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trans-Bis(pyridine)bis[3,3,3-trifluoro-1-(4-methoxybenzoyl)prop-1-en-2-olato]-cobalt(II)

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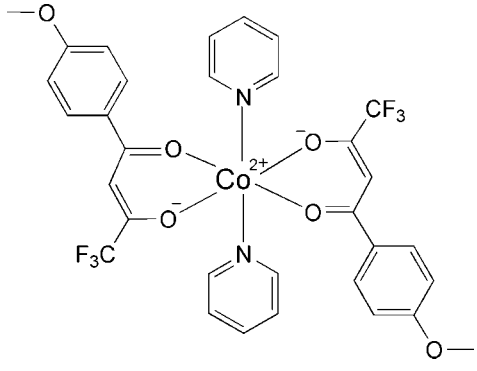
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; R factor = 0.048; wR factor = 0.117; data-to-parameter ratio = 14.1.

The title compound, $[Co(C_{11}H_9F_3O_3)_2(C_5H_5N)_2]$, has an octahedral cobalt(II) centre. The crystal structure is stabilized by weak C—H$\cdots\pi$ interactions between a benzene H atom and a neighboring pyridine ring.

Related literature

For the applications of the title compound, see: Soldatov *et al.* (2003). For the synthesis, see: Sloopa *et al.* (2002)



Experimental

Crystal data

$[Co(C_{11}H_8F_3O_3)_2(C_5H_5N)_2]$
M_r = 707.48
Triclinic, $P\overline{1}$
a = 7.3199 (10) Å
b = 10.2375 (15) Å
c = 11.9968 (17) Å
α = 66.641 (2)°
β = 84.821 (2)°
γ = 71.477 (2)°
V = 781.91 (19) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.63 mm^{-1}
T = 295 (2) K
0.20 × 0.20 × 0.10 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)
T_{min} = 0.866, T_{max} = 0.940
5023 measured reflections
3027 independent reflections
2326 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.117
S = 0.97
3027 reflections
215 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

Cg is the centroid of the C2–C7 benzene ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C6—H6$\cdots Cg^{i}$	0.93	3.22	3.884 (3)	131

Symmetry code: (i) $-x, -y+1, -z+1$.

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 Xiangfan University, Dr Guo-Dong Yin and Ling Fan (Central China Normal University).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LX2035).

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supplementary materials

Acta Cryst. (2007). E**63**, m3182 [**doi:10.1107/S160053680706237X**]

trans-Bis(pyridine)bis[3,3,3-trifluoro-1-(4-methoxybenzoyl)prop-1-en-2-olato]cobalt(II)

H. Cheng and X. Shi

Comment

Coordination complexes of divalent transition metal ions with β-diketonate ligands have proven useful in a wide range of applications (Soldatov *et al.*, 2003).

In the title compound, the coordination of the Co^{II} centre (Fig. 1) is distorted octahedral, with the O donor atoms of the β-diketonate ligand occupying equatorial positions and N atoms of two pyridine ligands in the axial positions. Co cation shows positive bivalence, and β-diketones show negative bivalence after loss of two hydrogen protons. The molecular packing (Fig. 2) is stabilized by weak C—H···π interactions between the benzene-H atom and the neighboring pyridine ring unit, with a C6—H6···Cg^{i} separation of 3.22 Å (Fig. 2 & Table 1) (*Cg* is the centroid of C2—C7 benzene ring, symmetry code as in Fig. 2).

Experimental

The ligand 4,4,4-trifluoro-1-(4-methoxyphenyl)-2-butene-1,3-dione was synthesized according to the reported literature (Sloopa *et al.*, 2002). The coordination compound was prepared as follows: The ligand (0.344 g, 1.4 mmol) and pyridine (0.111 g, 1.4 mmol) in 20 ml hot acetone was added slowly to the $Co(CH_3COO)_2{\cdot}4H_2O$ (0.174 g, 0.7 mmol) solution of 10 ml water. The mixture was stirred for 3 h. After filtration, the red solution was allowed to stand at room temperature. Red block-shaped crystals suitable for X-ray analysis were obtained in several days.

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 $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

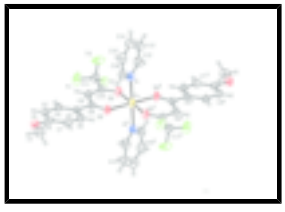

Fig. 1. The molecular structure of the title compound. Showing displacement ellipsoids drawn at the 30% probability level. [Symmetry code: (i) $-x + 1, -y + 1, -z + 1$.]

