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Bis(1,3-diphenylpropane-1,3-dionato-κ^2O,O')bis(morpholine-κN)cobalt(II)

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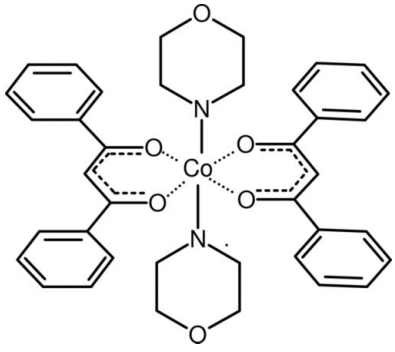
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(Co–O) = 0.0014 Å; R factor = 0.056; wR factor = 0.164; data-to-parameter ratio = 22.4.

The title compound, $[Co(C_{15}H_{11}O_2)_2(C_4H_4NO)_2]$, was obtained from bis(1-phenylpropane-1,3-dionato)cobalt(II) after crystallization from morpholine. The Co atom is located on a crystallographic inversion centre with an octahedral environment formed by four O atoms of the two 1,3-diphenylpropane-1,3-dione ligands and two N atoms from two morpholine molecules. Both morpholine molecules are additionally involved in N—H$\cdots\pi$ interactions with the chelate ring (N$\cdots$centroid = 2.70 Å).

Related literature

For background information, see: Soldatov *et al.* (1999, 2001, 2002, 2003); Bučar & Meštrović (2003); Meštrović *et al.* (2004); Meštrović & Kaitner (2006). The corresponding complex has the Co atom in an octahedral environment formed by two dibenzoylmethane units and two morpholine molecules analogous to the compex with thiomorpholine (Judaš *et al.*, 2006).

For related literature, see: Cotton & Elder (1965); Etter *et al.* (1987); Kaitner & Meštrović (1993); Ozturk *et al.* (1997); Soldatov & Ripmeester (2001*a*,*b*).



Experimental

Crystal data

$[Co(C_{15}H_{11}O_2)_2(C_4H_4NO)_2]$
M_r = 679.65
Monoclinic, $P2_1/n$
a = 11.310 (1) Å
b = 8.064 (1) Å
c = 18.642 (1) Å
β = 96.09 (2)°
V = 1690.6 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.56 mm^{-1}
T = 293 (2) K
0.57 × 0.57 × 0.43 mm

Data collection

Philips PW1100 diffractometer upgraded by Stoe
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.784, T_{max} = 0.861 (expected range = 0.717–0.787)
5060 measured reflections
4924 independent reflections
3152 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
3 standard reflections
frequency: 90 min
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.164
S = 0.99
4924 reflections
220 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.84 e Å^{-3}
$\Delta\rho_{min}$ = −0.55 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co—O2	2.0286 (14)	Co—O1	2.0556 (14)
O2—Co—O1	89.12 (6)	O1—Co—N	95.07 (7)
O2—Co—N	95.15 (7)		

Data collection: *STADI4* (Stoe & Cie, 1994); cell refinement: *X-RED32* (Stoe & Cie, 1994); data reduction: *X-RED32*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2100).

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supplementary materials

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Bis(1,3-diphenylpropane-1,3-dionato-κ^2O,O')bis(morpholine-κN)cobalt(II)

