

***trans*-Dimethanolbis(1,1,1-trifluoro-5,5-dimethylhexane-2,4-dionato)cobalt(II)**

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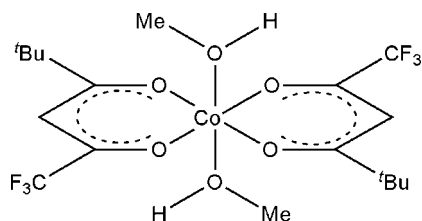
Received 10 September 2007; accepted 11 September 2007

Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.043; wR factor = 0.114; data-to-parameter ratio = 17.7.

The Co atom of the title compound, $[\text{Co}(\text{C}_8\text{H}_{10}\text{F}_3\text{O}_2)_2(\text{CH}_3\text{OH})_2]$, which is located on a crystallographic inversion center, exhibits a distorted octahedral geometry. The bidentate acetylacetonate-like ligands are in a *trans* arrangement. The plane through the acetylacetonate unit is tilted with respect to the CoO_4 plane by $17.41(7)^\circ$, which is in the same range as observed for similar $\text{Co}(\text{acac})_2\text{OR}_2$ derivatives. *Via* the methanol hydroxy groups, each molecule participates in two pairs of intermolecular hydrogen bonds that create a network of hydrogen-bonded chains along the direction of the a axis.

Related literature

For information regarding the synthesis of various metal- β -diketonates see Skopenko *et al.* (2004) and Watson & Lin (1966). For similar metal-acetylacetonates refer to Bullen (1959) and Werndrup & Kessler (2001). Varying uses of metal- β -diketonates can be found in Mayo *et al.* (2000), Katok *et al.* (2006), Bessergenev (2004) and Fahlmen (2006). The paper by Bernstein *et al.* (1995) describes graph-set motifs. For related mass spectrometry work see Majer & Perry (1969) and Schilderout (1976).

**Experimental***Crystal data*
 $[\text{Co}(\text{C}_8\text{H}_{10}\text{F}_3\text{O}_2)_2(\text{CH}_4\text{O})_2]$
 $M_r = 513.33$

 Triclinic, $P\bar{1}$
 $a = 5.4390(7)$ Å

 $b = 8.7181(11)$ Å
 $c = 12.0169(15)$ Å
 $\alpha = 78.835(2)^\circ$
 $\beta = 80.571(2)^\circ$
 $\gamma = 87.946(2)^\circ$
 $V = 551.47(12)$ Å³
 $Z = 1$
 Mo $K\alpha$ radiation
 $\mu = 0.86$ mm⁻¹
 $T = 100(2)$ K
 $0.49 \times 0.23 \times 0.08$ mm
Data collection
 Bruker SMART APEX CCD
 diffractometer
 Absorption correction: multi-scan
 (SADABS in SAINT-Plus;
 Bruker, 2003)
 $T_{\min} = 0.572$, $T_{\max} = 0.934$

 4542 measured reflections
 2637 independent reflections
 2380 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.021$
Refinement
 $R[F^2 > 2\sigma(F^2)] = 0.043$
 $wR(F^2) = 0.114$
 $S = 1.07$
 2637 reflections
 149 parameters
 1 restraint

 H atoms treated by a mixture of
 independent and constrained
 refinement
 $\Delta\rho_{\max} = 0.89$ e Å⁻³
 $\Delta\rho_{\min} = -0.79$ e Å⁻³
Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O3}-\text{H3A}\cdots\text{O1}^i$	0.840 (17)	2.032 (18)	2.867 (2)	172 (3)

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

Data collection: SMART (Bruker, 2003); cell refinement: SAINT-Plus (Bruker, 2003); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXTL (Bruker, 2003); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

The Cushwa/Commercial Shearing Graduate Fellowship is acknowledged. The diffractometer was funded by NSF grant 0087210, by Ohio Board of Regents grant CAP-491, and by Youngstown State University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2505).

