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Bis(2-benzyliminomethyl-4,6-dihydro-selenophenolato)iron(II)

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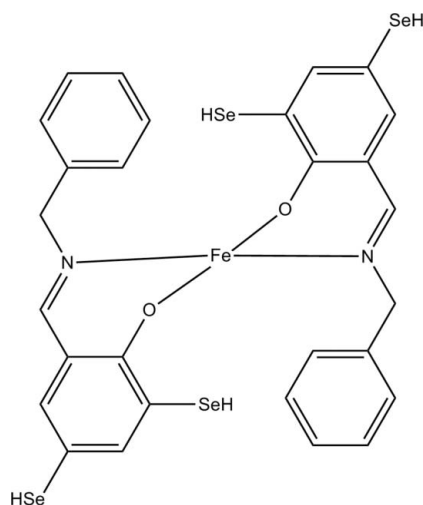
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.040; wR factor = 0.105; data-to-parameter ratio = 18.5.

In the title compound, $[\text{Fe}(\text{C}_{14}\text{H}_{12}\text{NOSe}_2)_2]$, the Fe^{II} ion (site symmetry $\bar{1}$) is four-coordinated by two *N,O*-bidentate Schiff base ligands, resulting in a slightly distorted *trans*- FeN_2O_2 square-planar coordination for the metal ion.

Related literature

For background, see: Shi *et al.* (2008); Xu *et al.* (2009). For reference structural data, see: Allen *et al.* (1987).



Experimental

Crystal data

$[\text{Fe}(\text{C}_{14}\text{H}_{12}\text{NOSe}_2)_2]$
 $M_r = 792.18$
Monoclinic, $P2_1/c$

$a = 10.6065$ (5) Å
 $b = 6.1055$ (5) Å
 $c = 20.7125$ (15) Å

$\beta = 102.435$ (5)°
 $V = 1309.83$ (16) Å³
 $Z = 2$
Mo $K\alpha$ radiation

$\mu = 6.16$ mm⁻¹
 $T = 296$ K
 $0.32 \times 0.26 \times 0.24$ mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
 $T_{\min} = 0.243$, $T_{\max} = 0.319$
(expected range = 0.174–0.228)
8208 measured reflections

2321 independent reflections
2133 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.044$
3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.040$
 $wR(F^2) = 0.105$
 $S = 1.05$
3231 reflections
175 parameters
2 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.68$ e Å⁻³
 $\Delta\rho_{\min} = -0.61$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Fe1—O1	1.845 (2)	Fe1—N1	1.945 (3)
O1—Fe1—N1	91.85 (12)		

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: HB5048).

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Shi, L., Fang, R.-Q., Xue, J.-Y., Xiao, Z.-P., Tan, S.-H. & Zhu, H.-L. (2008). *Aust. J. Chem.* **61**, 288–296.
Xu, S.-P., Shi, L., Lv, P.-C., Fang, R.-Q. & Zhu, H.-L. (2009). *J. Coord. Chem.* **62**, 2048–2057.

supplementary materials

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Bis(2-benzyliminomethyl-4,6-dihydro-selenophenolato)iron(II)

H.-Y. Li, L.-J. Wang, J. Hou and Q.-F. Zeng

Comment

There has been much research interest in Schiff base metal complexes due to their molecular architectures and biological activities (Shi *et al.*, 2008; Xu *et al.*, 2009). In this work, we report here the crystal structure of the title compound, (I). In (I), all bond lengths are within normal ranges (Allen *et al.*, 1987) (Fig. 1). The Fe^{II} is four-coordinated in a slightly distort square-planar configuration by two N atoms and two O atoms of the Schiff base ligands.

Experimental

A mixture of 3,5-dihydro-seleno-2-hydroxybenzaldehyde (564 mg, 2 mmol), phenylmethanamine (107 mg, 2 mmol) and FeCl₂·4H₂O (1 mmol, 198 mg) in methanol (10 ml) was stirred for 1 h. After keeping the filtrate in air for 7 d, green blocks of (I) were formed.

Refinement

All H atoms were positioned geometrically (C—H = 0.93 Å for the aromatic H atoms and C—H = 0.96 Å for the aliphatic H atoms) and were refined as riding, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$.

Figures

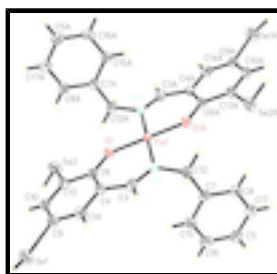


Fig. 1. The molecular structure of (I) showing 30% probability displacement ellipsoids, Atoms with an A suffix to their labels are generated by the symmetry operation (1-x, 1-y, -z).

