bis[4,4,4-trifluoro-1-(4-fluorophenyl)butane-1,3-dionato-$\kappa^2 O,O'$]cobalt(II)

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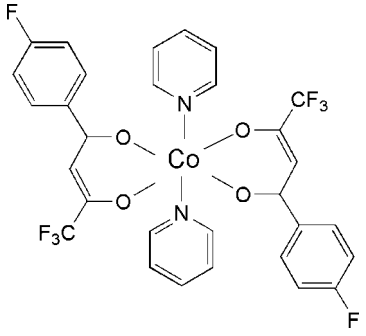
Received 1 November 2007; accepted 20 December 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.060; wR factor = 0.139; data-to-parameter ratio = 16.1.

In the structure of the title compound, $[Co(C_{10}H_5F_4O_2)_2(C_5H_5N)_2]$, cobalt(II) forms a complex with two 4,4,4-trifluoro-1-(4-fluorophenyl)butane-1,3-dionate anions and two pyridine molecules in an octahedral coordination environment, where the two dionate ligands are in equatorial positions and the two pyridine molecules in axial positions. The complex is located on a crystallographic inversion centre.

Related literature

For related literature, see: Fan *et al.* (2007); Feng (2002); Lu *et al.* (2003); Sloopa *et al.* (2002).



Experimental

Crystal data

$[Co(C_{10}H_5F_4O_2)_2(C_5H_5N)_2]$
M_r = 683.41
Monoclinic, $P2_1/c$
a = 8.5181 (6) Å
b = 17.0379 (13) Å
c = 10.0150 (7) Å
β = 90.374 (2)°
V = 1453.45 (18) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.68 mm^{-1}
T = 293 (2) K
0.40 × 0.10 × 0.10 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.772, T_{max} = 0.935
16450 measured reflections
3299 independent reflections
2136 reflections with $I > 2\sigma(I)$
R_{int} = 0.063

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.138
S = 1.09
3299 reflections
205 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O1	2.055 (2)	Co1—N1	2.195 (3)
Co1—O2	2.033 (2)		
O1—Co1—O2	88.35 (8)	O2—Co1—N1	90.24 (9)
O1—Co1—N1	93.58 (9)		

Data collection: *SMART* (Bruker, 1997); 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, 2001); software used to prepare material for publication: *SHELXTL*.

The authors are grateful to Hubei Normal University and the Natural Science Foundation of the Educational Commission of Hubei Province (grant Nos. J200522002 and Z200622001) for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KJ2078).

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 doi:10.1107/S1600536807067955

supporting information

Acta Cryst. (2008). E**64**, m347 [doi:10.1107/S1600536807067955]

Bis(pyridine-κN)bis[4,4,4-trifluoro-1-(4-fluorophenyl)butane-1,3-dionato-κ^2O,O']cobalt(II)

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S1. Comment

The chelating group 1,3-diketone, widely used in coordination chemistry for a long time (Fan *et al.*, 2007; Lu *et al.*, 2003; Feng, 2002), has been increasingly encountered as a constituent of polydentate ligands in the context of metallo-supramolecular chemistry. In this paper, we report the crystal structure of the title compound, $Co(C_{10}H_5O_2F_4)_2(C_5H_5N)_2$. The Co(II) ion is located on a crystallographic inversion centre and is coordinated by two 4,4,4-trifluoro-1-(4-fluoro-phenyl)butane-1,3-dione oxygen atoms and two nitrogen atoms of pyridines, forming a distorted octahedron coordination geometry (Fig. 1). The chelate fragment is planar and the both lengths imply strong conjugation in chelate rings (Table 1).

S2. Experimental

The ligand 4,4,4-trifluoro-1-(4-fluorophenyl)butane-1,3-dione was synthesized according to the reported literature (Sloopa *et al.*, 2002). The coordination compound was prepared according to the following procedure: a mixture of ligand (0.328 g, 1.4 mmol) and pyridine (0.111 g, 1.4 mmol), dissolved in hot acetone (20 ml) was added slowly to a solution of $Co(CH_3COO)_2\cdot 4H_2O$ (0.174 g, 0.7 mmol) in water (10 ml). The mixture was stirred for 3 h. After filtration, the red solution was allowed to stand at room temperature. Brown block-shaped crystals suitable for X-ray analysis were obtained in several days. C, H and N content analyses were performed on a Perkin Elmer 2400 analytical instrument. Anal. Calcd. (%) for $C_{30}H_{20}CoF_8N_2O_4$: C, 52.72; H, 2.95; N, 4.10. Found (%): C, 53.01; H, 2.72; N, 4.20.