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supplementary materials

Acta Cryst. (2007). E63, m2639 [doi:10.1107/S1600536807044340]

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Comment

β -Diketones such as acetylacetonate (acac), and the metal complexes of their anions, have been used as in a variety of areas including catalysis in sol-gel synthesis (Mayo *et al.*, 2000), carbon nanotube formation (Katok *et al.*, 2006) and also as precursors for metal organic chemical vapor deposition (MOCVD) (Bessergenev, 2004). The synthesis of metal- β -diketonates has also been studied thoroughly (Skopenko *et al.*, 2004). We are especially interested in fluorinated metal- β -diketonates, which, due to their increased volatility, are ideally suited as precursors for vapor deposition processes (Fahlmen, 2006) and allow for the detailed study of gas phase metal and ligand association reactions by mass spectrometry (Majer & Perry, 1969; Schildcrout, 1976). Varying the substituent identity and degree of fluorination are some of the routes used to tune the properties of MOCVD precursors and are currently under investigation in the gas phase. In the course of these studies the title compound was prepared by reaction of 1,1,1-trifluoro-5,5-dimethyl-2,4-hexanedione (tftm) with CoCl_2 in a basic aqueous medium and subsequent recrystallization from methanol.

The β -diketonate ligand, as well as the methanol substituents in this crystal structure, are arranged in a *trans* geometry with the cobalt atom being localized on a crystallographic inversion center (Fig. 1). The CoO_4 plane, formed by the oxygen atoms of the chelating ligands and the Co atom, is planar. The Co—O bond distances and angles are within the expected range, with the tftm bite angle being the smallest at $89.82(5)^\circ$ and Co—O bonds ranging between 2.0338 (14) and 2.0388 (13) Å. The tftm ligands themselves are also nearly planar with an r.m.s. deviation from the mean plane formed by the two oxygen and five carbon atoms of the two ligands of only 0.0729. With respect to the CoO_4 plane however, the tftm ligands are tilted by $17.41(7)^\circ$ which compares well to values found for other similar Co compounds such as $\text{Co}(\text{acac})_2(\text{H}_2\text{O})_2$ and $\text{Co}(\text{acac})_2(\text{MeOH})_2$, with angles of 16.70° and 9.71° respectively (Bullen, 1959; Werndrup & Kessler, 2001).

The hydroxyl groups of the methanol ligands are involved in O—H \cdots O hydrogen bonds towards O1^i of a tftm ligand in a neighboring molecule (symmetry operator $i: x - 1, y, z$). Each molecule functions as both H donor and acceptor towards each two neighboring molecules. Chains of H-bound molecules extend along the a axis due to this network of H-bonds (Fig. 2). Also, each two of the O—H \cdots O bonds are related to each other by an inversion center located between two neighboring molecules, resulting in an $R^2_2(8)$ graph set motif (Bernstein *et al.*, 1995).

Experimental

The synthesis of the title compound was adapted from Watson & Lin (1966). 0.2 ml (1.2 mmol) of the β -diketonate ligand was added to a solution of 0.11 g $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ (0.5 mmol) in 100 ml de-ionized water. Diluted 1:1 (v/v) NH_4OH was added dropwise to the solution until no additional precipitate formed. The solution was stirred for 2 h and the precipitate was isolated by filtration. The desired product was separated from any impurities by extraction with toluene and filtration. Toluene was removed *in vacuo* and the product was subsequently re-crystallized from methanol.

Refinement

The hydroxyl H atom was located in a difference density Fourier map. The O—H distance was restrained to 0.84 (2) Å. The other H atoms were placed in calculated positions with C—H distances of 0.980 (methyl) and 0.950 Å (CH). The methyl and hydroxyl H's were refined with an isotropic displacement parameter U_{iso} of 1.5 times U_{eq} of the adjacent carbon or oxygen atom, and the C—H hydrogen atom with $U_{\text{iso}} = 1.2 U_{\text{eq}}(\text{C})$. Methyl hydrogen atoms were allowed to rotate to best fit the experimental electron density.