B. Kaitner and E. Mestrovic

Comment

High potential of metal complexes with β-diketonesas hosts in soft (and smart) supramolecular materials was recognized several years ago (Soldatov *et al.*, 1999). These materials have a lot of attributes which qualify them for use as supramolecular ion exchange materials, flexible and smart sorbents and as functional organic zeolite analogues. Based on this results Soldatov and his group have prepared a series of modified metal β-diketonate complexes in the design of supramolecular host–guest materials (Soldatov *et al.*, 1999, 2001, 2002, 2003). Based on molecular structural properties of metal(II)(β-diketonato)$_2$ units different types of supramolecular assemblies can be achieved (Bučar and Meštrović, 2003, Meštrović *et al.*, 2004, Meštrović and Kaitner 2006). Using this concepts soft supramolecular materials of specific property can be prepared. As β-diketones we used 1,3-diphenylpropane-1,3-dione (dibenzoylmethane, Hdbm) because the phenyl rings prevent formation of oligomers as in the case of cobalt(II)(acetylacetonate)$_2$ complex (Cotton and Elder, 1965) In further research, among other neutral molecules, morpholine was introduced to the basic metal bis-chelate unit of Co(dbm). Morpholine with two different heteroatoms can be bound to the metal centre. This ligand was expected to bind to the metal ion through the N atom and with possibility for additional interaction involving oxygen atoms. After recrystallization of Co(dbm)$_2$ from morpholine we obtained Co(dbm)$_2$(morpholine)$_2$. The title compound crystallizes in the monoclinic space group $P2_1/n$. The asymmetric unit comprises a half of the title complex. The complex unit is of C_i symmetry with Co atom located in the crystallographic inversion centre. The Co atom is in an octahedral environment formed by two dibenzoilmethanate moieties and two morpholine molecules. The Co—O bond distances are 2.029 (1) Å and 2.056 (1) Å. The Co—N bond distance is 2.262 (2) Å. The observed Co—N bond lengths are longer than the ones previously observed in adducts of Co(DBM)$_2$(thiomorpholine-N)$_2$ (2.211 Å Judaš *et al.*, 2006). The chelate rings, formed by two benzoylacetonate anions and cobalt are almost planar. The bite distance O1···O2 is 2.910 (2) Å and it is significantly longer than in any of the polymorphs of the free ligand (2.452 Å Etter *et al.*, 1987), 2.461 Å (Kaitner and Meštrović, 1993) and 2.459Å (Ozturk *et al.*, 1997). The morpholine molecules are additionally involved in a N—H···π interaction between the hydrogen atoms of the morpholine molecule and the chelate rings with distance of 2.700Å (Fig. 2.) Molecules in the crystal are linked by van der Waals interactions.

Experimental

Bis(1-phenyl-1,3-butanedionato)cobalt(II), Co(dbm), was prepared by methods previously published (Meštrović and Kaitner, 2006). The methanol adduct was formed after dissolving of Co(dbm)2 in morpholine. Crystals suitable for single-crystal X-ray-diffraction were obtained by evaporation of solution for two weeks.

Figures

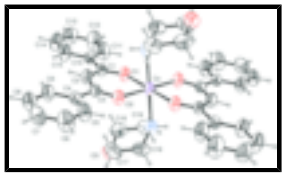

Fig. 1. A view of the title compound, showing the atom-numbering sheme and displacement ellipsoids drawn at the 30% probability level.

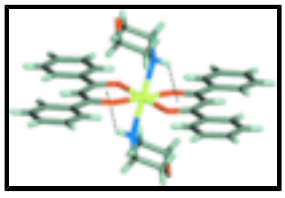

Fig. 2. The N—H···π interaction in Co(dbm)2(morpholine)2 shown by dashed line.

Bis(1,3-diphenylpropane-1,3-dionato-κ^2*O*,*O*')bis(morpholine-κ*N*)cobalt(II)

Crystal data

$[Co(C_{15}H_{11}O_2)_2(C_4H_4NO)_2]$	F_{000} = 714
M_r = 679.65	D_x = 1.335 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 25 reflections
a = 11.310 (1) Å	θ = 15–30º
b = 8.064 (1) Å	μ = 0.56 mm^{-1}
c = 18.642 (1) Å	T = 293 (2) K
β = 96.09 (2)º	Prism, dark red
V = 1690.6 (3) Å^3	0.57 × 0.57 × 0.43 mm
Z = 2	

Data collection

Philips Stoe upgrade diffractometer	R_{int} = 0.042
Radiation source: fine-focus sealed tube	θ_{max} = 30.0º
Monochromator: graphite	θ_{min} = 2.0º
T = 293(2) K	h = −15→15
ω scans	k = 0→11
Absorption correction: ψ scan (North et al., 1968)	l = 0→26
T_{min} = 0.784, T_{max} = 0.861	3 standard reflections
5060 measured reflections	every 90 min
4924 independent reflections	intensity decay: 1%
3152 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.056$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.164$	$w = 1/[\sigma^2(F_o^2) + (0.1132P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.99$	$(\Delta/\sigma)_{max} < 0.001$
4924 reflections	$\Delta\rho_{max} = 0.84$ e Å^{-3}
220 parameters	$\Delta\rho_{min} = -0.55$ 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}
Co	0.0000	0.0000	0.0000	0.04124 (14)
O1	0.17031 (12)	0.0848 (2)	0.02704 (8)	0.0473 (3)
O2	−0.04433 (12)	0.0846 (2)	0.09607 (8)	0.0486 (4)
O3	0.1758 (2)	−0.3391 (3)	0.17174 (11)	0.0758 (6)
N	0.03864 (17)	−0.2621 (2)	0.03876 (11)	0.0493 (4)
C1	0.20576 (17)	0.1773 (2)	0.07989 (10)	0.0387 (4)
C2	0.13570 (19)	0.2269 (3)	0.13436 (12)	0.0480 (5)
H2	0.1704	0.2992	0.1694	0.058*
C3	0.01808 (17)	0.1766 (2)	0.14047 (10)	0.0386 (4)
C4	−0.04179 (18)	0.2334 (3)	0.20448 (10)	0.0408 (4)
C5	−0.1584 (2)	0.1854 (4)	0.20850 (14)	0.0636 (7)
H5	−0.1974	0.1226	0.1714	0.076*
C6	−0.2179 (3)	0.2292 (5)	0.26685 (16)	0.0804 (9)
H6	−0.2960	0.1949	0.2691	0.096*
C7	−0.1611 (3)	0.3239 (4)	0.32154 (14)	0.0705 (8)
H7	−0.2008	0.3541	0.3608	0.085*
C8	−0.0462 (3)	0.3733 (4)	0.31806 (13)	0.0687 (7)
H8	−0.0081	0.4373	0.3551	0.082*
C9	0.0141 (2)	0.3295 (3)	0.26016 (12)	0.0582 (6)
H9	0.0922	0.3643	0.2584	0.070*
C10	0.33239 (17)	0.2368 (2)	0.08363 (10)	0.0405 (4)