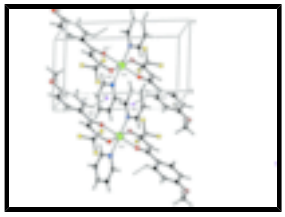

Fig. 2. C—H···π interaction (dotted lines) in the title compound. *Cg* denotes ring centroid. [Symmetry code: (i) *x* + 1, *y*, *z*; (ii) −*x* + 1, −*y* + 1, −*z* + 1.]

trans-Dipyridinebis[3,3,3-trifluoro-1-(4-methoxybenzoyl)prop-1-en-2- olato]cobalt(II)

Crystal data

$[Co(C_{11}H_8F_3O_3)_2(C_5H_5N)_2]$	$Z = 1$
$M_r = 707.48$	$F_{000} = 361$
Triclinic, $P\overline{1}$	$D_x = 1.502$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.3199$ (10) Å	Cell parameters from 1762 reflections
$b = 10.2375$ (15) Å	$\theta = 2.3$–23.8º
$c = 11.9968$ (17) Å	$\mu = 0.63$ mm^{-1}
$\alpha = 66.641$ (2)º	$T = 295$ (2) K
$\beta = 84.821$ (2)º	Plate, red
$\gamma = 71.477$ (2)º	0.20 × 0.20 × 0.10 mm
$V = 781.91$ (19) Å^3	

Data collection

Bruker SMART 4K CCD area-detector diffractometer	3027 independent reflections
Radiation source: fine-focus sealed tube	2326 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.045$
$T = 295$(2) K	$\theta_{max} = 26.0$º
φ and ω scans	$\theta_{min} = 1.9$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1997)	$h = -8 \rightarrow 8$
$T_{min} = 0.866$, $T_{max} = 0.940$	$k = -11 \rightarrow 12$
5023 measured reflections	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.048$	H-atom parameters constrained
$wR(F^2) = 0.117$	$w = 1/[\sigma^2(F_o^2) + (0.0597P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.97$	$(\Delta/\sigma)_{max} = <0.001$
3027 reflections	$\Delta\rho_{max} = 0.54$ e Å^{-3}

215 parameters	$\Delta\rho_{min} = -0.31$ 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 $F^2 > 2\text{sigma}(F^2)$ 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}
C1	−0.3653 (4)	0.6315 (4)	−0.0412 (3)	0.0843 (10)
H1A	−0.2862	0.5297	−0.0206	0.126*
H1B	−0.4541	0.6601	−0.1071	0.126*
H1C	−0.4359	0.6409	0.0282	0.126*
C2	−0.1157 (4)	0.7072 (3)	0.0068 (2)	0.0542 (6)
C3	−0.0098 (4)	0.8064 (3)	−0.0296 (2)	0.0579 (7)
H3	−0.0317	0.8812	−0.1073	0.069*
C4	0.1267 (4)	0.7967 (3)	0.0468 (2)	0.0509 (6)
H4	0.1958	0.8650	0.0201	0.061*
C5	0.1635 (3)	0.6863 (3)	0.16331 (19)	0.0427 (5)
C6	0.0564 (4)	0.5885 (3)	0.1974 (2)	0.0569 (7)
H6	0.0790	0.5131	0.2749	0.068*
C7	−0.0828 (4)	0.5970 (3)	0.1223 (2)	0.0605 (7)
H7	−0.1531	0.5295	0.1491	0.073*
C8	0.3086 (3)	0.6684 (3)	0.2516 (2)	0.0447 (6)
C9	0.4020 (4)	0.7779 (3)	0.2259 (2)	0.0523 (6)
H9	0.3685	0.8606	0.1528	0.063*
C10	0.5388 (3)	0.7713 (3)	0.3010 (2)	0.0469 (6)
C11	0.6189 (4)	0.9035 (3)	0.2584 (2)	0.0579 (7)
C12	0.2994 (5)	0.7244 (4)	0.6183 (3)	0.0737 (8)
H12	0.4270	0.7102	0.6363	0.088*
C13	0.1576 (6)	0.8161 (4)	0.6588 (3)	0.0904 (10)
H13	0.1888	0.8618	0.7044	0.108*
C14	−0.0307 (5)	0.8407 (4)	0.6321 (3)	0.0876 (10)
H14	−0.1299	0.9036	0.6585	0.105*
C15	−0.0693 (5)	0.7698 (4)	0.5654 (3)	0.0795 (9)
H15	−0.1959	0.7841	0.5454	0.095*
C16	0.0803 (5)	0.6780 (3)	0.5285 (2)	0.0702 (8)
H16	0.0521	0.6303	0.4835	0.084*
Co	0.5000	0.5000	0.5000	0.0551 (2)