Figures

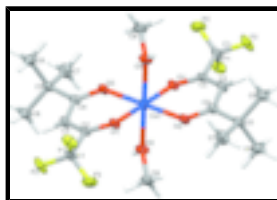


Fig. 1. ORTEP representation of the title compound, with anisotropic displacement parameters for the non-H atoms of 50% probability.

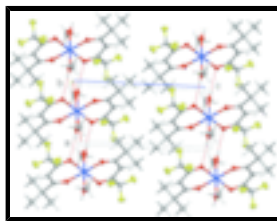


Fig. 2. Packing diagram showing the H-bonding network down the *b* axis at 50% probability.

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Crystal data

[Co(C₈H₁₀F₃O₂)₂(CH₄O)₂]

$M_r = 513.33$

Triclinic, $P\bar{1}$

$a = 5.4390$ (7) Å

$b = 8.7181$ (11) Å

$c = 12.0169$ (15) Å

$\alpha = 78.835$ (2)°

$\beta = 80.571$ (2)°

$\gamma = 87.946$ (2)°

$V = 551.47$ (12) Å³

$Z = 1$

$F_{000} = 265$

$D_x = 1.546$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 3517 reflections

$\theta = 2.4$ – 30.4 °

$\mu = 0.86$ mm⁻¹

$T = 100$ (2) K

Plate, red

$0.49 \times 0.23 \times 0.08$ mm

Data collection

Bruker SMART APEX CCD
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

2637 independent reflections

2380 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.021$

$T = 100(2)$ K $\theta_{\max} = 28.3^\circ$
 ω scans $\theta_{\min} = 1.8^\circ$
 Absorption correction: multi-scan
 (SADABS in SAINT-Plus; Bruker, 2003) $h = -7 \rightarrow 7$
 $T_{\min} = 0.572$, $T_{\max} = 0.934$ $k = -11 \rightarrow 11$
 4542 measured reflections $l = -15 \rightarrow 15$

Refinement

Refinement on F^2 Secondary atom site location: difference Fourier map
 Least-squares matrix: full Hydrogen site location: inferred from neighbouring sites
 $R[F^2 > 2\sigma(F^2)] = 0.043$ H atoms treated by a mixture of independent and constrained refinement
 $wR(F^2) = 0.114$ $w = 1/[\sigma^2(F_o^2) + (0.0734P)^2 + 0.1036P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $S = 1.07$ $(\Delta/\sigma)_{\max} < 0.001$
 2637 reflections $\Delta\rho_{\max} = 0.89 \text{ e } \text{\AA}^{-3}$
 149 parameters $\Delta\rho_{\min} = -0.79 \text{ e } \text{\AA}^{-3}$
 1 restraint Extinction correction: none
 Primary atom site location: structure-invariant direct methods

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 $F^2 > 2\sigma(F^2)$ 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	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.6715 (4)	1.2223 (2)	0.26390 (17)	0.0224 (4)
C2	0.5746 (3)	1.0953 (2)	0.21029 (16)	0.0187 (4)
C3	0.4063 (4)	0.9910 (2)	0.27916 (17)	0.0209 (4)
H3	0.3564	1.0027	0.3566	0.025*
C4	0.3002 (3)	0.8652 (2)	0.24211 (17)	0.0190 (4)
C5	0.1482 (3)	0.7401 (2)	0.33239 (17)	0.0198 (4)
C6	-0.0258 (4)	0.8130 (2)	0.42237 (18)	0.0246 (4)
H6A	-0.1322	0.8919	0.3836	0.037*
H6B	0.0738	0.8624	0.4666	0.037*
H6C	-0.1302	0.7313	0.4744	0.037*

