

Retraction of articles

This article reports the retraction of 39 articles published in *Acta Crystallographica Section E* between 2004 and 2009.

After thorough investigation (see Harrison *et al.*, 2010), 39 additional articles are retracted as a result of problems with the data sets or incorrect atom assignments. Full details of all the articles are given in Table 1.

Table 1

Details of articles to be retracted, in order of publication.

Title	Reference	Retracted by	DOI	Refcode
<i>trans</i> -Bis[1-[3-(cyclohexylamino)propyliminomethyl]-2-naphtholato]copper(II) dichloride dihydrate	Zhang (2004)	Journal	10.1107/S1600536804028296	BIPDUA
Bis(4-bromo-2-formylphenolato- $\kappa^2 O, O'$)copper(II)	Sun & Gao (2005)	Author	10.1107/S160053680500187X	FEYSUY
Bis(salicylaldehyde)zinc(II)	Xiong & Liu (2005)	Journal	10.1107/S1600536805010913	GAMDUU
Bis(4-bromo-2-formylphenolato- $\kappa^2 O, O'$)zinc(II)	Chen (2006)	Journal	10.1107/S1600536805040432	SAZCUS
Bis(2-formylphenolato- $\kappa^2 O, O'$)nickel(II)	Li & Chen (2006)	Journal	10.1107/S1600536806012931	IDAZAP
Bis(2-formylphenolato)cobalt(II)	Qiu (2006)	Journal	10.1107/S1600536806015704	GEJDUV
Bis(2-formylphenolato- $\kappa^2 O, O'$)manganese(II)	Wang & Fang (2006)	Journal	10.1107/S1600536806021039	IDOVED
Tetraaqua(1,10-phenanthroline- $\kappa^2 N, N'$)copper(II) naphthalene-1,5-disulfonate dihydrate	Liu <i>et al.</i> (2006)	Author	10.1107/S1600536806030637	GENYOO
Tetraaqua(1,10-phenanthroline- $\kappa^2 N, N'$)nickel(II) naphthalene-1,5-disulfonate dihydrate	Liu & Fan (2006)	Author	10.1107/S1600536806035410	KERBEP
{6,6'-Diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratolutetium(III)copper(II)	Sui <i>et al.</i> (2006)	Journal	10.1107/S160053680604565X	HESPEP
Bis(2-formylphenolato- $\kappa^2 O, O'$)iron(II)	Yang <i>et al.</i> (2007)	Author	10.1107/S1600536807021721	PIFCAJ
2,6-Dimethoxybenzohydrazide	Qadeer <i>et al.</i> (2007a)	Journal	10.1107/S1600536807022593	PIFHES
2-(2,4-Dichlorophenylsulfanyl)acetohydrazide	Qadeer <i>et al.</i> (2007b)	Journal	10.1107/S1600536807022891	YIFSOW
{6,6'-Diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratoeuropium(III)zinc(II)	Hu <i>et al.</i> (2007)	Author	10.1107/S1600536807031121	WIHKEE
{ μ -6,6'-Diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratocerium(III)zinc(II)	Sui, Zhang, Hu & Yin (2007)	Author	10.1107/S1600536807032564	WIHREL
{ μ -6,6'-Diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratopraseodymium(III)zinc(II)	Chen <i>et al.</i> (2007)	Author	10.1107/S1600536807032540	WIHRIP
{ μ -6,6'-Diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratopraseodymium(III)nickel(II)	Sui, Li <i>et al.</i> (2007)	Author	10.1107/S1600536807032618	UFACUA
{6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-1 $\kappa^4 O^1, O^2, O^3, O^4, O^5, O^6, O^7, O^8, O^9, O^{10}, O^{11}, O^{12}, O^{13}, O^{14}, O^{15}, O^{16}, O^{17}, O^{18}, O^{19}, O^{20}, O^{21}, O^{22}, O^{23}, O^{24}, O^{25}, O^{26}, O^{27}, O^{28}, O^{29}, O^{30}, O^{31}, O^{32}, O^{33}, O^{34}, O^{35}, O^{36}, O^{37}, O^{38}, O^{39}, O^{40}, O^{41}, O^{42}, O^{43}, O^{44}, O^{45}, O^{46}, O^{47}, O^{48}, O^{49}, O^{50}, O^{51}, O^{52}, O^{53}, O^{54}, O^{55}, O^{56}, O^{57}, O^{58}, O^{59}, O^{60}, O^{61}, O^{62}, O^{63}, O^{64}, O^{65}, O^{66}, O^{67}, O^{68}, O^{69}, O^{70}, O^{71}, O^{72}, O^{73}, O^{74}, O^{75}, O^{76}, O^