S3. Refinement

All the H atoms were placed at their idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, with $U_{iso}(H) = 1.2U_{eq}(C)$.

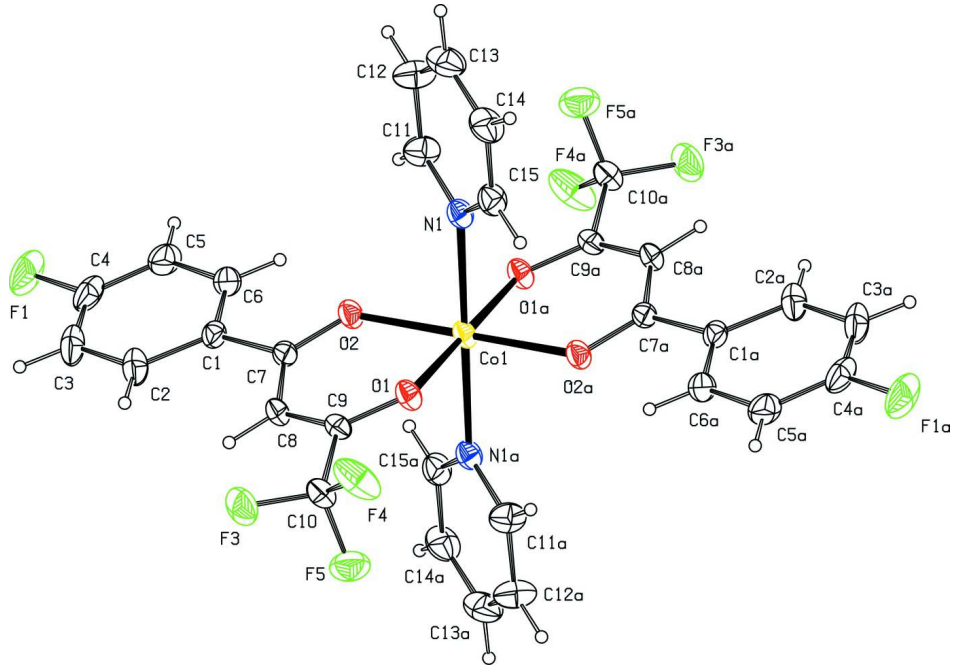

Figure 1

View of the title compound, showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 30% probability level. H-atoms are represented by circles of arbitrary size. Symmetry codes: a: (2 - *x*, 2 - *y*, 2 - *z*).

Bis(pyridine-*κN*)bis[4,4,4-trifluoro-1-(4-fluorophenyl)butane-1,3-dionato-\ *κ*^{2}*O,O′*]cobalt(II)