supplementary materials

C7	-0.0022 (4)	0.6457 (3)	0.27254 (19)	0.0277 (4)
H7A	0.1114	0.5960	0.2178	0.042*
H7B	-0.1169	0.7155	0.2314	0.042*
H7C	-0.0977	0.5652	0.3300	0.042*
C8	0.3351 (4)	0.6316 (2)	0.39236 (19)	0.0255 (4)
H8A	0.2446	0.5499	0.4508	0.038*
H8B	0.4352	0.6923	0.4290	0.038*
H8C	0.4449	0.5832	0.3355	0.038*
C9	0.2186 (4)	1.3202 (2)	0.0062 (2)	0.0283 (4)
H9A	0.2177	1.3465	0.0820	0.042*
H9B	0.0805	1.3743	-0.0284	0.042*
H9C	0.3768	1.3530	-0.0433	0.042*
Co1	0.5000	1.0000	0.0000	0.01756 (13)
F1	0.9170 (2)	1.20843 (16)	0.26299 (12)	0.0330 (3)
F2	0.6323 (3)	1.36435 (15)	0.20402 (13)	0.0374 (3)
F3	0.5676 (3)	1.22055 (17)	0.37246 (12)	0.0377 (4)
O1	0.6700 (2)	1.10554 (15)	0.10421 (12)	0.0201 (3)
O2	0.3314 (3)	0.84840 (16)	0.13993 (12)	0.0208 (3)
O3	0.1904 (3)	1.15484 (17)	0.01845 (13)	0.0244 (3)
H3A	0.042 (4)	1.134 (3)	0.049 (2)	0.037*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0234 (9)	0.0219 (9)	0.0237 (10)	-0.0037 (7)	-0.0007 (7)	-0.0108 (8)
C2	0.0193 (9)	0.0174 (9)	0.0216 (9)	-0.0001 (7)	-0.0033 (7)	-0.0091 (7)
C3	0.0212 (9)	0.0228 (9)	0.0202 (9)	-0.0023 (7)	-0.0007 (7)	-0.0094 (7)
C4	0.0170 (8)	0.0184 (9)	0.0222 (9)	0.0001 (7)	-0.0012 (7)	-0.0073 (7)
C5	0.0188 (9)	0.0193 (9)	0.0222 (9)	-0.0032 (7)	0.0003 (7)	-0.0083 (7)
C6	0.0220 (9)	0.0249 (10)	0.0253 (10)	-0.0023 (8)	0.0040 (8)	-0.0064 (8)
C7	0.0262 (10)	0.0320 (11)	0.0258 (10)	-0.0128 (8)	-0.0009 (8)	-0.0082 (8)
C8	0.0242 (10)	0.0216 (10)	0.0293 (11)	-0.0016 (8)	-0.0014 (8)	-0.0039 (8)
C9	0.0318 (11)	0.0192 (10)	0.0339 (11)	0.0005 (8)	-0.0016 (9)	-0.0087 (8)
Co1	0.0185 (2)	0.0168 (2)	0.0188 (2)	-0.00344 (13)	-0.00057 (13)	-0.00835 (14)
F1	0.0239 (6)	0.0389 (7)	0.0430 (8)	-0.0064 (5)	-0.0069 (5)	-0.0221 (6)
F2	0.0544 (9)	0.0184 (6)	0.0456 (8)	-0.0014 (6)	-0.0175 (7)	-0.0132 (6)
F3	0.0436 (8)	0.0443 (8)	0.0287 (7)	-0.0183 (6)	0.0080 (6)	-0.0242 (6)
O1	0.0195 (6)	0.0202 (7)	0.0223 (7)	-0.0038 (5)	-0.0002 (5)	-0.0101 (5)
O2	0.0228 (7)	0.0193 (7)	0.0214 (7)	-0.0041 (5)	0.0003 (5)	-0.0091 (5)
O3	0.0197 (7)	0.0202 (7)	0.0340 (8)	-0.0015 (5)	-0.0003 (6)	-0.0104 (6)

Geometric parameters (\AA , $^\circ$)

C1—F3	1.332 (2)	C7—H7B	0.9800
C1—F1	1.335 (2)	C7—H7C	0.9800
C1—F2	1.336 (2)	C8—H8A	0.9800
C1—C2	1.532 (3)	C8—H8B	0.9800
C2—O1	1.282 (2)	C8—H8C	0.9800
C2—C3	1.368 (3)	C9—O3	1.432 (2)