C11	0.3989 (2)	0.1924 (4)	0.02880 (15)	0.0739 (8)
H11	0.3649	0.1265	−0.0088	0.089*
C12	0.5161 (3)	0.2449 (6)	0.02903 (19)	0.0966 (13)
H12	0.5597	0.2136	−0.0084	0.116*
C13	0.5684 (2)	0.3428 (4)	0.08424 (17)	0.0792 (9)
H13	0.6466	0.3781	0.0843	0.095*
C14	0.5038 (2)	0.3868 (4)	0.13844 (17)	0.0743 (8)
H14	0.5381	0.4534	0.1757	0.089*
C15	0.3873 (2)	0.3339 (4)	0.13909 (14)	0.0619 (6)
H15	0.3451	0.3639	0.1773	0.074*
C16	−0.0166 (2)	−0.3232 (4)	0.10135 (15)	0.0654 (7)
H16A	−0.0240	−0.4430	0.0989	0.078*
H16B	−0.0957	−0.2764	0.1012	0.078*
C17	0.0582 (3)	−0.2747 (4)	0.16943 (15)	0.0785 (9)
H17A	0.0617	−0.1547	0.1728	0.094*
H17B	0.0213	−0.3158	0.2106	0.094*
C18	0.2303 (2)	−0.2745 (4)	0.11232 (18)	0.0762 (9)
H18A	0.3110	−0.3164	0.1139	0.091*
H18B	0.2342	−0.1546	0.1159	0.091*
C19	0.1622 (2)	−0.3223 (4)	0.04198 (15)	0.0641 (7)
H19A	0.2003	−0.2751	0.0025	0.077*
H19B	0.1624	−0.4420	0.0369	0.077*
H111	−0.001 (2)	−0.296 (5)	0.0032 (17)	0.073 (10)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co	0.0365 (2)	0.0505 (2)	0.0363 (2)	−0.00666 (16)	0.00202 (13)	−0.00943 (16)
O1	0.0397 (7)	0.0591 (9)	0.0430 (7)	−0.0065 (7)	0.0029 (6)	−0.0117 (7)
O2	0.0425 (7)	0.0612 (10)	0.0423 (8)	−0.0091 (7)	0.0055 (6)	−0.0110 (7)
O3	0.0928 (14)	0.0659 (12)	0.0636 (11)	0.0021 (11)	−0.0161 (10)	0.0100 (9)
N	0.0457 (9)	0.0539 (10)	0.0471 (10)	−0.0028 (8)	0.0003 (8)	−0.0046 (8)
C1	0.0364 (9)	0.0401 (9)	0.0387 (9)	−0.0024 (7)	−0.0010 (7)	−0.0008 (7)
C2	0.0440 (10)	0.0568 (12)	0.0433 (10)	−0.0101 (9)	0.0058 (8)	−0.0122 (9)
C3	0.0401 (9)	0.0401 (9)	0.0352 (9)	0.0001 (8)	0.0024 (7)	−0.0008 (7)
C4	0.0435 (10)	0.0432 (10)	0.0356 (9)	0.0034 (8)	0.0039 (7)	0.0004 (8)
C5	0.0463 (12)	0.094 (2)	0.0511 (12)	−0.0078 (13)	0.0092 (10)	−0.0190 (13)
C6	0.0522 (14)	0.125 (3)	0.0668 (16)	−0.0032 (16)	0.0209 (12)	−0.0211 (17)
C7	0.0693 (16)	0.092 (2)	0.0521 (14)	0.0182 (15)	0.0172 (12)	−0.0086 (13)
C8	0.0816 (18)	0.0786 (18)	0.0464 (12)	0.0000 (14)	0.0096 (12)	−0.0172 (12)
C9	0.0580 (13)	0.0718 (15)	0.0451 (11)	−0.0082 (12)	0.0063 (10)	−0.0120 (11)
C10	0.0371 (9)	0.0441 (10)	0.0396 (9)	−0.0035 (8)	0.0007 (7)	0.0015 (8)
C11	0.0555 (14)	0.113 (2)	0.0556 (14)	−0.0280 (15)	0.0160 (11)	−0.0254 (15)
C12	0.0650 (17)	0.152 (4)	0.077 (2)	−0.039 (2)	0.0307 (16)	−0.032 (2)
C13	0.0512 (14)	0.101 (2)	0.086 (2)	−0.0270 (15)	0.0102 (13)	−0.0083 (17)
C14	0.0489 (13)	0.092 (2)	0.0806 (18)	−0.0205 (14)	0.0030 (12)	−0.0293 (16)
C15	0.0446 (12)	0.0789 (17)	0.0621 (14)	−0.0103 (11)	0.0055 (10)	−0.0236 (13)
C16	0.0547 (14)	0.0678 (16)	0.0761 (17)	0.0000 (12)	0.0177 (12)	0.0171 (13)