F1	0.5934 (3)	0.9857 (2)	0.13895 (16)	0.0954 (6)
F2	0.8062 (2)	0.86269 (19)	0.28260 (16)	0.0767 (5)
F3	0.5351 (3)	0.9960 (2)	0.3128 (2)	0.0957 (6)
N	0.2648 (3)	0.6535 (2)	0.55390 (18)	0.0608 (6)
O1	−0.2461 (3)	0.7266 (2)	−0.07681 (18)	0.0753 (6)
O2	0.3404 (3)	0.55291 (19)	0.34842 (14)	0.0601 (5)
O3	0.6076 (3)	0.67465 (19)	0.40365 (14)	0.0590 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0606 (19)	0.105 (3)	0.109 (3)	−0.0285 (19)	−0.0118 (16)	−0.058 (2)
C2	0.0478 (15)	0.0556 (16)	0.0588 (16)	−0.0093 (13)	−0.0077 (12)	−0.0250 (13)
C3	0.0676 (17)	0.0510 (16)	0.0460 (14)	−0.0186 (14)	−0.0099 (12)	−0.0070 (12)
C4	0.0566 (15)	0.0470 (14)	0.0459 (13)	−0.0210 (12)	−0.0008 (11)	−0.0102 (11)
C5	0.0452 (13)	0.0414 (13)	0.0413 (12)	−0.0148 (11)	0.0017 (10)	−0.0147 (10)
C6	0.0664 (17)	0.0542 (16)	0.0476 (14)	−0.0300 (14)	−0.0048 (12)	−0.0071 (12)
C7	0.0607 (17)	0.0616 (17)	0.0644 (17)	−0.0313 (14)	−0.0010 (13)	−0.0196 (14)
C8	0.0518 (14)	0.0433 (14)	0.0388 (12)	−0.0180 (11)	0.0016 (10)	−0.0133 (11)
C9	0.0586 (15)	0.0467 (14)	0.0486 (14)	−0.0225 (12)	−0.0051 (11)	−0.0090 (11)
C10	0.0499 (14)	0.0419 (14)	0.0501 (14)	−0.0194 (11)	0.0045 (11)	−0.0157 (12)
C11	0.0579 (17)	0.0478 (15)	0.0644 (17)	−0.0232 (13)	−0.0014 (13)	−0.0121 (13)
C12	0.077 (2)	0.081 (2)	0.081 (2)	−0.0419 (18)	0.0028 (16)	−0.0355 (18)
C13	0.102 (3)	0.097 (3)	0.103 (3)	−0.051 (2)	0.020 (2)	−0.059 (2)
C14	0.088 (3)	0.083 (2)	0.090 (2)	−0.030 (2)	0.0171 (19)	−0.032 (2)
C15	0.071 (2)	0.090 (2)	0.0695 (19)	−0.033 (2)	0.0002 (16)	−0.0151 (18)
C16	0.082 (2)	0.071 (2)	0.0597 (17)	−0.0391 (18)	−0.0038 (15)	−0.0146 (15)
Co	0.0734 (4)	0.0517 (3)	0.0401 (3)	−0.0326 (3)	−0.0113 (2)	−0.0045 (2)
F1	0.1143 (15)	0.0826 (13)	0.0786 (12)	−0.0660 (12)	−0.0169 (10)	0.0115 (10)
F2	0.0534 (10)	0.0692 (11)	0.1055 (12)	−0.0299 (8)	−0.0028 (8)	−0.0223 (9)
F3	0.0876 (13)	0.0705 (12)	0.1550 (18)	−0.0335 (10)	0.0235 (12)	−0.0668 (13)
N	0.0734 (16)	0.0577 (14)	0.0544 (12)	−0.0338 (12)	−0.0040 (11)	−0.0129 (11)
O1	0.0648 (12)	0.0808 (14)	0.0792 (13)	−0.0190 (11)	−0.0264 (10)	−0.0268 (11)
O2	0.0833 (13)	0.0539 (11)	0.0436 (9)	−0.0371 (10)	−0.0132 (8)	−0.0036 (8)
O3	0.0740 (12)	0.0568 (11)	0.0474 (10)	−0.0340 (10)	−0.0108 (8)	−0.0080 (9)

Geometric parameters (Å, °)

