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1-(4-{[(*E*)-3-Ethoxy-2-hydroxybenzylidene]amino}phenyl)ethanone oxime

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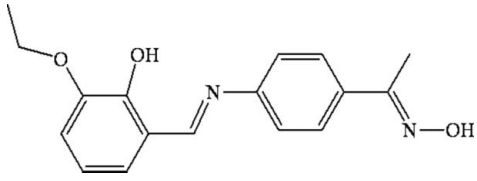
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.068; wR factor = 0.168; data-to-parameter ratio = 12.7.

In the title compound, $C_{17}H_{18}N_2O_3$, the benzene rings form a dihedral angle of 3.34 (2)°. There is a strong intramolecular O—H···N hydrogen bonds (which induces planarity of the structure). In the crystal, molecules are linked by pairs of O—H···N hydrogen bonds, forming inversion dimers.

Related literature

For background to oxime-type compounds, see: Dong *et al.*, (2009); Narasaka & Kitamura (2005). For their syntheses and structures, see: Dong *et al.* (2008); Akine *et al.* (2002); Wu *et al.* (2010).



Experimental

Crystal data

$C_{17}H_{18}N_2O_3$
M_r = 298.33
Triclinic, $P\overline{1}$
a = 7.0556 (7) Å
b = 7.4852 (9) Å
c = 14.7821 (16) Å
α = 96.890 (1)°
β = 98.762 (1)°
γ = 102.105 (2)°
V = 745.03 (14) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 K
0.32 × 0.21 × 0.13 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.971, T_{max} = 0.988
3664 measured reflections
2561 independent reflections
1376 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.168
S = 1.02
2561 reflections
201 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1^{i}	0.82	2.07	2.817 (4)	152
O2—H2···N2	0.82	1.84	2.567 (3)	147

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; 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: HG5155).

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supporting information

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1-(4-{[(*E*)-3-Ethoxy-2-hydroxybenzylidene]amino}phenyl)ethanone oxime

Li Zhao, Xu-Tao Dong, Si-Jia Xing, Qian Cheng and Ji-Xing Zhao

S1. Comment

Oxime-type compounds are a traditional class of chelating ligands widely used in coordination and analytical chemistry and extraction metallurgy (Dong *et al.*, 2009; Narasaka *et al.*, 2005). In the last few years, a large number of oxime-type compounds and their complexes have been reported (Dong *et al.*, 2008; Akine *et al.*, 2002). However, the oxime-type compounds derived the 4-aminophenylethanone have never been reported. In this paper, the crystal structure of new oxime-type compound, 1-(4-{[(*E*)-3-ethoxy-2-hydroxybenzylidene] amino}phenyl)ethanone oxime, derived from the reaction of 4-amino-phenylethanone oxime and 3-ethoxysalicylaldehyde (I), (Fig. 1) is reported.

The single-crystal structure of the title compound was determined by X-ray crystallography. The crystal structure of the title compound is only built up by the $C_{17}H_{18}N_2O_3$ molecules, in which all bond lengths are in normal ranges. The two benzene rings form a dihedral angle of 3.34 (2) °. There is a strong intramolecular O2–H2···N2 hydrogen bonds (which induces planarity on the structure). In the crystal structure, the molecules form dimers disposed about two pairs of intermolecular O—H..N hydrogen bonds. (Table 1)(Wu *et al.*, 2010).

S2. Experimental

To an ethanol solution (5 ml) of 3-ethoxysalicylaldehyde(166.2 mg, 1.00 mmol) was added an ethanol solution (5 ml) of 4-aminophenylethanone oxime (151.7 mg, 1.00 mmol). After the solution had been stirred at 328 K for 5 h, the mixture was filtered. The residue was washed successively with ethanol and n-hexane, respectively. The isolated compound was dried under reduced pressure to yield 281.1 mg of yellow solid (yield 80%, m.p. 436–437 K). Elemental analysis also supports composition of the title compound. Anal. calcd. for $C_{17}H_{18}N_2O_3$: C 68.44; H 6.08; N 9.39; Found: C, 68.30; H, 6.02; N, 9.52. The single crystals were obtained by slow evaporation from an acetonitrile solution at room temperature.

