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1-(4-{[(*E*)-4-Methylbenzylidene]amino}-phenyl)ethanone oxime

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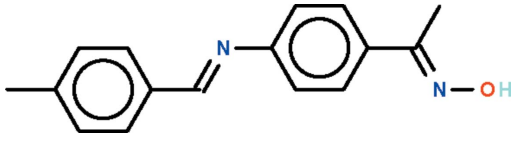
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.047; wR factor = 0.136; data-to-parameter ratio = 13.5.

In the title compound, $C_{16}H_{16}N_2O$, the dihedral angle formed by the two benzene rings is 50.3 (1)°. In the crystal structure, molecules are linked into an infinite one-dimensional supramolecular structure by intermolecular O—H···N hydrogen-bond interactions.

Related literature

For background to oxime-type compounds, see: Dong *et al.* (2009*a*,*b*). For the synthesis, see: Rafiq *et al.* (2008); Dong *et al.* (2009*c*).



Experimental

Crystal data

$C_{16}H_{16}N_2O$
M_r = 252.31
Monoclinic, $P2_1/n$
a = 5.7785 (6) Å
b = 14.581 (2) Å
c = 16.226 (2) Å
β = 94.285 (1)°
V = 1363.4 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 K
0.45 × 0.15 × 0.10 mm

Data collection

Bruker SMART diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.966, T_{max} = 0.992
6860 measured reflections
2396 independent reflections
1480 reflections with $I > 2\sigma(I)$
R_{int} = 0.054

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.136
S = 0.95
2396 reflections
178 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N2^{i}	0.86 (1)	2.06 (1)	2.919 (2)	175 (3)

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

Data collection: *SMART* (Bruker, 1996); cell refinement: *SAINT* (Bruker, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2705).

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supplementary materials

Acta Cryst. (2010). E**66**, o2473 [**doi:10.1107/S1600536810034598**]

1-(4-{[(*E*)-4-Methylbenzylidene]amino}phenyl)ethanone oxime

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Comment

Oxime-type compounds are a great important ligands in modern coordination chemistry (Dong *et al.*, 2009*a*; Dong *et al.*, 2009*b*). Structures of oxime-type compounds derived from substituted benzaldehydes and 1-(4-aminophenyl)ethanone haven't been reported so far (Rafiq *et al.*, 2008). Here we report the synthesis and crystal structure of (*E*)-4-[1-(Hydroxyimino)ethyl]-*N*-(4-methylbenzylidene)aniline (I), (Fig. 1).

The single-crystal structure of the title compound is built up by discrete $C_{16}H_{16}N_2O$ molecules, in which all bond lengths are in normal ranges. Within the molecule, the dihedral angle formed by the two benzene rings is 50.3 (1)°. In the crystal structure, the molecules are linked into infinite one-dimensional supramolecular structure by intermolecular O—H···N hydrogen bond interaction (Table 1 and Fig. 2).

Experimental

4-Aminophenylethanone oxime was prepared by 1-(4-aminophenyl)ethanone, hydroxylamine sulfate and sodium acetate (Rafiq *et al.*, 2008; Dong *et al.*, 2009*c*). To an ethanol solution (7 ml) of 4-aminophenylethanone oxime (151.0 mg, 1.00 mmol) was added dropwise an ethanol solution (8 ml) of 4-methylbenzaldehyde (121.6 mg, 1.00 mmol). The mixture solution was stirred at 330 K for 4 h. After cooling to room temperature, the precipitate was filtered off, and washed successively three times with ethanol. The product was dried *in vacuo* and purified by recrystallization from ethanol to yield 220.3 mg (Yield, 80.8%) of solid; m.p. 471–472 K. Pale-yellow block-like single crystals suitable for X-ray diffraction studies were obtained by slow evaporation from a solution of acetone of (I) at room temperature for about two weeks. Anal. Calcd. for $C_{16}H_{16}N_2O$: C, 76.16; H, 6.39; N, 11.10; Found: C, 76.08; H, 6.45; N, 11.02.

Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.93 to 0.96 Å) and were included in the refinement in the riding model approximation, with U(H) set to 1.2 to 1.5U(C).

The hydroxy H-atom was located in a difference Fourier map, and was refined with a distance restraint of O–H of 0.85±0.01 Å; its temperature factor was freely refined.