C1—O1	1.426 (4)	C10—C11	1.529 (3)
C1—H1A	0.9600	C11—F3	1.322 (3)
C1—H1B	0.9600	C11—F2	1.323 (3)
C1—H1C	0.9600	C11—F1	1.337 (3)
C2—O1	1.360 (3)	C12—N	1.335 (4)
C2—C7	1.378 (4)	C12—C13	1.359 (4)
C2—C3	1.382 (4)	C12—H12	0.9300
C3—C4	1.370 (3)	C13—C14	1.364 (5)
C3—H3	0.9300	C13—H13	0.9300
C4—C5	1.388 (3)	C14—C15	1.370 (5)
C4—H4	0.9300	C14—H14	0.9300

C5—C6	1.379 (3)	C15—C16	1.367 (4)
C5—C8	1.486 (3)	C15—H15	0.9300
C6—C7	1.381 (3)	C16—N	1.334 (3)
C6—H6	0.9300	C16—H16	0.9300
C7—H7	0.9300	Co—O2	2.0408 (15)
C8—O2	1.259 (3)	Co—O2^{i}	2.0408 (15)
C8—C9	1.412 (3)	Co—O3^{i}	2.0603 (17)
C9—C10	1.374 (3)	Co—O3	2.0603 (17)
C9—H9	0.9300	Co—N^{i}	2.177 (2)
C10—O3	1.257 (3)	Co—N	2.177 (2)
O1—C1—H1A	109.5	F1—C11—C10	114.0 (2)
O1—C1—H1B	109.5	N—C12—C13	123.3 (3)
H1A—C1—H1B	109.5	N—C12—H12	118.4
O1—C1—H1C	109.5	C13—C12—H12	118.4
H1A—C1—H1C	109.5	C12—C13—C14	119.6 (3)
H1B—C1—H1C	109.5	C12—C13—H13	120.2
O1—C2—C7	124.8 (2)	C14—C13—H13	120.2
O1—C2—C3	116.2 (2)	C13—C14—C15	118.0 (3)
C7—C2—C3	119.0 (2)	C13—C14—H14	121.0
C4—C3—C2	121.3 (2)	C15—C14—H14	121.0
C4—C3—H3	119.4	C16—C15—C14	119.3 (3)
C2—C3—H3	119.4	C16—C15—H15	120.3
C3—C4—C5	121.0 (2)	C14—C15—H15	120.3
C3—C4—H4	119.5	N—C16—C15	123.1 (3)
C5—C4—H4	119.5	N—C16—H16	118.5
C6—C5—C4	116.7 (2)	C15—C16—H16	118.5
C6—C5—C8	119.0 (2)	O2—Co—O2^{i}	179.999 (1)
C4—C5—C8	124.3 (2)	O2—Co—O3^{i}	91.06 (6)
C5—C6—C7	123.2 (2)	O2^{i}—Co—O3^{i}	88.94 (6)
C5—C6—H6	118.4	O2—Co—O3	88.94 (6)
C7—C6—H6	118.4	O2^{i}—Co—O3	91.06 (6)
C2—C7—C6	118.8 (2)	O3^{i}—Co—O3	180.000 (1)
C2—C7—H7	120.6	O2—Co—N^{i}	90.34 (8)
C6—C7—H7	120.6	O2^{i}—Co—N^{i}	89.66 (8)
O2—C8—C9	123.1 (2)	O3^{i}—Co—N^{i}	88.90 (8)
O2—C8—C5	116.5 (2)	O3—Co—N^{i}	91.10 (8)
C9—C8—C5	120.4 (2)	O2—Co—N	89.66 (8)
C10—C9—C8	124.9 (2)	O2^{i}—Co—N	90.34 (8)
C10—C9—H9	117.6	O3^{i}—Co—N	91.10 (8)
C8—C9—H9	117.6	O3—Co—N	88.90 (8)
O3—C10—C9	130.4 (2)	N^{i}—Co—N	179.998 (2)
O3—C10—C11	112.6 (2)	C16—N—C12	116.7 (3)
C9—C10—C11	116.9 (2)	C16—N—Co	122.3 (2)
F3—C11—F2	106.2 (2)	C12—N—Co	121.0 (2)
F3—C11—F1	106.3 (2)	C2—O1—C1	118.1 (2)
F2—C11—F1	105.7 (2)	C8—O2—Co	128.63 (15)