S3. Refinement

H atoms were treated as riding atoms with distances C—H = 0.96 (CH_3), C—H = 0.97 (CH_2), 0.93 Å (CH), 0.82 Å (OH), and the values of U_{iso}(H) for the thermal parameters for aromatic, methylene and hydroxy protons U_{iso}(H) = 1.2 U_{eq}(C) (aromatic), U_{iso}(H) = 1.5 U_{eq}(*C*)(methylene) and U_{iso}(H) = 1.5 U_{eq}(*C*)(hydroxy), respectively.

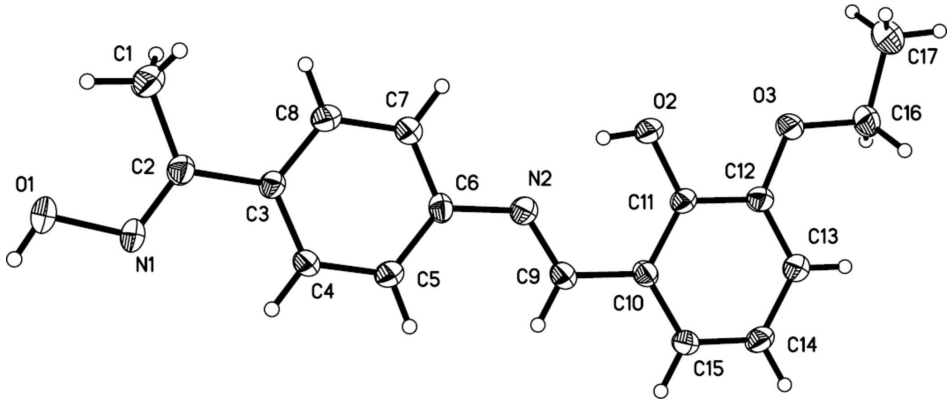

Figure 1

The molecule structure of the title compound with atom numbering scheme. Displacement ellipsoids for non-hydrogen atoms are drawn at the 30% probability level.

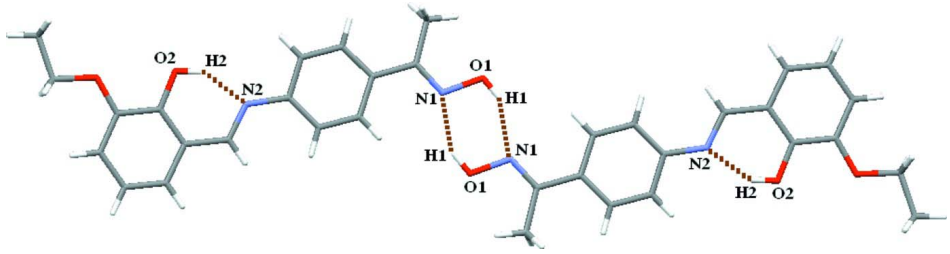

Figure 2

Digram showing the intramolecular O—H···N and intermolecular O—H···N hydrogen bonding interactions. Hydrogen atoms not involved have been deleted for clarity.

