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Bis(2-formylphenolato- κ^2 O,O')iron(II)

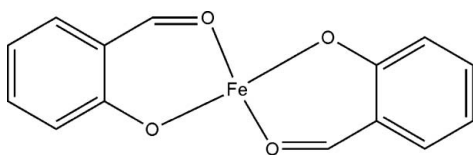
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.035; wR factor = 0.100; data-to-parameter ratio = 12.1.

The title complex, $[\text{Fe}(\text{C}_7\text{H}_5\text{O}_2)_2]$, is a mononuclear iron(II) complex with a distorted square planar coordination geometry and has the central Fe^{2+} ion located on an inversion centre, with four O atoms from two 2-formylphenolate ligands.



Experimental

Crystal data

$[\text{Fe}(\text{C}_7\text{H}_5\text{O}_2)_2]$
 $M_r = 298.07$
Monoclinic, $P2_1/n$
 $a = 8.801$ (5) Å
 $b = 6.236$ (3) Å
 $c = 11.408$ (6) Å
 $\beta = 105.642$ (7)°

$V = 602.9$ (5) Å³
 $Z = 2$
Mo $K\alpha$ radiation
 $\mu = 1.26$ mm⁻¹
 $T = 298$ (2) K
 $0.35 \times 0.30 \times 0.13$ mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{\min} = 0.668$, $T_{\max} = 0.854$

3023 measured reflections
1068 independent reflections
841 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.026$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.035$
 $wR(F^2) = 0.100$
 $S = 1.02$
1068 reflections

88 parameters
H-atom parameters constrained
 $\Delta\rho_{\max} = 0.37$ e Å⁻³
 $\Delta\rho_{\min} = -0.29$ e Å⁻³

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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, 1996); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2082).

References

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Sheldrick, G. M. (1997). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
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supplementary materials

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Bis(2-formylphenolato- κ^2O,O')iron(II)

Y.-M. Yang, P.-C. Lu, T.-T. Zhu and C.-H. Liu

Experimental

Equimolar iron(II) acetate and salicylaldehyde were put into a Teflon vessel, and aqueous ethanol solution ($H_2O: EtOH = 1: 1 v/v$) was added. The vessel was then put in a stainless steel tank to make hydrothermal treatment. The tank was heated to $140^\circ C$ for 48 h. After the autoclave was cooled to room temperature, red crystals were formed. They were filtered, washed with aqueous ethanol solution for three times, and dried in a vacuo using $CaCl_2$, yield 71%.

Refinement

C-bound H atoms were included in the riding model approximation with $C-H = 0.93 - 0.97 \text{ \AA}$, and with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

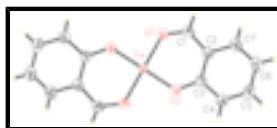


Fig. 1. A view of the molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability label and H atoms are shown as small spheres of arbitrary radii. Unlabeled atoms are related to labeled atoms by the symmetry code $(-x + 1, -y, -z + 2)$.

Bis(2-formylphenolato- κ^2O,O')iron(II)

Crystal data

$[Fe(C_7H_5O_2)_2]$

$M_r = 298.07$

Monoclinic, $P2_1/n$

Hall symbol: $-P 2_1n$

$a = 8.801 (5) \text{ \AA}$

$b = 6.236 (3) \text{ \AA}$

$c = 11.408 (6) \text{ \AA}$

$\beta = 105.642 (7)^\circ$

$V = 602.9 (5) \text{ \AA}^3$

$Z = 2$

$F_{000} = 304$

$D_x = 1.642 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073 \text{ \AA}$

Cell parameters from 658 reflections

$\theta = 3.6-26.1^\circ$

$\mu = 1.26 \text{ mm}^{-1}$

$T = 298 (2) \text{ K}$

Prism, red

$0.35 \times 0.30 \times 0.13 \text{ mm}$

Data collection

Bruker SMART CCD
diffractometer

1068 independent reflections

supplementary materials

Radiation source: fine-focus sealed tube	841 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.026$
$T = 298(2)$ K	$\theta_{\text{max}} = 25.0^\circ$
φ and ω scans	$\theta_{\text{min}} = 2.6^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -9 \rightarrow 10$
$T_{\text{min}} = 0.668$, $T_{\text{max}} = 0.854$	$k = -6 \rightarrow 7$
3023 measured reflections	$l = -13 \rightarrow 7$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.035$	H-atom parameters constrained
$wR(F^2) = 0.100$	$w = 1/[\sigma^2(F_o^2) + (0.0643P)^2]$
$S = 1.02$	where $P = (F_o^2 + 2F_c^2)/3$
1068 reflections	$(\Delta/\sigma)_{\text{max}} = 0.009$
88 parameters	$\Delta\rho_{\text{max}} = 0.37 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.29 \text{ e } \text{\AA}^{-3}$
	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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Fe	0.5000	0.0000	1.0000	0.0375 (2)
O1	0.3768 (2)	0.1172 (3)	0.8467 (2)	0.0613 (6)
O2	0.6619 (2)	0.2057 (3)	1.01596 (19)	0.0577 (6)
C1	0.4067 (4)	0.2879 (5)	0.7994 (3)	0.0566 (8)
H1A	0.3347	0.3292	0.7272	0.068*
C2	0.5378 (4)	0.4246 (5)	0.8436 (3)	0.0480 (7)
C3	0.6593 (3)	0.3772 (5)	0.9496 (3)	0.0478 (7)
C4	0.7849 (4)	0.5252 (5)	0.9844 (4)	0.0629 (10)
H4A	0.8673	0.4982	1.0533	0.075*
C5	0.7869 (4)	0.7082 (5)	0.9180 (4)	0.0694 (10)