C17	0.110 (3)	0.0733 (19)	0.0538 (15)	0.0222 (17)	0.0170 (16)	0.0115 (13)
C18	0.0531 (14)	0.0732 (18)	0.098 (2)	−0.0045 (13)	−0.0120 (15)	0.0229 (16)
C19	0.0597 (14)	0.0685 (16)	0.0671 (16)	0.0155 (12)	0.0202 (12)	0.0062 (13)

Geometric parameters (Å, °)

Co—O2	2.0286 (14)	C7—H7	0.9300
Co—O2^{i}	2.0286 (14)	C8—C9	1.383 (3)
Co—O1^{i}	2.0556 (14)	C8—H8	0.9300
Co—O1	2.0556 (14)	C9—H9	0.9300
Co—N^{i}	2.262 (2)	C10—C11	1.379 (3)
Co—N	2.262 (2)	C10—C15	1.390 (3)
O1—C1	1.267 (2)	C11—C12	1.392 (4)
O2—C3	1.269 (2)	C11—H11	0.9300
O3—C18	1.423 (4)	C12—C13	1.380 (4)
O3—C17	1.425 (4)	C12—H12	0.9300
N—C16	1.466 (3)	C13—C14	1.355 (4)
N—C19	1.475 (3)	C13—H13	0.9300
N—H111	0.81 (3)	C14—C15	1.386 (3)
C1—C2	1.411 (3)	C14—H14	0.9300
C1—C10	1.505 (3)	C15—H15	0.9300
C2—C3	1.407 (3)	C16—C17	1.501 (4)
C2—H2	0.9300	C16—H16A	0.9700
C3—C4	1.504 (3)	C16—H16B	0.9700
C4—C5	1.384 (3)	C17—H17A	0.9700
C4—C9	1.392 (3)	C17—H17B	0.9700
C5—C6	1.385 (3)	C18—C19	1.499 (4)
C5—H5	0.9300	C18—H18A	0.9700
C6—C7	1.377 (4)	C18—H18B	0.9700
C6—H6	0.9300	C19—H19A	0.9700
C7—C8	1.367 (4)	C19—H19B	0.9700
O2—Co—O2^{i}	180.00 (8)	C9—C8—H8	119.6
O2—Co—O1^{i}	90.88 (6)	C8—C9—C4	120.1 (2)
O2^{i}—Co—O1^{i}	89.12 (6)	C8—C9—H9	119.9
O2—Co—O1	89.12 (6)	C4—C9—H9	119.9
O2^{i}—Co—O1	90.88 (6)	C11—C10—C15	117.5 (2)
O1^{i}—Co—O1	180.00 (8)	C11—C10—C1	118.30 (19)
O2—Co—N^{i}	84.85 (7)	C15—C10—C1	124.18 (19)
O2^{i}—Co—N^{i}	95.15 (7)	C10—C11—C12	120.9 (3)
O1^{i}—Co—N^{i}	95.07 (7)	C10—C11—H11	119.6
O1—Co—N^{i}	84.93 (7)	C12—C11—H11	119.6
O2—Co—N	95.15 (7)	C13—C12—C11	120.6 (3)
O2^{i}—Co—N	84.85 (7)	C13—C12—H12	119.7
O1^{i}—Co—N	84.93 (7)	C11—C12—H12	119.7
O1—Co—N	95.07 (7)	C14—C13—C12	119.0 (2)
N^{i}—Co—N	180.00 (10)	C14—C13—H13	120.5