{77}, O^{78}, O^{79}, O^{80}, O^{81}, O^{82}, O^{83}, O^{84}, O^{85}, O^{86}, O^{87}, O^{88}, O^{89}, O^{90}, O^{91}, O^{92}, O^{93}, O^{94}, O^{95}, O^{96}, O^{97}, O^{98}, O^{99}, O^{100}, O^{101}, O^{102}, O^{103}, O^{104}, O^{105}, O^{106}, O^{107}, O^{108}, O^{109}, O^{110}, O^{111}, O^{112}, O^{113}, O^{114}, O^{115}, O^{116}, O^{117}, O^{118}, O^{119}, O^{120}, O^{121}, O^{122}, O^{123}, O^{124}, O^{125}, O^{126}, O^{127}, O^{128}, O^{129}, O^{130}, O^{131}, O^{132}, O^{133}, O^{134}, O^{135}, O^{136}, O^{137}, O^{138}, O^{139}, O^{140}, O^{141}, O^{142}, O^{143}, O^{144}, O^{145}, O^{146}, O^{147}, O^{148}, O^{149}, O^{150}, O^{151}, O^{152}, O^{153}, O^{154}, O^{155}, O^{156}, O^{157}, O^{158}, O^{159}, O^{160}, O^{161}, O^{162}, O^{163}, O^{164}, O^{165}, O^{166}, O^{167}, O^{168}, O^{169}, O^{170}, O^{171}, O^{172}, O^{173}, O^{174}, O^{175}, O^{176}, O^{177}, O^{178}, O^{179}, O^{180}, O^{181}, O^{182}, O^{183}, O^{184}, O^{185}, O^{186}, O^{187}, O^{188}, O^{189}, O^{190}, O^{191}, O^{192}, O^{193}, O^{194}, O^{195}, O^{196}, O^{197}, O^{198}, O^{199}, O^{200}, O^{201}, O^{202}, O^{203}, O^{204}, O^{205}, O^{206}, O^{207}, O^{208}, O^{209}, O^{210}, O^{211}, O^{212}, O^{213}, O^{214}, O^{215}, O^{216}, O^{217}, O^{218}, O^{219}, O^{220}, O^{221}, O^{222}, O^{223}, O^{224}, O^{225}, O^{226}, O^{227}, O^{228}, O^{229}, O^{230}, O^{231}, O^{232}, O^{233}, O^{234}, O^{235}, O^{236}, O^{237}, O^{238}, O^{239}, O^{240}, O^{241}, O^{242}, O^{243}, O^{244}, O^{245}, O^{246}, O^{247}, O^{248}, O^{249}, O^{250}, O^{251}, O^{252}, O^{253}, O^{254}, O^{255}, O^{256}, O^{257}, O^{258}, O^{259}, O^{260}, O^{261}, O^{262}, O^{263}, O^{264}, O^{265}, O^{266}, O^{267}, O^{268}, O^{269}, O^{270}, O^{271}, O^{272}, O^{273}, O^{274}, O^{275}, O^{276}, O^{277}, O^{278}, O^{279}, O^{280}, O^{281}, O^{282}, O^{283}, O^{284}, O^{285}, O^{286}, O^{287}, O^{288}, O^{289}, O^{290}, O^{291}, O^{292}, O^{293}, O^{294}, O^{295}, O^{296}, O^{297}, O^{298}, O^{299}, O^{300}, O^{301}, O^{302}, O^{303}, O^{304}, O^{305}, O^{306}, O^{307}, O^{308}, O^{309}, O^{310}, O^{311}, O^{312}, O^{313}, O^{314}, O^{315}, O^{316}, O^{317}, O^{318}, O^{319}, O^{320}, O^{321}, O^{322}, O^{323}, O^{324}, O^{325}, O^{326}, O^{327}, O^{328}, O^{329}, O^{330}, O^{331}, O^{332}, O^{333}, O^{334}, O^{335}, O^{336}, O^{337}, 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O^{893}, O^{894}, O^{895}, O^{896}, O^{897}, O^{898}, O^{899}, O^{900}, O^{901}, O^{902}, O^{903}, O^{904}, O^{905}, O^{906}, O^{907}, O^{908}, O^{909}, O^{910}, O^{911}, O^{912}, O^{913}, O^{914}, O^{915}, O^{916}, O^{917}, O^{918}, O^{919}, O^{920}, O^{921}, O^{922}, O^{923}, O^{924}, O^{925}, O^{926}, O^{927}, O^{928}, O^{929}, O^{930}, O^{931}, O^{932}, O^{933}, O^{934}, O^{935}, O^{936}, O^{937}, O^{938}, O^{939}, O^{940}, O^{941}, O^{942}, O^{943}, O^{944}, O^{945}, O^{946}, O^{947}, O^{948}, O^{949}, O^{950}, O^{951}, O^{952}, O^{953}, O^{954}, O^{955}, O^{956}, O^{957}, O^{958}, O^{959}, O^{960}, O^{961}, O^{962}, O^{963}, O^{964}, O^{965}, O^{966}, O^{967}, O^{968}, O^{969}, O^{970}, O^{971}, O^{972}, O^{973}, O^{974}, O^{975}, O^{976}, O^{977}, O^{978}, O^{979}, O^{980}, O^{981}, O^{982}, O^{983}, O^{984}, O^{985}, O^{986}, O^{987}, O^{988}, O^{989}, O^{990}, O^{991}, O^{992}, O^{993}, O^{994}, O^{995}, O^{996}, O^{997}, O^{998}, O^{999}, O^{1000}$				