1-(4-{[(*E*)-3-Ethoxy-2-hydroxybenzylidene]amino}phenyl)ethanone oxime

Crystal data

$C_{17}H_{18}N_2O_3$
$M_r = 298.33$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.0556\ (7)$ Å
$b = 7.4852\ (9)$ Å
$c = 14.7821\ (16)$ Å
$\alpha = 96.890\ (1)°$
$\beta = 98.762\ (1)°$
$\gamma = 102.105\ (2)°$
$V = 745.03\ (14)$ Å^3
$Z = 2$
$F(000) = 316$
$D_x = 1.330$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 818 reflections
$\theta = 2.8–27.5°$
$\mu = 0.09$ mm^{-1}
$T = 298$ K
Prismatical, yellow
0.32 × 0.21 × 0.13 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.971$, $T_{max} = 0.988$
3664 measured reflections
2561 independent reflections
1376 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.8°$
$h = -8\rightarrow8$
$k = -8\rightarrow8$
$l = -17\rightarrow9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.068$
$wR(F^2) = 0.168$
$S = 1.02$
2561 reflections
201 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0613P)^2 + 0.2977P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.3517 (4)	0.5142 (4)	0.91196 (19)	0.0451 (8)
N2	0.4699 (4)	0.7402 (4)	0.51348 (18)	0.0399 (7)
O1	0.2676 (4)	0.4614 (4)	0.98854 (17)	0.0644 (8)
H1	0.3548	0.4525	1.0301	0.097*
O2	0.3342 (3)	0.8040 (3)	0.35234 (16)	0.0518 (7)
H2	0.3308	0.7783	0.4046	0.078*
O3	0.3898 (3)	0.8888 (4)	0.19161 (16)	0.0522 (7)
C1	0.0075 (5)	0.5044 (6)	0.8478 (3)	0.0667 (13)
H1A	−0.0132	0.4861	0.9090	0.100*
H1B	−0.0658	0.3980	0.8041	0.100*
H1C	−0.0362	0.6120	0.8325	0.100*
C2	0.2226 (5)	0.5310 (5)	0.8443 (2)	0.0396 (9)
C3	0.2949 (5)	0.5820 (4)	0.7593 (2)	0.0332 (8)
C4	0.4926 (5)	0.6169 (5)	0.7524 (2)	0.0443 (10)
H4	0.5844	0.6042	0.8020	0.053*
C5	0.5573 (5)	0.6699 (5)	0.6740 (2)	0.0465 (10)
H5	0.6913	0.6937	0.6720	0.056*
C6	0.4246 (5)	0.6879 (4)	0.5984 (2)	0.0351 (8)
C7	0.2268 (5)	0.6483 (5)	0.6030 (2)	0.0446 (10)
H7	0.1352	0.6561	0.5522	0.053*
C8	0.1624 (5)	0.5971 (5)	0.6820 (2)	0.0449 (10)
H8	0.0282	0.5724	0.6836	0.054*
C9	0.6452 (5)	0.7803 (4)	0.4955 (2)	0.0376 (9)
H9	0.7514	0.7766	0.5404	0.045*
C10	0.6814 (5)	0.8313 (4)	0.4067 (2)	0.0344 (8)