Bis(2-benzyliminomethyl-4,6-dihydro-selenophenolato)iron(II)

Crystal data

[Fe(C₁₄H₁₂NOSe₂)₂]

$M_r = 792.18$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 10.6065$ (5) Å

$b = 6.1055$ (5) Å

$F_{000} = 768$

$D_x = 2.009$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 25 reflections

$\theta = 9\text{--}12^\circ$

$\mu = 6.16$ mm⁻¹

supplementary materials

$c = 20.7125 (15) \text{ \AA}$
 $\beta = 102.435 (5)^\circ$
 $V = 1309.83 (16) \text{ \AA}^3$
 $Z = 2$

$T = 296 \text{ K}$
Block, green
 $0.32 \times 0.26 \times 0.24 \text{ mm}$

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Monochromator: graphite
 $T = 296 \text{ K}$
 $\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
 $T_{\min} = 0.243$, $T_{\max} = 0.319$
8208 measured reflections
3231 independent reflections
2133 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.044$
 $\theta_{\max} = 28.6^\circ$
 $\theta_{\min} = 2.0^\circ$
 $h = -13 \rightarrow 12$
 $k = -8 \rightarrow 8$
 $l = -27 \rightarrow 24$
3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.040$
 $wR(F^2) = 0.105$
 $S = 1.05$
3231 reflections
175 parameters
2 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0464P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.015$
 $\Delta\rho_{\max} = 0.68 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.61 \text{ e \AA}^{-3}$
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	$U_{\text{iso}}^*/U_{\text{eq}}$
Fe1	0.5000	0.5000	0.0000	0.02627 (19)
Se1	0.39624 (5)	1.46692 (8)	0.19627 (3)	0.06046 (19)
Se2	0.11313 (4)	0.76022 (9)	0.06333 (3)	0.05734 (19)
N1	0.6354 (3)	0.6850 (5)	0.05035 (16)	0.0338 (7)
O1	0.3733 (2)	0.6579 (5)	0.02791 (13)	0.0383 (7)
C3	0.6153 (4)	0.8701 (7)	0.0771 (2)	0.0370 (9)
H3	0.6877	0.9562	0.0930	0.044*
C4	0.4943 (3)	0.9565 (6)	0.08496 (19)	0.0333 (9)
C5	0.8814 (4)	0.1903 (9)	0.2276 (2)	0.0519 (12)
H5	0.9044	0.0960	0.2635	0.062*
C6	0.3792 (3)	0.8364 (6)	0.06265 (18)	0.0322 (9)
C7	0.8111 (3)	0.4726 (6)	0.12025 (19)	0.0339 (9)
C8	0.8905 (4)	0.2934 (7)	0.1180 (2)	0.0433 (10)
H8	0.9206	0.2664	0.0798	0.052*
C9	0.3884 (4)	1.2227 (6)	0.1388 (2)	0.0393 (9)
C10	0.2727 (4)	1.1107 (7)	0.11830 (19)	0.0403 (10)
H10	0.1978	1.1635	0.1293	0.048*
C12	0.7746 (3)	0.6234 (7)	0.0611 (2)	0.0359 (9)
H12A	0.8275	0.7544	0.0684	0.043*
H12B	0.7905	0.5504	0.0220	0.043*
C13	0.2689 (4)	0.9232 (7)	0.08202 (19)	0.0370 (9)
C14	0.4963 (4)	1.1457 (6)	0.1226 (2)	0.0398 (10)
H14	0.5737	1.2204	0.1368	0.048*
C15	0.7687 (4)	0.5074 (7)	0.1783 (2)	0.0425 (10)
H15	0.7167	0.6274	0.1820	0.051*
C16	0.8040 (4)	0.3632 (8)	0.2308 (2)	0.0504 (12)
H16	0.7734	0.3864	0.2691	0.061*
C17	0.9257 (4)	0.1547 (8)	0.1713 (2)	0.0498 (11)
H17	0.9798	0.0364	0.1689	0.060*
H1	0.318 (3)	1.461 (7)	0.2300 (18)	0.060*
H2	0.064 (4)	0.795 (7)	0.1091 (14)	0.060*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0184 (3)	0.0306 (4)	0.0295 (4)	-0.0017 (3)	0.0046 (3)	-0.0018 (3)
Se1	0.0802 (4)	0.0432 (3)	0.0599 (4)	0.0061 (2)	0.0195 (3)	-0.0142 (2)
Se2	0.0286 (2)	0.0838 (4)	0.0631 (4)	-0.0073 (2)	0.0177 (2)	-0.0260 (3)
N1	0.0228 (15)	0.0406 (19)	0.0364 (19)	0.0003 (13)	0.0028 (13)	0.0025 (15)
O1	0.0262 (13)	0.0458 (17)	0.0436 (17)	-0.0017 (11)	0.0092 (12)	-0.0112 (14)
C3	0.0283 (19)	0.035 (2)	0.047 (3)	-0.0040 (16)	0.0069 (18)	0.004 (2)
C4	0.0310 (19)	0.032 (2)	0.037 (2)	-0.0006 (15)	0.0079 (17)	0.0007 (18)
C5	0.047 (3)	0.066 (3)	0.039 (3)	0.003 (2)	0.000 (2)	0.006 (2)
C6	0.0314 (19)	0.035 (2)	0.030 (2)	0.0012 (16)	0.0070 (16)	0.0023 (18)