Crystal data

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b = 17.0379 (13) Å
c = 10.0150 (7) Å
β = 90.374 (2)°
V = 1453.45 (18) Å^3
Z = 2
$F(000)$ = 690
D_x = 1.562 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1950 reflections
θ = 2.4–20.8°
μ = 0.68 mm^{-1}
T = 293 K
Block, brown
0.40 × 0.10 × 0.10 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.772, T_{max} = 0.935
16450 measured reflections
3299 independent reflections
2136 reflections with $I > 2\sigma(I)$
R_{int} = 0.063
θ_{max} = 27.5°, θ_{min} = 2.4°
h = −11→11
k = −22→21
l = −12→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.059$
$wR(F^2) = 0.138$
$S = 1.10$
3299 reflections
205 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.059P)^2 + 0.1443P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.44$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	1.0000	1.0000	1.0000	0.0428 (2)
C1	1.1943 (3)	0.9984 (2)	0.6036 (3)	0.0479 (8)
C2	1.2093 (4)	0.9561 (3)	0.4859 (3)	0.0659 (10)
H2	1.1591	0.9079	0.4765	0.079*
C3	1.2988 (5)	0.9855 (3)	0.3824 (4)	0.0766 (12)
H3	1.3085	0.9574	0.3033	0.092*
C4	1.3713 (4)	1.0548 (3)	0.3971 (4)	0.0754 (12)
C5	1.3597 (4)	1.0991 (2)	0.5103 (4)	0.0732 (11)
H5	1.4099	1.1474	0.5178	0.088*
C6	1.2700 (4)	1.0691 (2)	0.6137 (3)	0.0599 (9)
H6	1.2611	1.0978	0.6922	0.072*
C7	1.0984 (3)	0.97134 (18)	0.7195 (3)	0.0432 (7)
C8	1.0258 (4)	0.89683 (18)	0.7204 (3)	0.0495 (8)
H8	1.0478	0.8627	0.6506	0.059*
C9	0.9242 (3)	0.87138 (17)	0.8183 (3)	0.0442 (7)
C10	0.8602 (4)	0.7887 (2)	0.8059 (3)	0.0568 (9)
C11	0.8337 (4)	1.1450 (2)	0.8834 (4)	0.0673 (10)
H11	0.9344	1.1531	0.8509	0.081*
C12	0.7186 (5)	1.1979 (2)	0.8505 (5)	0.0860 (13)
H12	0.7422	1.2414	0.7983	0.103*
C13	0.5687 (5)	1.1862 (3)	0.8949 (5)	0.0824 (12)
H13	0.4883	1.2206	0.8716	0.099*
C14	0.5405 (4)	1.1228 (3)	0.9741 (4)	0.0757 (11)
H14	0.4404	1.1136	1.0073	0.091*
C15	0.6617 (4)	1.0729 (2)	1.0041 (3)	0.0601 (9)

H15	0.6411	1.0299	1.0584	0.072*
F1	1.4601 (3)	1.08363 (17)	0.2953 (2)	0.1107 (9)
F3	0.8525 (3)	0.76125 (12)	0.6819 (2)	0.0869 (7)
F4	0.7189 (3)	0.78070 (13)	0.8566 (3)	0.1041 (9)
F5	0.9517 (3)	0.73792 (12)	0.8714 (2)	0.0910 (7)
N1	0.8080 (3)	1.08270 (15)	0.9594 (2)	0.0481 (6)
O1	0.8796 (2)	0.90574 (12)	0.9225 (2)	0.0506 (5)
O2	1.0882 (2)	1.01973 (12)	0.8149 (2)	0.0505 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0456 (3)	0.0427 (4)	0.0403 (3)	−0.0036 (3)	0.0131 (2)	−0.0079 (3)
C1	0.0444 (17)	0.062 (2)	0.0373 (17)	0.0143 (16)	0.0035 (13)	0.0043 (15)
C2	0.057 (2)	0.097 (3)	0.043 (2)	0.004 (2)	0.0051 (17)	−0.0090 (19)
C3	0.065 (2)	0.127 (4)	0.037 (2)	0.014 (2)	0.0073 (17)	−0.003 (2)
C4	0.059 (2)	0.115 (4)	0.053 (2)	0.023 (2)	0.0165 (19)	0.035 (2)
C5	0.077 (3)	0.073 (3)	0.070 (3)	0.011 (2)	0.026 (2)	0.022 (2)
C6	0.069 (2)	0.060 (2)	0.051 (2)	0.0100 (18)	0.0191 (17)	0.0066 (17)
C7	0.0398 (16)	0.0505 (18)	0.0393 (18)	0.0114 (14)	0.0037 (13)	−0.0001 (14)
C8	0.0566 (19)	0.0513 (19)	0.0408 (18)	0.0110 (15)	0.0085 (15)	−0.0100 (14)
C9	0.0413 (17)	0.0419 (17)	0.0494 (19)	0.0061 (14)	0.0017 (14)	−0.0087 (14)
C10	0.060 (2)	0.049 (2)	0.061 (2)	−0.0014 (17)	0.0095 (17)	−0.0132 (17)
C11	0.059 (2)	0.056 (2)	0.088 (3)	−0.0057 (18)	0.0111 (19)	0.011 (2)
C12	0.086 (3)	0.055 (2)	0.117 (4)	0.007 (2)	−0.001 (3)	0.019 (2)
C13	0.072 (3)	0.071 (3)	0.105 (3)	0.023 (2)	−0.005 (2)	−0.013 (3)
C14	0.051 (2)	0.091 (3)	0.084 (3)	0.016 (2)	0.0119 (19)	−0.013 (2)
C15	0.056 (2)	0.067 (2)	0.057 (2)	0.0000 (18)	0.0144 (17)	−0.0027 (18)
F1	0.0994 (17)	0.166 (3)	0.0678 (15)	0.0212 (17)	0.0392 (13)	0.0496 (15)
F3	0.1210 (19)	0.0674 (14)	0.0721 (15)	−0.0174 (13)	−0.0008 (13)	−0.0267 (11)
F4	0.0790 (16)	0.0701 (15)	0.164 (2)	−0.0272 (12)	0.0479 (16)	−0.0429 (15)
F5	0.1182 (19)	0.0515 (13)	0.1031 (19)	0.0003 (12)	−0.0169 (15)	0.0079 (12)
N1	0.0459 (15)	0.0505 (16)	0.0479 (15)	−0.0032 (12)	0.0095 (12)	−0.0060 (12)
O1	0.0502 (12)	0.0512 (13)	0.0506 (13)	−0.0053 (10)	0.0154 (10)	−0.0114 (10)
O2	0.0610 (13)	0.0467 (13)	0.0440 (13)	−0.0027 (10)	0.0178 (10)	−0.0046 (9)