Figures

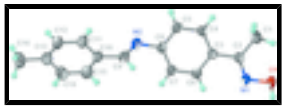

Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $C_{16}H_{16}N_2O$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

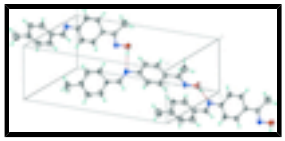

Fig. 2. Part of one-dimensional supramolecular structure is formed by O—H···N intermolecular interaction with H bonds drawn as dotted lines.

1-(4-{[(*E*)-4-Methylbenzylidene]amino}phenyl)ethanone oxime

Crystal data

$C_{16}H_{16}N_2O$	$F(000) = 536$
$M_r = 252.31$	$D_x = 1.229$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 1735 reflections
$a = 5.7785$ (6) Å	$\theta = 2.5$–$25.3°$
$b = 14.581$ (2) Å	$\mu = 0.08$ mm^{-1}
$c = 16.226$ (2) Å	$T = 293$ K
$\beta = 94.285$ (1)°	Block, yellow
$V = 1363.4$ (2) Å^3	0.45 × 0.15 × 0.10 mm
$Z = 4$	

Data collection

Bruker SMART diffractometer	2396 independent reflections
Radiation source: fine-focus sealed tube	1480 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.054$
φ and ω scans	$\theta_{max} = 25.0°$, $\theta_{min} = 1.9°$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$h = -6 \rightarrow 6$
$T_{min} = 0.966$, $T_{max} = 0.992$	$k = -17 \rightarrow 14$
6860 measured reflections	$l = -18 \rightarrow 19$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.047$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.136$	H atoms treated by a mixture of independent and constrained refinement
$S = 0.95$	$w = 1/[\sigma^2(F_o^2) + (0.0748P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
2396 reflections	$(\Delta/\sigma)_{max} = 0.001$
178 parameters	$\Delta\rho_{max} = 0.15$ e Å^{-3}
1 restraint	$\Delta\rho_{min} = -0.17$ 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.7517 (3)	0.26556 (12)	0.05236 (8)	0.0674 (5)
H1	0.861 (4)	0.2274 (16)	0.0445 (16)	0.107 (11)*
N1	0.7670 (3)	0.27459 (12)	0.13916 (9)	0.0529 (5)
N2	0.6350 (3)	0.35564 (11)	0.51824 (10)	0.0512 (5)
C1	0.4032 (4)	0.36066 (17)	0.11219 (13)	0.0710 (7)
H1A	0.4313	0.3513	0.0552	0.106*
H1B	0.3934	0.4252	0.1231	0.106*
H1C	0.2599	0.3316	0.1236	0.106*
C2	0.5974 (4)	0.32006 (13)	0.16606 (11)	0.0457 (5)
C3	0.6050 (3)	0.32942 (12)	0.25745 (11)	0.0419 (5)
C4	0.4248 (4)	0.36780 (14)	0.29717 (12)	0.0515 (5)
H4	0.2943	0.3890	0.2659	0.062*
C5	0.4343 (4)	0.37537 (14)	0.38259 (12)	0.0531 (6)
H5	0.3091	0.4001	0.4078	0.064*
C6	0.6290 (4)	0.34636 (13)	0.43064 (11)	0.0451 (5)
C7	0.8106 (4)	0.30705 (14)	0.39156 (11)	0.0508 (5)
H7	0.9415	0.2861	0.4228	0.061*
C8	0.7974 (4)	0.29896 (13)	0.30692 (12)	0.0506 (5)
H8	0.9206	0.2724	0.2819	0.061*
C9	0.8175 (4)	0.39055 (13)	0.55448 (12)	0.0502 (5)
H9	0.9316	0.4104	0.5211	0.060*
C10	0.8639 (4)	0.40224 (12)	0.64333 (12)	0.0470 (5)
C11	0.7108 (4)	0.37421 (14)	0.70052 (12)	0.0554 (6)
H11	0.5694	0.3481	0.6823	0.066*
C12	0.7675 (4)	0.38494 (14)	0.78433 (12)	0.0605 (6)
H12	0.6630	0.3658	0.8217	0.073*
C13	0.9766 (4)	0.42353 (14)	0.81375 (13)	0.0555 (6)
C14	1.1268 (4)	0.45209 (14)	0.75684 (13)	0.0624 (6)
H14	1.2677	0.4786	0.7752	0.075*
C15	1.0720 (4)	0.44209 (14)	0.67304 (13)	0.0593 (6)
H15	1.1759	0.4623	0.6359	0.071*
C16	1.0399 (5)	0.43398 (18)	0.90515 (13)	0.0821 (8)
H16A	1.1710	0.3958	0.9210	0.123*
H16B	0.9106	0.4160	0.9354	0.123*
H16C	1.0783	0.4968	0.9173	0.123*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0689 (12)	0.0968 (13)	0.0364 (9)	0.0112 (10)	0.0044 (7)	−0.0072 (8)
N1	0.0546 (12)	0.0723 (12)	0.0319 (9)	0.0032 (9)	0.0043 (8)	−0.0032 (8)
N2	0.0532 (11)	0.0621 (11)	0.0388 (10)	−0.0012 (9)	0.0078 (8)	−0.0002 (8)
C1	0.0772 (18)	0.0874 (17)	0.0466 (13)	0.0216 (14)	−0.0075 (12)	−0.0056 (11)
C2	0.0468 (13)	0.0492 (12)	0.0411 (11)	−0.0013 (10)	0.0027 (9)	0.0008 (9)
C3	0.0436 (12)	0.0441 (11)	0.0383 (10)	−0.0009 (9)	0.0034 (9)	0.0033 (8)
C4	0.0461 (13)	0.0631 (13)	0.0449 (12)	0.0082 (10)	0.0015 (10)	0.0029 (9)
C5	0.0472 (13)	0.0670 (14)	0.0462 (12)	0.0069 (11)	0.0110 (10)	−0.0012 (9)
C6	0.0503 (13)	0.0503 (11)	0.0356 (11)	−0.0028 (9)	0.0078 (9)	0.0025 (8)
C7	0.0469 (13)	0.0632 (13)	0.0422 (12)	0.0074 (10)	0.0016 (10)	0.0018 (9)
C8	0.0481 (13)	0.0610 (13)	0.0430 (12)	0.0088 (10)	0.0065 (10)	−0.0019 (9)
C9	0.0543 (14)	0.0529 (12)	0.0447 (12)	−0.0008 (10)	0.0122 (10)	0.0012 (9)
C10	0.0556 (14)	0.0451 (11)	0.0406 (11)	0.0013 (10)	0.0050 (10)	−0.0027 (8)
C11	0.0566 (14)	0.0648 (13)	0.0448 (12)	−0.0067 (11)	0.0048 (10)	−0.0059 (10)
C12	0.0717 (16)	0.0685 (15)	0.0419 (12)	−0.0052 (12)	0.0078 (11)	−0.0055 (10)
C13	0.0699 (16)	0.0499 (12)	0.0459 (12)	0.0042 (11)	−0.0017 (11)	−0.0061 (9)
C14	0.0628 (16)	0.0594 (13)	0.0629 (15)	−0.0095 (11)	−0.0096 (12)	−0.0083 (11)
C15	0.0609 (15)	0.0594 (14)	0.0582 (14)	−0.0098 (11)	0.0084 (12)	−0.0013 (10)
C16	0.101 (2)	0.0889 (18)	0.0538 (15)	0.0072 (15)	−0.0125 (14)	−0.0117 (12)