C11	0.5221 (5)	0.8398 (4)	0.3389 (2)	0.0355 (8)
C12	0.5558 (5)	0.8854 (5)	0.2518 (2)	0.0382 (9)
C13	0.7458 (5)	0.9199 (5)	0.2339 (2)	0.0412 (9)
H13	0.7682	0.9488	0.1764	0.049*
C14	0.9048 (5)	0.9119 (5)	0.3015 (2)	0.0427 (9)
H14	1.0321	0.9360	0.2890	0.051*
C15	0.8720 (5)	0.8682 (5)	0.3863 (2)	0.0384 (9)
H15	0.9781	0.8630	0.4309	0.046*
C16	0.4125 (5)	0.9423 (5)	0.1031 (2)	0.0506 (10)
H16A	0.4586	0.8501	0.0659	0.061*
H16B	0.5070	1.0601	0.1109	0.061*
C17	0.2127 (6)	0.9575 (7)	0.0572 (3)	0.0781 (15)
H17A	0.1228	0.8383	0.0466	0.117*
H17B	0.2220	1.0006	−0.0009	0.117*
H17C	0.1655	1.0433	0.0966	0.117*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0459 (19)	0.059 (2)	0.0336 (18)	0.0094 (15)	0.0162 (14)	0.0153 (14)
N2	0.0371 (18)	0.0485 (19)	0.0364 (18)	0.0112 (14)	0.0100 (13)	0.0084 (14)
O1	0.0549 (18)	0.103 (2)	0.0438 (17)	0.0163 (16)	0.0224 (13)	0.0324 (15)
O2	0.0305 (15)	0.085 (2)	0.0447 (16)	0.0123 (13)	0.0110 (11)	0.0243 (13)
O3	0.0358 (15)	0.085 (2)	0.0345 (15)	0.0073 (13)	0.0001 (11)	0.0229 (13)
C1	0.043 (3)	0.111 (4)	0.048 (3)	0.014 (2)	0.0157 (19)	0.018 (2)
C2	0.038 (2)	0.046 (2)	0.033 (2)	0.0060 (17)	0.0095 (16)	0.0061 (17)
C3	0.033 (2)	0.037 (2)	0.031 (2)	0.0085 (15)	0.0097 (14)	0.0051 (15)
C4	0.034 (2)	0.071 (3)	0.032 (2)	0.0155 (18)	0.0049 (15)	0.0166 (19)
C5	0.031 (2)	0.071 (3)	0.043 (2)	0.0136 (19)	0.0118 (17)	0.0162 (19)
C6	0.042 (2)	0.038 (2)	0.030 (2)	0.0128 (17)	0.0108 (15)	0.0097 (16)
C7	0.037 (2)	0.063 (3)	0.038 (2)	0.0144 (19)	0.0075 (16)	0.0171 (19)
C8	0.032 (2)	0.062 (3)	0.044 (2)	0.0126 (18)	0.0096 (16)	0.0113 (19)
C9	0.038 (2)	0.043 (2)	0.032 (2)	0.0111 (17)	0.0029 (15)	0.0089 (16)
C10	0.035 (2)	0.039 (2)	0.030 (2)	0.0110 (16)	0.0047 (14)	0.0077 (15)
C11	0.030 (2)	0.044 (2)	0.035 (2)	0.0091 (16)	0.0106 (15)	0.0081 (16)
C12	0.032 (2)	0.045 (2)	0.034 (2)	0.0044 (17)	0.0019 (15)	0.0063 (16)
C13	0.038 (2)	0.046 (2)	0.040 (2)	0.0087 (17)	0.0090 (16)	0.0100 (17)
C14	0.031 (2)	0.051 (2)	0.047 (2)	0.0067 (17)	0.0134 (16)	0.0093 (18)
C15	0.031 (2)	0.049 (2)	0.036 (2)	0.0109 (17)	0.0047 (15)	0.0102 (17)
C16	0.054 (3)	0.060 (3)	0.037 (2)	0.009 (2)	0.0047 (17)	0.0163 (19)
C17	0.064 (3)	0.110 (4)	0.059 (3)	0.013 (3)	−0.003 (2)	0.038 (3)

Geometric parameters (Å, º)

N1—C2	1.283 (4)	C7—C8	1.383 (5)
N1—O1	1.416 (3)	C7—H7	0.9300
N2—C9	1.286 (4)	C8—H8	0.9300
N2—C6	1.420 (4)	C9—C10	1.454 (4)

O1—H1	0.8200	C9—H9	0.9300
O2—C11	1.346 (4)	C10—C15	1.401 (4)
O2—H2	0.8200	C10—C11	1.406 (4)
O3—C12	1.366 (4)	C11—C12	1.411 (4)
O3—C16	1.435 (4)	C12—C13	1.384 (4)
C1—C2	1.498 (5)	C13—C14	1.400 (4)
C1—H1A	0.9600	C13—H13	0.9300
C1—H1B	0.9600	C14—C15	1.374 (4)
C1—H1C	0.9600	C14—H14	0.9300
C2—C3	1.488 (4)	C15—H15	0.9300
C3—C4	1.387 (4)	C16—C17	1.502 (5)
C3—C8	1.393 (4)	C16—H16A	0.9700
C4—C5	1.379 (5)	C16—H16B	0.9700
C4—H4	0.9300	C17—H17A	0.9600
C5—C6	1.384 (4)	C17—H17B	0.9600
C5—H5	0.9300	C17—H17C	0.9600
C6—C7	1.378 (5)		