supplementary materials

C7	0.0201 (16)	0.044 (2)	0.035 (2)	-0.0050 (16)	-0.0009 (15)	-0.0045 (18)
C8	0.037 (2)	0.055 (3)	0.038 (2)	0.0061 (19)	0.0076 (18)	-0.005 (2)
C9	0.051 (2)	0.034 (2)	0.035 (2)	0.0071 (18)	0.0113 (19)	0.0010 (18)
C10	0.040 (2)	0.048 (3)	0.035 (2)	0.0138 (19)	0.0132 (19)	0.006 (2)
C12	0.0211 (17)	0.041 (2)	0.046 (2)	-0.0033 (15)	0.0070 (17)	-0.0012 (19)
C13	0.033 (2)	0.046 (3)	0.034 (2)	0.0039 (17)	0.0106 (17)	0.0013 (19)
C14	0.042 (2)	0.034 (2)	0.043 (2)	-0.0020 (18)	0.0059 (19)	0.003 (2)
C15	0.040 (2)	0.046 (3)	0.041 (3)	0.0009 (19)	0.0073 (19)	-0.011 (2)
C16	0.048 (3)	0.072 (3)	0.030 (2)	-0.009 (2)	0.007 (2)	-0.005 (2)
C17	0.046 (2)	0.054 (3)	0.046 (3)	0.010 (2)	0.003 (2)	0.003 (2)

Geometric parameters (Å, °)

Fe1—O1	1.845 (2)	C6—C13	1.419 (5)
Fe1—O1 ⁱ	1.845 (2)	C7—C8	1.387 (5)
Fe1—N1 ⁱ	1.945 (3)	C7—C15	1.388 (5)
Fe1—N1	1.945 (3)	C7—C12	1.516 (5)
Se1—C9	1.898 (4)	C8—C17	1.378 (6)
Se1—H1	1.191 (10)	C8—H8	0.9300
Se2—C13	1.896 (4)	C9—C14	1.345 (5)
Se2—H2	1.196 (10)	C9—C10	1.390 (6)
N1—C3	1.296 (5)	C10—C13	1.365 (6)
N1—C12	1.493 (4)	C10—H10	0.9300
O1—C6	1.300 (4)	C12—H12A	0.9700
C3—C4	1.429 (5)	C12—H12B	0.9700
C3—H3	0.9300	C14—H14	0.9300
C4—C14	1.391 (5)	C15—C16	1.387 (6)
C4—C6	1.414 (5)	C15—H15	0.9300
C5—C16	1.348 (6)	C16—H16	0.9300
C5—C17	1.366 (6)	C17—H17	0.9300
C5—H5	0.9300		
O1—Fe1—O1 ⁱ	180.0	C7—C8—H8	119.3
O1—Fe1—N1 ⁱ	88.15 (12)	C14—C9—C10	119.6 (4)
O1 ⁱ —Fe1—N1 ⁱ	91.85 (12)	C14—C9—Se1	120.5 (3)
O1—Fe1—N1	91.85 (12)	C10—C9—Se1	119.7 (3)
O1 ⁱ —Fe1—N1	88.15 (12)	C13—C10—C9	120.1 (4)
N1 ⁱ —Fe1—N1	180.0	C13—C10—H10	120.0
C9—Se1—H1	114 (2)	C9—C10—H10	120.0
C13—Se2—H2	105 (2)	N1—C12—C7	110.2 (3)
C3—N1—C12	113.9 (3)	N1—C12—H12A	109.6
C3—N1—Fe1	124.4 (3)	C7—C12—H12A	109.6
C12—N1—Fe1	121.7 (3)	N1—C12—H12B	109.6
C6—O1—Fe1	131.3 (2)	C7—C12—H12B	109.6
N1—C3—C4	127.2 (4)	H12A—C12—H12B	108.1
N1—C3—H3	116.4	C10—C13—C6	122.7 (4)
C4—C3—H3	116.4	C10—C13—Se2	118.3 (3)
C14—C4—C6	121.4 (3)	C6—C13—Se2	118.8 (3)

C14—C4—C3	117.7 (3)	C9—C14—C4	121.3 (4)
C6—C4—C3	120.4 (3)	C9—C14—H14	119.4
C16—C5—C17	119.4 (4)	C4—C14—H14	119.4
C16—C5—H5	120.3	C16—C15—C7	119.9 (4)
C17—C5—H5	120.3	C16—C15—H15	120.0
O1—C6—C4	123.4 (3)	C7—C15—H15	120.0
O1—C6—C13	121.7 (3)	C5—C16—C15	121.6 (4)
C4—C6—C13	114.9 (4)	C5—C16—H16	119.2
C8—C7—C15	117.5 (4)	C15—C16—H16	119.2
C8—C7—C12	120.2 (3)	C5—C17—C8	120.2 (4)
C15—C7—C12	122.2 (3)	C5—C17—H17	119.9
C17—C8—C7	121.3 (4)	C8—C17—H17	119.9
C17—C8—H8	119.3		

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

Fig. 1