C3—C4	1.432 (3)	C9—H9A	0.9800
C3—H3	0.9500	C9—H9B	0.9800
C4—O2	1.248 (2)	C9—H9C	0.9800
C4—C5	1.537 (3)	Co1—O2	2.0338 (14)
C5—C7	1.528 (3)	Co1—O2 ⁱ	2.0339 (14)
C5—C8	1.535 (3)	Co1—O1 ⁱ	2.0388 (13)
C5—C6	1.535 (3)	Co1—O1	2.0388 (13)
C6—H6A	0.9800	Co1—O3	2.1301 (15)
C6—H6B	0.9800	Co1—O3 ⁱ	2.1302 (15)
C6—H6C	0.9800	O3—H3A	0.840 (17)
C7—H7A	0.9800		
F3—C1—F1	106.65 (17)	C5—C8—H8A	109.5
F3—C1—F2	107.19 (17)	C5—C8—H8B	109.5
F1—C1—F2	106.60 (16)	H8A—C8—H8B	109.5
F3—C1—C2	114.14 (16)	C5—C8—H8C	109.5
F1—C1—C2	111.10 (16)	H8A—C8—H8C	109.5
F2—C1—C2	110.78 (16)	H8B—C8—H8C	109.5
O1—C2—C3	130.15 (17)	O3—C9—H9A	109.5
O1—C2—C1	112.25 (16)	O3—C9—H9B	109.5
C3—C2—C1	117.60 (17)	H9A—C9—H9B	109.5
C2—C3—C4	124.26 (18)	O3—C9—H9C	109.5
C2—C3—H3	117.9	H9A—C9—H9C	109.5
C4—C3—H3	117.9	H9B—C9—H9C	109.5
O2—C4—C3	123.37 (17)	O2—Co1—O2 ⁱ	180.00 (6)
O2—C4—C5	117.62 (16)	O2—Co1—O1 ⁱ	90.18 (5)
C3—C4—C5	118.97 (17)	O2 ⁱ —Co1—O1 ⁱ	89.82 (5)
C7—C5—C8	109.26 (17)	O2—Co1—O1	89.82 (5)
C7—C5—C6	110.21 (16)	O2 ⁱ —Co1—O1	90.18 (5)
C8—C5—C6	109.09 (17)	O1 ⁱ —Co1—O1	180.00 (6)
C7—C5—C4	109.43 (16)	O2—Co1—O3	89.28 (6)
C8—C5—C4	107.12 (15)	O2 ⁱ —Co1—O3	90.72 (6)
C6—C5—C4	111.66 (15)	O1 ⁱ —Co1—O3	90.09 (6)
C5—C6—H6A	109.5	O1—Co1—O3	89.91 (6)
C5—C6—H6B	109.5	O2—Co1—O3 ⁱ	90.72 (6)
H6A—C6—H6B	109.5	O2 ⁱ —Co1—O3 ⁱ	89.28 (6)
C5—C6—H6C	109.5	O1 ⁱ —Co1—O3 ⁱ	89.91 (6)
H6A—C6—H6C	109.5	O1—Co1—O3 ⁱ	90.09 (6)
H6B—C6—H6C	109.5	O3—Co1—O3 ⁱ	179.999 (1)
C5—C7—H7A	109.5	C2—O1—Co1	119.97 (12)
C5—C7—H7B	109.5	C4—O2—Co1	127.11 (13)
H7A—C7—H7B	109.5	C9—O3—Co1	122.65 (12)
C5—C7—H7C	109.5	C9—O3—H3A	107 (2)
H7A—C7—H7C	109.5	Co1—O3—H3A	129 (2)
H7B—C7—H7C	109.5		
F3—C1—C2—O1	176.81 (17)	C3—C2—O1—Co1	19.4 (3)