C2—N1—O1	112.6 (3)	N2—C9—H9	119.2
C9—N2—C6	124.4 (3)	C10—C9—H9	119.2
N1—O1—H1	109.5	C15—C10—C11	119.0 (3)
C11—O2—H2	109.5	C15—C10—C9	121.4 (3)
C12—O3—C16	118.0 (3)	C11—C10—C9	119.6 (3)
C2—C1—H1A	109.5	O2—C11—C10	122.8 (3)
C2—C1—H1B	109.5	O2—C11—C12	117.3 (3)
H1A—C1—H1B	109.5	C10—C11—C12	119.9 (3)
C2—C1—H1C	109.5	O3—C12—C13	125.9 (3)
H1A—C1—H1C	109.5	O3—C12—C11	114.6 (3)
H1B—C1—H1C	109.5	C13—C12—C11	119.5 (3)
N1—C2—C3	117.0 (3)	C12—C13—C14	120.7 (3)
N1—C2—C1	123.4 (3)	C12—C13—H13	119.7
C3—C2—C1	119.5 (3)	C14—C13—H13	119.7
C4—C3—C8	116.9 (3)	C15—C14—C13	119.8 (3)
C4—C3—C2	122.9 (3)	C15—C14—H14	120.1
C8—C3—C2	120.2 (3)	C13—C14—H14	120.1
C5—C4—C3	122.0 (3)	C14—C15—C10	121.1 (3)
C5—C4—H4	119.0	C14—C15—H15	119.4
C3—C4—H4	119.0	C10—C15—H15	119.4
C4—C5—C6	120.6 (3)	O3—C16—C17	106.4 (3)
C4—C5—H5	119.7	O3—C16—H16A	110.5
C6—C5—H5	119.7	C17—C16—H16A	110.5
C7—C6—C5	118.2 (3)	O3—C16—H16B	110.5
C7—C6—N2	115.2 (3)	C17—C16—H16B	110.5
C5—C6—N2	126.6 (3)	H16A—C16—H16B	108.7
C6—C7—C8	121.1 (3)	C16—C17—H17A	109.5
C6—C7—H7	119.4	C16—C17—H17B	109.5
C8—C7—H7	119.4	H17A—C17—H17B	109.5
C7—C8—C3	121.2 (3)	C16—C17—H17C	109.5

C7—C8—H8	119.4	H17A—C17—H17C	109.5
C3—C8—H8	119.4	H17B—C17—H17C	109.5
N2—C9—C10	121.7 (3)		

O1—N1—C2—C3	−178.6 (3)	N2—C9—C10—C15	−177.6 (3)
O1—N1—C2—C1	2.1 (5)	N2—C9—C10—C11	0.9 (5)
N1—C2—C3—C4	−2.2 (5)	C15—C10—C11—O2	179.1 (3)
C1—C2—C3—C4	177.1 (3)	C9—C10—C11—O2	0.6 (5)
N1—C2—C3—C8	178.0 (3)	C15—C10—C11—C12	−0.1 (5)
C1—C2—C3—C8	−2.7 (5)	C9—C10—C11—C12	−178.6 (3)
C8—C3—C4—C5	2.0 (5)	C16—O3—C12—C13	−3.5 (5)
C2—C3—C4—C5	−177.8 (3)	C16—O3—C12—C11	177.2 (3)
C3—C4—C5—C6	−0.8 (6)	O2—C11—C12—O3	0.6 (4)
C4—C5—C6—C7	−1.2 (5)	C10—C11—C12—O3	179.8 (3)
C4—C5—C6—N2	−179.7 (3)	O2—C11—C12—C13	−178.8 (3)
C9—N2—C6—C7	−179.2 (3)	C10—C11—C12—C13	0.5 (5)
C9—N2—C6—C5	−0.6 (5)	O3—C12—C13—C14	−179.9 (3)
C5—C6—C7—C8	1.9 (5)	C11—C12—C13—C14	−0.6 (5)
N2—C6—C7—C8	−179.4 (3)	C12—C13—C14—C15	0.4 (5)
C6—C7—C8—C3	−0.7 (5)	C13—C14—C15—C10	0.0 (5)
C4—C3—C8—C7	−1.3 (5)	C11—C10—C15—C14	−0.1 (5)
C2—C3—C8—C7	178.6 (3)	C9—C10—C15—C14	178.4 (3)
C6—N2—C9—C10	179.5 (3)	C12—O3—C16—C17	−172.9 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1^{i}	0.82	2.07	2.817 (4)	152
O2—H2···N2	0.82	1.84	2.567 (3)	147

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+2.