Geometric parameters (Å, °)

O1—N1	1.4107 (19)	C7—H7	0.9300
O1—H1	0.860 (10)	C8—H8	0.9300
N1—C2	1.286 (2)	C9—C10	1.457 (3)
N2—C9	1.275 (2)	C9—H9	0.9300
N2—C6	1.426 (2)	C10—C15	1.389 (3)
C1—C2	1.492 (3)	C10—C11	1.390 (3)
C1—H1A	0.9600	C11—C12	1.384 (3)
C1—H1B	0.9600	C11—H11	0.9300
C1—H1C	0.9600	C12—C13	1.385 (3)
C2—C3	1.487 (2)	C12—H12	0.9300
C3—C4	1.383 (3)	C13—C14	1.378 (3)
C3—C8	1.394 (3)	C13—C16	1.509 (3)
C4—C5	1.387 (3)	C14—C15	1.381 (3)
C4—H4	0.9300	C14—H14	0.9300
C5—C6	1.386 (3)	C15—H15	0.9300
C5—H5	0.9300	C16—H16A	0.9600
C6—C7	1.389 (3)	C16—H16B	0.9600
C7—C8	1.375 (3)	C16—H16C	0.9600
N1—O1—H1	102.5 (18)	C3—C8—H8	119.0
C2—N1—O1	113.22 (16)	N2—C9—C10	126.0 (2)
C9—N2—C6	117.10 (18)	N2—C9—H9	117.0
C2—C1—H1A	109.5	C10—C9—H9	117.0