F3—C11—C10	110.9 (2)	C10—O3—Co	122.64 (15)
F2—C11—C10	113.1 (2)		
O1—C2—C3—C4	−179.5 (2)	C14—C15—C16—N	−0.3 (5)
C7—C2—C3—C4	0.2 (4)	C15—C16—N—C12	−0.2 (4)
C2—C3—C4—C5	0.1 (4)	C15—C16—N—Co	177.6 (2)
C3—C4—C5—C6	0.0 (4)	C13—C12—N—C16	0.8 (4)
C3—C4—C5—C8	−179.9 (2)	C13—C12—N—Co	−177.0 (2)
C4—C5—C6—C7	−0.5 (4)	O2—Co—N—C16	32.4 (2)
C8—C5—C6—C7	179.4 (2)	O2^{i}—Co—N—C16	−147.6 (2)
O1—C2—C7—C6	179.0 (2)	O3^{i}—Co—N—C16	−58.6 (2)
C3—C2—C7—C6	−0.6 (4)	O3—Co—N—C16	121.4 (2)
C5—C6—C7—C2	0.8 (4)	O2—Co—N—C12	−149.9 (2)
C6—C5—C8—O2	8.0 (3)	O2^{i}—Co—N—C12	30.1 (2)
C4—C5—C8—O2	−172.1 (2)	O3^{i}—Co—N—C12	119.0 (2)
C6—C5—C8—C9	−171.5 (2)	O3—Co—N—C12	−61.0 (2)
C4—C5—C8—C9	8.4 (4)	C7—C2—O1—C1	3.5 (4)
O2—C8—C9—C10	1.0 (4)	C3—C2—O1—C1	−176.9 (2)
C5—C8—C9—C10	−179.5 (2)	C9—C8—O2—Co	8.0 (4)
C8—C9—C10—O3	−0.9 (4)	C5—C8—O2—Co	−171.42 (15)
C8—C9—C10—C11	−178.3 (2)	O3^{i}—Co—O2—C8	168.1 (2)
O3—C10—C11—F3	−78.0 (3)	O3—Co—O2—C8	−11.9 (2)
C9—C10—C11—F3	99.9 (3)	N^{i}—Co—O2—C8	−103.0 (2)
O3—C10—C11—F2	41.2 (3)	N—C1—O2—C8	−94.49 (19)
C9—C10—C11—F2	−140.9 (2)	C9—C10—O3—Co	−7.6 (4)
O3—C10—C11—F1	162.1 (2)	C11—C10—O3—Co	169.87 (16)
C9—C10—C11—F1	−20.1 (3)	O2—Co—O3—C10	11.02 (19)
N—C12—C13—C14	−1.0 (5)	O2^{i}—Co—O3—C10	−168.98 (19)
C12—C13—C14—C15	0.5 (5)	N^{i}—Co—O3—C10	101.3 (2)
C13—C14—C15—C16	0.1 (5)	N—Co—O3—C10	−78.7 (2)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···Cg^{ii}	0.93	3.22	3.884 (3)	131

Symmetry codes: (ii) −*x*, −*y*+1, −*z*+1.

Fig. 1

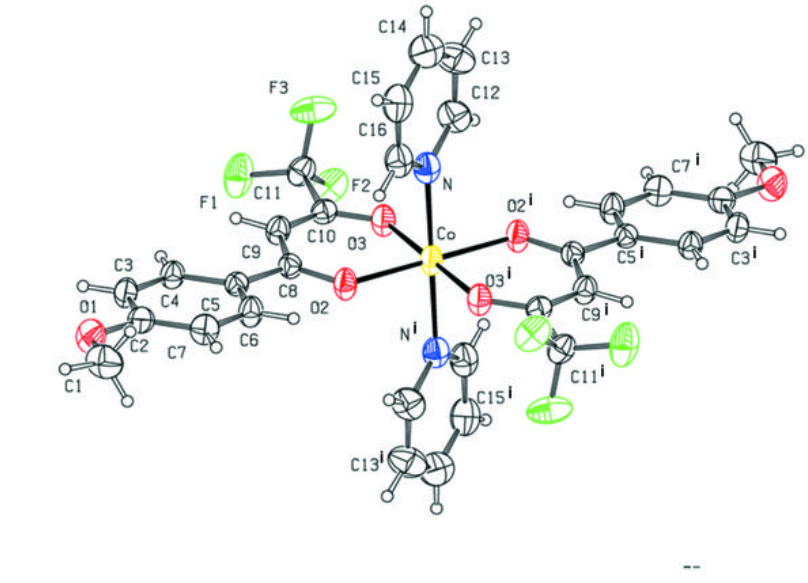
C14
C13
C15
C12
F3
C16
N
F2
F1
C11
C10
O3
Co
O2i
C7i
C5i
C3i
C9
C3
C4
C5
C8
O2
O3i
C9i
O1
C2
C7
C6
Ni
C11i
C1
C15i
C13i

Fig. 2