supplementary materials

F1—C1—C2—O1	-62.6 (2)	C1—C2—O1—Co1	-160.77 (12)
F2—C1—C2—O1	55.7 (2)	O2—Co1—O1—C2	-23.55 (14)
F3—C1—C2—C3	-3.3 (3)	O2 ⁱ —Co1—O1—C2	156.45 (14)
F1—C1—C2—C3	117.3 (2)	O3—Co1—O1—C2	65.73 (14)
F2—C1—C2—C3	-124.4 (2)	O3 ⁱ —Co1—O1—C2	-114.27 (14)
O1—C2—C3—C4	0.3 (3)	C3—C4—O2—Co1	-7.2 (3)
C1—C2—C3—C4	-179.48 (18)	C5—C4—O2—Co1	175.20 (12)
C2—C3—C4—O2	-7.8 (3)	O1 ⁱ —Co1—O2—C4	-160.79 (16)
C2—C3—C4—C5	169.72 (18)	O1—Co1—O2—C4	19.21 (16)
O2—C4—C5—C7	-17.5 (2)	O3—Co1—O2—C4	-70.70 (16)
C3—C4—C5—C7	164.78 (18)	O3 ⁱ —Co1—O2—C4	109.30 (16)
O2—C4—C5—C8	100.8 (2)	O2—Co1—O3—C9	137.10 (16)
C3—C4—C5—C8	-76.9 (2)	O2 ⁱ —Co1—O3—C9	-42.90 (16)
O2—C4—C5—C6	-139.84 (19)	O1 ⁱ —Co1—O3—C9	-132.72 (16)
C3—C4—C5—C6	42.5 (2)	O1—Co1—O3—C9	47.28 (16)

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H3A \cdots O1 ⁱⁱ	0.840 (17)	2.032 (18)	2.867 (2)	172 (3)

Symmetry codes: (ii) $x-1, y, z$.

Fig. 1

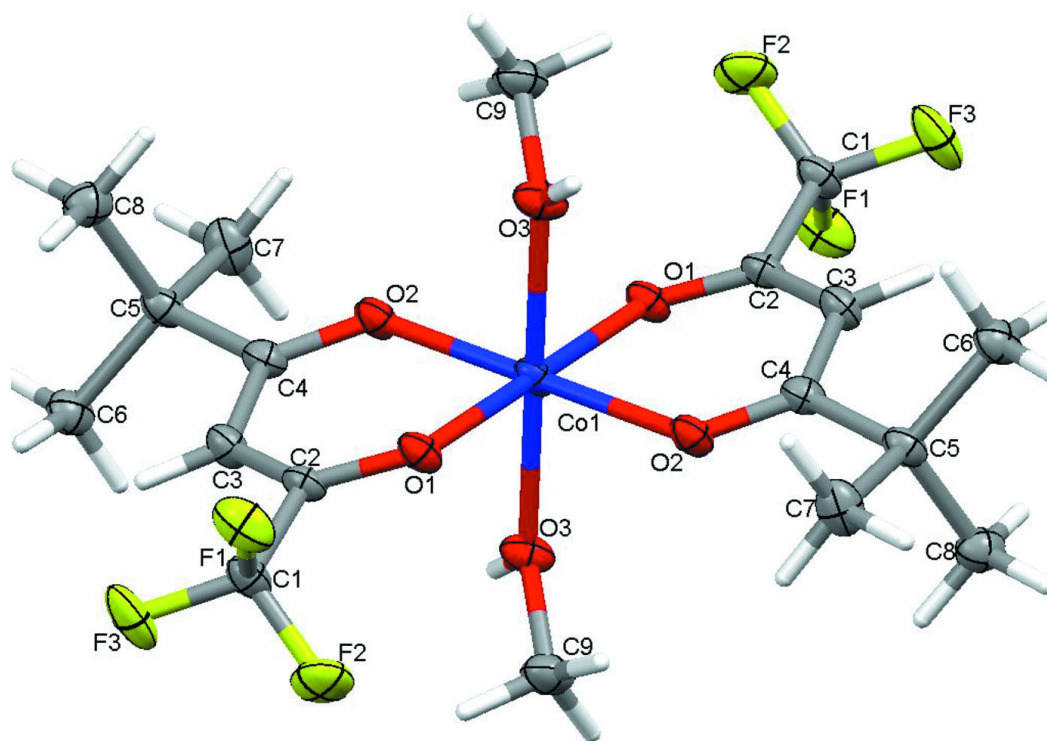


Fig. 2