C1—O1—Co	126.71 (13)	C12—C13—H13	120.5
C3—O2—Co	126.88 (13)	C13—C14—C15	120.9 (3)
C18—O3—C17	108.9 (2)	C13—C14—H14	119.5
C16—N—C19	109.84 (19)	C15—C14—H14	119.5
C16—N—Co	118.94 (16)	C14—C15—C10	121.1 (2)
C19—N—Co	118.09 (16)	C14—C15—H15	119.4
C16—N—H111	107 (2)	C10—C15—H15	119.4
C19—N—H111	111 (2)	N—C16—C17	109.6 (2)
Co—N—H111	89 (3)	N—C16—H16A	109.7
O1—C1—C2	124.84 (18)	C17—C16—H16A	109.7
O1—C1—C10	116.41 (17)	N—C16—H16B	109.7
C2—C1—C10	118.75 (18)	C17—C16—H16B	109.7
C3—C2—C1	125.80 (19)	H16A—C16—H16B	108.2
C3—C2—H2	117.1	O3—C17—C16	111.8 (2)
C1—C2—H2	117.1	O3—C17—H17A	109.3
O2—C3—C2	125.52 (18)	C16—C17—H17A	109.3
O2—C3—C4	115.42 (17)	O3—C17—H17B	109.3
C2—C3—C4	119.06 (18)	C16—C17—H17B	109.3
C5—C4—C9	118.4 (2)	H17A—C17—H17B	107.9
C5—C4—C3	118.00 (19)	O3—C18—C19	111.2 (2)
C9—C4—C3	123.61 (19)	O3—C18—H18A	109.4
C4—C5—C6	121.1 (2)	C19—C18—H18A	109.4
C4—C5—H5	119.4	O3—C18—H18B	109.4
C6—C5—H5	119.4	C19—C18—H18B	109.4
C7—C6—C5	119.7 (3)	H18A—C18—H18B	108.0
C7—C6—H6	120.2	N—C19—C18	110.4 (2)
C5—C6—H6	120.2	N—C19—H19A	109.6
C8—C7—C6	119.9 (2)	C18—C19—H19A	109.6
C8—C7—H7	120.1	N—C19—H19B	109.6
C6—C7—H7	120.1	C18—C19—H19B	109.6
C7—C8—C9	120.8 (2)	H19A—C19—H19B	108.1
C7—C8—H8	119.6		

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

Fig. 1

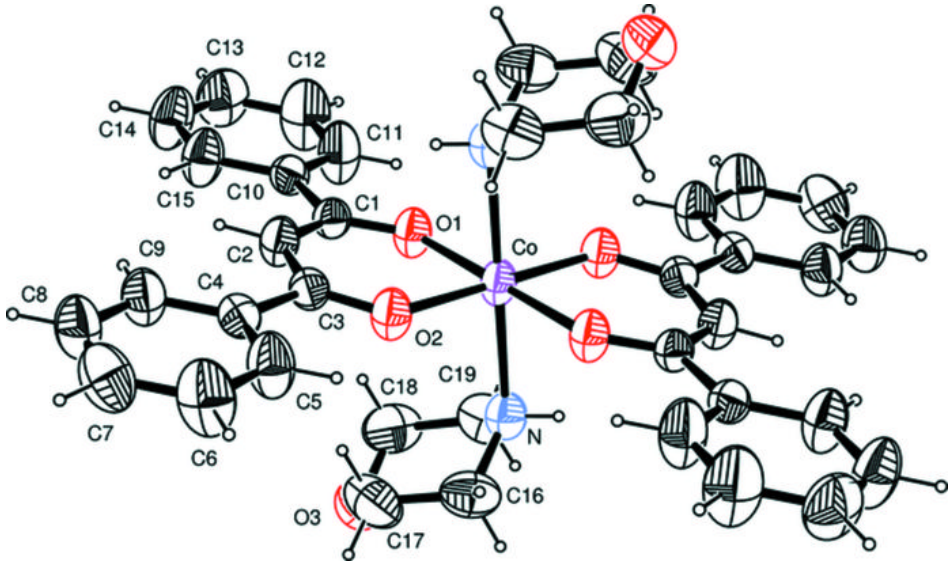
C13
C12
C14
C11
C15
C10
C1
O1
Co
C9
C2
C4
C8
C3
O2
C19
C18
C5
C7
C6
N
C16
O3
C17

Fig. 2