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Bis(2-formylphenolato)cobalt(II)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.051
wR factor = 0.153
Data-to-parameter ratio = 14.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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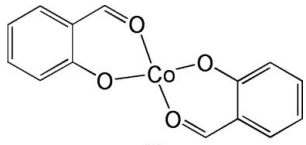
In the title compound, $[Co(C_7H_5O_2)_2]$, the Co atom is connected to four O atoms from two 2-formylphenolate ligands in a square-planar coordination. The molecule possesses a crystallographically imposed centre of symmetry.

Comment

The ability of some cobalt(II) complexes to bind dioxygen reversibly was discovered decades ago. Since then, many cobalt(II) dioxygen carriers have been discovered (Rybak-Akimova *et al.*, 1997), some of them having properties which make them good candidates for industrial and medicinal applications. Here, the structure of a new cobalt(II) complex, (I), derived from salicylaldehyde is reported.



(I)

In the title mononuclear cobalt(II) compound, the Co atom is four-coordinated by four O atoms from two 2-formylphenolate ligands, forming a square-planar coordination (Fig. 1). The Co atom lies on a centre of symmetry. The whole complex molecule is essentially planar, with a mean deviation of 0.047 (3) Å. The Co—O bond lengths (Table 1) are comparable with the corresponding values observed in other cobalt(II) complexes (De Angelis *et al.*, 1996; Ruiz-Molina *et al.*, 2000; Henson *et al.*, 1999). The molecular packing in (I) is stabilized only by van der Waals interactions (Fig. 2).

Experimental

A mixture of salicylaldehyde (1.0 mmol, 122.1 mg) and $Co(CH_3COO)_2{\cdot}4H_2O$ (1.0 mmol, 249.1 mg) was dissolved in ethanol (50 ml).

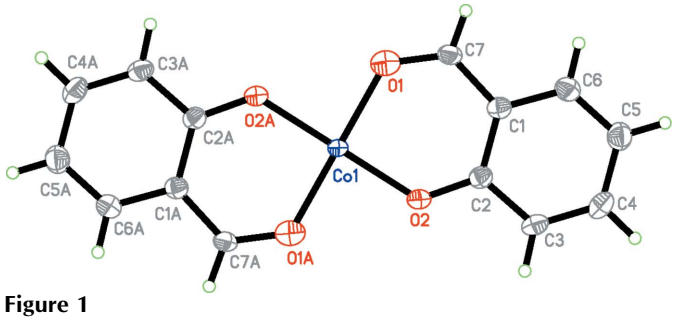


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level. Atoms with the suffix A are generated by the symmetry code $(2-x, 2-y, 2-z)$.

The mixture was stirred for about 1 h at room temperature to give a clear brown solution. After allowing the solution to evaporate slowly in air for a week, brown flake-like crystals were obtained.

Crystal data

$[Co(C_7H_5O_2)_2]$
M_r = 301.15
Monoclinic, $P2_1/c$
a = 12.955 (2) Å
b = 5.846 (1) Å
c = 8.050 (2) Å
β = 94.72 (2)°
V = 607.6 (2) Å^3
Z = 2
D_x = 1.646 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.42 mm^{-1}
T = 298 (2) K
Flake, brown
0.19 × 0.17 × 0.09 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.774, T_{max} = 0.883
4072 measured reflections
1312 independent reflections
1084 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 27.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.153
S = 1.07
1312 reflections
88 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0811P)^2 + 0.9211P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.80 e Å^{-3}
$\Delta\rho_{min}$ = −0.70 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O2	1.909 (3)	Co1—O1	1.921 (3)
O2^i—Co1—O2	180	O2—Co1—O1	92.73 (13)
O2^i—Co1—O1	87.27 (13)	O1—Co1—O1^i	180

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

H atoms were placed in calculated positions and constrained to ride on their parent atoms, with C—H distances of 0.93 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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*.

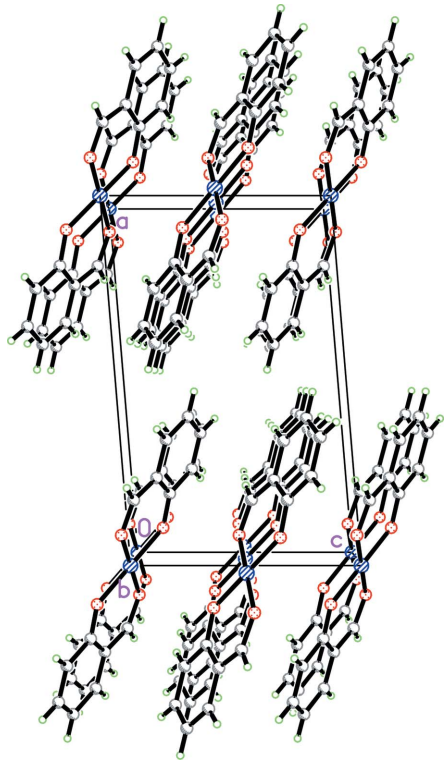


Figure 2
The molecular packing of (I), viewed along the *b* axis.

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