H5A	0.8708	0.8033	0.9433	0.083*
C6	0.6667 (4)	0.7555 (5)	0.8137 (4)	0.0682 (10)
H6A	0.6696	0.8802	0.7696	0.082*
C7	0.5447 (4)	0.6140 (5)	0.7779 (3)	0.0619 (9)
H7A	0.4639	0.6435	0.7084	0.074*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe	0.0355 (3)	0.0346 (3)	0.0344 (4)	-0.0034 (2)	-0.0043 (2)	0.0028 (2)
O1	0.0597 (13)	0.0552 (14)	0.0568 (14)	-0.0066 (11)	-0.0052 (11)	0.0086 (12)
O2	0.0571 (13)	0.0556 (13)	0.0498 (13)	-0.0091 (10)	-0.0039 (10)	0.0068 (11)
C1	0.0536 (19)	0.0568 (19)	0.052 (2)	0.0065 (15)	0.0010 (15)	0.0093 (16)
C2	0.0500 (18)	0.0448 (14)	0.0499 (19)	0.0071 (14)	0.0146 (14)	0.0032 (15)
C3	0.0527 (19)	0.0456 (17)	0.0448 (17)	0.0001 (14)	0.0125 (14)	-0.0028 (15)
C4	0.065 (2)	0.063 (2)	0.056 (2)	-0.0143 (16)	0.0078 (17)	-0.0014 (17)
C5	0.075 (2)	0.061 (2)	0.078 (3)	-0.0172 (19)	0.030 (2)	-0.005 (2)
C6	0.076 (2)	0.0538 (19)	0.082 (3)	0.0027 (18)	0.034 (2)	0.0130 (19)
C7	0.062 (2)	0.059 (2)	0.067 (2)	0.0129 (18)	0.0206 (17)	0.0132 (19)

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

Fe—O2 ⁱ	1.889 (2)	C2—C3	1.413 (4)
Fe—O2	1.889 (2)	C3—C4	1.412 (4)
Fe—O1 ⁱ	1.936 (2)	C4—C5	1.373 (4)
Fe—O1	1.936 (2)	C4—H4A	0.9300
O1—C1	1.253 (3)	C5—C6	1.394 (5)
O2—C3	1.307 (3)	C5—H5A	0.9300
C1—C2	1.413 (4)	C6—C7	1.365 (5)
C1—H1A	0.9300	C6—H6A	0.9300
C2—C7	1.409 (5)	C7—H7A	0.9300
O2 ⁱ —Fe—O2	180.0	O2—C3—C2	123.9 (3)
O2 ⁱ —Fe—O1 ⁱ	93.15 (9)	C4—C3—C2	117.3 (3)
O2—Fe—O1 ⁱ	86.85 (9)	C5—C4—C3	120.9 (3)
O2 ⁱ —Fe—O1	86.85 (9)	C5—C4—H4A	119.5
O2—Fe—O1	93.15 (9)	C3—C4—H4A	119.5
O1 ⁱ —Fe—O1	180.000 (1)	C4—C5—C6	121.8 (3)
C1—O1—Fe	125.3 (2)	C4—C5—H5A	119.1
C3—O2—Fe	127.21 (19)	C6—C5—H5A	119.1
O1—C1—C2	127.2 (3)	C7—C6—C5	118.3 (3)
O1—C1—H1A	116.4	C7—C6—H6A	120.9
C2—C1—H1A	116.4	C5—C6—H6A	120.9
C7—C2—C3	120.0 (3)	C6—C7—C2	121.8 (3)
C7—C2—C1	117.7 (3)	C6—C7—H7A	119.1
C3—C2—C1	122.4 (3)	C2—C7—H7A	119.1
O2—C3—C4	118.8 (3)		
O2 ⁱ —Fe—O1—C1	172.5 (3)	C7—C2—C3—O2	179.8 (3)

supplementary materials

O2—Fe—O1—C1	-7.5 (3)	C1—C2—C3—O2	-0.1 (5)
O1 ⁱ —Fe—O1—C1	33 (100)	C7—C2—C3—C4	-0.5 (5)
O2 ⁱ —Fe—O2—C3	0(100)	C1—C2—C3—C4	179.6 (3)
O1 ⁱ —Fe—O2—C3	-170.2 (2)	O2—C3—C4—C5	-179.7 (3)
O1—Fe—O2—C3	9.8 (2)	C2—C3—C4—C5	0.7 (5)
Fe—O1—C1—C2	3.0 (5)	C3—C4—C5—C6	-0.4 (5)
O1—C1—C2—C7	-177.5 (3)	C4—C5—C6—C7	0.0 (6)
O1—C1—C2—C3	2.5 (5)	C5—C6—C7—C2	0.2 (5)
Fe—O2—C3—C4	172.7 (2)	C3—C2—C7—C6	0.1 (5)
Fe—O2—C3—C2	-7.6 (4)	C1—C2—C7—C6	-180.0 (3)

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

Fig. 1