Table 1 (continued)

Title	Reference	Retracted by	DOI	Refcode
{ μ -6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}- μ -nitrate-dinitratoeuropium(III)zinc(II)	Hu <i>et al.</i> (2008)	Author	10.1107/S160053680706151X	MIRPAF
Bis(4-chloro-2-formylphenolato)nickel(II)	Li <i>et al.</i> (2008)	Author	10.1107/S1600536807056309	RISTET
{ μ -6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}- μ -nitrate-dinitratoerbium(III)zinc(II)	Chen <i>et al.</i> (2008)	Author	10.1107/S1600536808006958	QIXHIP
Bis(2-ethoxy-6-formylphenolato- $\kappa^2 O^1, O^6$)nickel(II)	Han (2008)	Journal	10.1107/S160053680800809X	QIXLIT
{ μ -6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}- μ -nitrate-dinitratoholmium(III)zinc(II)	Xiao, Sui <i>et al.</i> (2008)	Author	10.1107/S1600536808013743	BIZTUA
{ μ -6,6'-Diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratoholmium(III)nickel(II)	Xiao, Fu <i>et al.</i> (2008)	Author	10.1107/S1600536808013755	BIZVAI
Hydrogen-bonding patterns in the cocrystal terephthalic acid-4,4'-bipyridine (2I)	Wang <i>et al.</i> (2009)	Journal	10.1107/S160053680903236X	DUCZEH
{6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato- $1\kappa^4 O^1, O^1, O^6, O^6:2\kappa^4 O^1, N, N', O^1$ }(ethanol- $1\kappa O$)- μ -nitrate- $1:2\kappa^2 O:O'$ -dinitrate- $1\kappa^2 O, O'$ -samarium(III)zinc(II)	Huang <i>et al.</i> (2009)	Journal	10.1107/S1600536809033558	YUCWAV

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Structure Reports

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

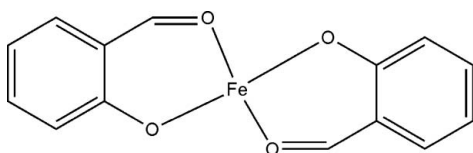
Yu-Min Yang, Peng-Cheng Lu, Tao-Tao Zhu and Chang-Hong Liu*

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

The title complex, $[Fe(C_7H_5O_2)_2]$, 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

$[Fe(C_7H_5O_2)_2]$
 $M_r = 298.07$
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 × 0.30 × 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 $I > 2\sigma(I)$
 $R_{int} = 0.026$

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*.

The work was supported by the Analytical Test Fund of Nanjing University awarded to Dr Chang-Hong Liu.

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

References

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supplementary materials

Article retracted

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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

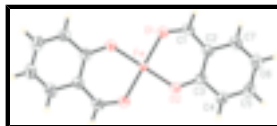


Fig. 1. A view of the molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability label and H atoms are shown as small spheres of arbitrary radii. Unlabeled atoms are related to labeled atoms by the symmetry code $(-x + 1, -y, -z + 2)$.

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: $-P 2_1/n$

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

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

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

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

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

$Z = 2$

$F_{000} = 304$

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

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)

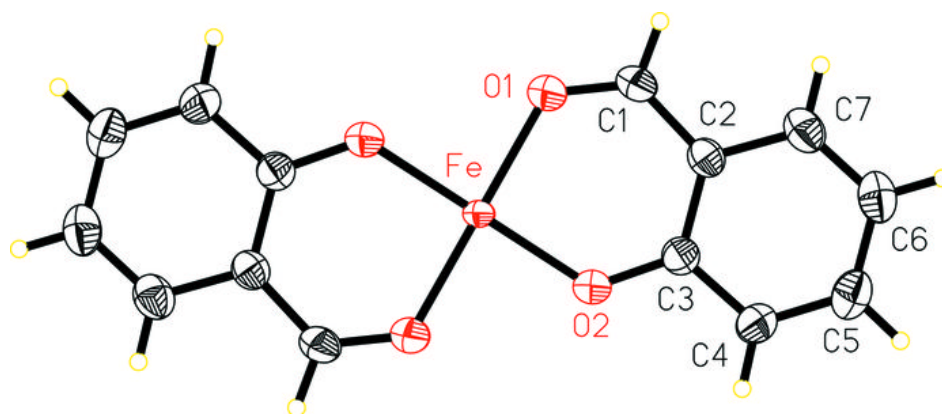
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O2—Fe—O1—C1	-7.5 (3)	C1—C2—C3—O2	-0.1 (5)
O1 ⁱ —Fe—O1—C1	33 (100)	C7—C2—C3—C4	-0.5 (5)
O2 ⁱ —Fe—O2—C3	0(100)	C1—C2—C3—C4	179.6 (3)
O1 ⁱ —Fe—O2—C3	-170.2 (2)	O2—C3—C4—C5	-179.7 (3)
O1—Fe—O2—C3	9.8 (2)	C2—C3—C4—C5	0.7 (5)
Fe—O1—C1—C2	3.0 (5)	C3—C4—C5—C6	-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) $-x+1, -y, -z+2$.

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Fig. 1



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