Geometric parameters (Å, º)

Co1—O1	2.055 (2)	C7—C8	1.412 (4)
Co1—O1^{i}	2.055 (2)	C8—H8	0.9300
Co1—O2	2.033 (2)	C8—C9	1.382 (4)
Co1—O2^{i}	2.033 (2)	C9—O1	1.257 (3)
Co1—N1^{i}	2.195 (3)	C9—C10	1.516 (4)
Co1—N1	2.195 (3)	C10—F3	1.328 (4)
C1—C2	1.388 (4)	C10—F4	1.316 (4)
C1—C6	1.370 (4)	C10—F5	1.334 (4)
C1—C7	1.496 (4)	C11—N1	1.325 (4)
C2—H2	0.9300	C11—H11	0.9300

C2—C3	1.385 (5)	C11—C12	1.370 (5)
C3—H3	0.9300	C12—H12	0.9300
C3—C4	1.339 (6)	C12—C13	1.370 (5)
C4—F1	1.365 (4)	C13—H13	0.9300
C4—C5	1.366 (5)	C13—C14	1.362 (6)
C5—H5	0.9300	C14—H14	0.9300
C5—C6	1.389 (5)	C14—C15	1.370 (5)
C6—H6	0.9300	C15—N1	1.338 (4)
C7—O2	1.266 (3)	C15—H15	0.9300

O1—Co1—N1^{i}	86.43 (9)	C9—C8—C7	124.3 (3)
O1^{i}—Co1—N1^{i}	93.58 (9)	C9—C8—H8	117.9
O1—Co1—O1^{i}	180	C9—O1—Co1	121.66 (19)
O1—Co1—O2	88.35 (8)	C11—C12—H12	120.2
O1—Co1—N1	93.58 (9)	C11—N1—C15	116.7 (3)
O2^{i}—Co1—O1	91.65 (8)	C11—N1—Co1	119.7 (2)
O2^{i}—Co1—O1^{i}	88.35 (8)	C12—C11—H11	118.5
O2—Co1—N1	90.24 (9)	C12—C13—H13	120.9
O2—Co1—N1^{i}	89.76 (9)	C13—C12—C11	119.6 (4)
O2^{i}—Co1—N1^{i}	90.24 (9)	C13—C12—H12	120.2
O2—Co1—O2^{i}	180	C13—C14—H14	120.5
N1^{i}—Co1—N1	180	C13—C14—C15	119.0 (4)
C1—C2—H2	119.9	C14—C13—C12	118.2 (4)
C1—C6—C5	122.0 (3)	C14—C13—H13	120.9
C1—C6—H6	119.0	C14—C15—H15	118.3
C2—C1—C7	123.6 (3)	C15—C14—H14	120.5
C2—C3—H3	120.2	C15—N1—Co1	123.6 (2)
C3—C2—C1	120.1 (4)	O1—C9—C8	129.5 (3)
C3—C2—H2	119.9	O1—C9—C10	113.0 (3)
C3—C4—F1	119.5 (4)	O2—C7—C1	115.2 (3)
C3—C4—C5	122.9 (4)	O2—C7—C8	123.2 (3)
C4—C3—C2	119.5 (4)	F1—C4—C5	117.6 (4)
C4—C3—H3	120.3	F3—C10—C9	114.8 (3)
C4—C5—H5	121.4	F3—C10—F5	104.9 (3)
C4—C5—C6	117.2 (4)	F4—C10—F3	106.5 (3)
C5—C6—H6	119.0	F4—C10—F5	106.1 (3)
C6—C1—C2	118.2 (3)	F4—C10—C9	113.2 (3)
C6—C1—C7	118.2 (3)	F5—C10—C9	110.7 (3)
C6—C5—H5	121.4	N1—C11—H11	118.5
C7—C8—H8	117.9	N1—C11—C12	123.0 (4)
C7—O2—Co1	127.5 (2)	N1—C15—C14	123.5 (4)
C8—C7—C1	121.5 (3)	N1—C15—H15	118.3
C8—C9—C10	117.4 (3)		