C2—C1—H1B	109.5	C15—C10—C11	117.95 (19)
H1A—C1—H1B	109.5	C15—C10—C9	118.88 (19)
C2—C1—H1C	109.5	C11—C10—C9	123.16 (19)
H1A—C1—H1C	109.5	C12—C11—C10	120.5 (2)
H1B—C1—H1C	109.5	C12—C11—H11	119.8
N1—C2—C3	114.78 (17)	C10—C11—H11	119.8
N1—C2—C1	124.35 (18)	C11—C12—C13	121.4 (2)
C3—C2—C1	120.87 (19)	C11—C12—H12	119.3
C4—C3—C8	117.15 (17)	C13—C12—H12	119.3
C4—C3—C2	122.31 (17)	C14—C13—C12	118.0 (2)
C8—C3—C2	120.54 (18)	C14—C13—C16	120.6 (2)
C3—C4—C5	121.51 (18)	C12—C13—C16	121.4 (2)
C3—C4—H4	119.2	C13—C14—C15	121.2 (2)
C5—C4—H4	119.2	C13—C14—H14	119.4
C6—C5—C4	120.5 (2)	C15—C14—H14	119.4
C6—C5—H5	119.8	C14—C15—C10	121.0 (2)
C4—C5—H5	119.8	C14—C15—H15	119.5
C5—C6—C7	118.56 (18)	C10—C15—H15	119.5
C5—C6—N2	119.34 (18)	C13—C16—H16A	109.5
C7—C6—N2	122.08 (18)	C13—C16—H16B	109.5
C8—C7—C6	120.26 (19)	H16A—C16—H16B	109.5
C8—C7—H7	119.9	C13—C16—H16C	109.5
C6—C7—H7	119.9	H16A—C16—H16C	109.5
C7—C8—C3	122.00 (19)	H16B—C16—H16C	109.5
C7—C8—H8	119.0		
O1—N1—C2—C3	178.84 (15)	C4—C3—C8—C7	−0.6 (3)
O1—N1—C2—C1	−0.6 (3)	C2—C3—C8—C7	179.64 (18)
N1—C2—C3—C4	−173.15 (18)	C6—N2—C9—C10	−176.97 (17)
C1—C2—C3—C4	6.3 (3)	N2—C9—C10—C15	−179.7 (2)
N1—C2—C3—C8	6.6 (3)	N2—C9—C10—C11	1.2 (3)
C1—C2—C3—C8	−173.93 (19)	C15—C10—C11—C12	−0.9 (3)
C8—C3—C4—C5	−0.3 (3)	C9—C10—C11—C12	178.23 (18)
C2—C3—C4—C5	179.52 (18)	C10—C11—C12—C13	0.0 (3)
C3—C4—C5—C6	1.6 (3)	C11—C12—C13—C14	0.7 (3)
C4—C5—C6—C7	−2.0 (3)	C11—C12—C13—C16	−179.1 (2)
C4—C5—C6—N2	179.47 (18)	C12—C13—C14—C15	−0.4 (3)
C9—N2—C6—C5	−132.4 (2)	C16—C13—C14—C15	179.4 (2)
C9—N2—C6—C7	49.1 (3)	C13—C14—C15—C10	−0.5 (3)
C5—C6—C7—C8	1.2 (3)	C11—C10—C15—C14	1.1 (3)
N2—C6—C7—C8	179.67 (18)	C9—C10—C15—C14	−178.03 (18)
C6—C7—C8—C3	0.1 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N2^{i}	0.86 (1)	2.06 (1)	2.919 (2)	175 (3)

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

Fig. 1

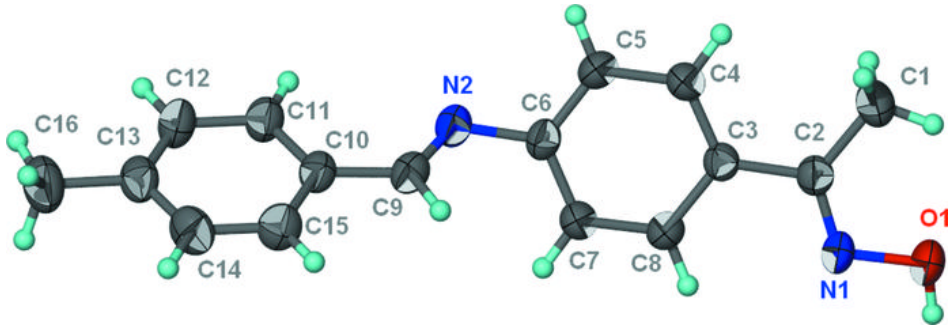

Fig. 2