C6—C1—C2—C3	−0.1 (5)	C12—C13—C14—C15	−1.1 (6)
C7—C1—C2—C3	179.3 (3)	C13—C14—C15—N1	−0.1 (6)
C1—C2—C3—C4	0.4 (5)	C12—C11—N1—C15	0.1 (5)
C2—C3—C4—F1	179.7 (3)	C12—C11—N1—Co1	178.0 (3)

C2—C3—C4—C5	−0.9 (6)	C14—C15—N1—C11	0.7 (5)
C3—C4—C5—C6	1.0 (6)	C14—C15—N1—Co1	−177.2 (3)
F1—C4—C5—C6	−179.6 (3)	O2—Co1—N1—C11	−33.8 (3)
C2—C1—C6—C5	0.2 (5)	O2^{i}—Co1—N1—C11	146.2 (3)
C7—C1—C6—C5	−179.1 (3)	O1—Co1—N1—C11	−122.2 (3)
C4—C5—C6—C1	−0.6 (5)	O1^{i}—Co1—N1—C11	57.8 (3)
C6—C1—C7—O2	4.3 (4)	O2—Co1—N1—C15	144.0 (3)
C2—C1—C7—O2	−175.0 (3)	O2^{i}—Co1—N1—C15	−36.0 (3)
C6—C1—C7—C8	−175.6 (3)	O1—Co1—N1—C15	55.6 (3)
C2—C1—C7—C8	5.1 (5)	O1^{i}—Co1—N1—C15	−124.4 (3)
O2—C7—C8—C9	6.5 (5)	C8—C9—O1—Co1	−17.9 (4)
C1—C7—C8—C9	−173.6 (3)	C10—C9—O1—Co1	158.9 (2)
C7—C8—C9—O1	−1.7 (5)	O2—Co1—O1—C9	23.5 (2)
C7—C8—C9—C10	−178.3 (3)	O2^{i}—Co1—O1—C9	−156.5 (2)
O1—C9—C10—F4	33.3 (4)	N1^{i}—Co1—O1—C9	−66.3 (2)
C8—C9—C10—F4	−149.5 (3)	N1—Co1—O1—C9	113.7 (2)
O1—C9—C10—F3	155.9 (3)	C8—C7—O2—Co1	10.3 (4)
C8—C9—C10—F3	−26.9 (4)	C1—C7—O2—Co1	−169.56 (18)
O1—C9—C10—F5	−85.6 (3)	O1—Co1—O2—C7	−21.1 (2)
C8—C9—C10—F5	91.5 (3)	O1^{i}—Co1—O2—C7	158.9 (2)
N1—C11—C12—C13	−1.3 (7)	N1^{i}—Co1—O2—C7	65.4 (2)
C11—C12—C13—C14	1.8 (7)	N1—Co1—O2—C7	−114.6 (2)

Symmetry code: (i) −*x*+2, −*y*+2, −*z*+2.