Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

(*E*)-1-(4-Aminophenyl)ethanone oxime

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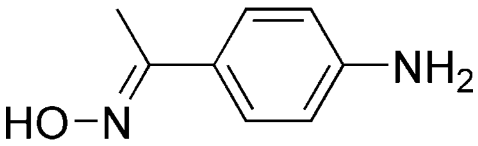
Received 13 October 2008; accepted 18 October 2008

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.040; wR factor = 0.108; data-to-parameter ratio = 15.6.

In the molecule of the title compound, $C_8H_{10}N_2O$, the oxime group is oriented at a dihedral angle of 5.58 (3)° with respect to the benzene ring. In the crystal structure, intermolecular O—H···N and N—H···O hydrogen bonds link the molecules, forming a three-dimensional network.

Related literature

For general background, see: Bertolasi *et al.* (1982); Degorre *et al.* (1998). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_8H_{10}N_2O$
M_r = 150.18
Monoclinic, $P2_1/n$
a = 4.8641 (2) Å
b = 9.2016 (3) Å
c = 17.1447 (7) Å
β = 95.535 (2)°
V = 763.78 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100 (2) K
0.34 × 0.28 × 0.26 mm

Data collection

Enraf–Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*DENZO*; Otwinowski & Minor, 1997)
T_{min} = 0.972, T_{max} = 0.979
6132 measured reflections
1761 independent reflections
1483 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.107
S = 1.04
1761 reflections
113 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1O···N2^{i}	0.92 (2)	1.88 (2)	2.7919 (14)	169.8 (18)
N2—H2N···O1^{ii}	0.916 (18)	2.165 (18)	3.0790 (13)	175.7 (15)
N2—H2M···N1^{iii}	0.929 (19)	2.525 (19)	3.3000 (14)	141.0 (14)

Symmetry codes: (i) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (ii) $x-\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (iii) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2007) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

The authors gratefully acknowledge funds from the Higher Education Commission, Islamabad, Pakistan.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2552).

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supplementary materials

Acta Cryst. (2008). E**64**, o2173 [**doi:10.1107/S1600536808034120**]

(*E*)-1-(4-Aminophenyl)ethanone oxime

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Comment

One of the richest sources of diversity for the medicinal chemist is small heterocyclic rings, which in addition to often exhibiting biological activity, may serve as rigid scaffolds for a further display of functionalities. Oximes are among those, that have been reported to posses a wide range of biological activities including anti-oxidants, anti-inflammatory and as reactivators of organophosphate inhibited acetylcholine esterases (Degorre *et al.*, 1998). The oxime moiety can both donate and accept hydrogen bonds, which makes it a very interesting building block in supramolecular chemistry (Bertolasi *et al.*, 1982). It is also a key intermediate, which undergoes the 1,3-dipolar cycloaddition reaction with mono substituted alkenes to form isoxazolines.Due to importance of these compounds, we decided to synthesize the title compound and report herein its crystal structure.

In the title compound (Fig. 1), the bond lengths (Allen *et al.*, 1987) and angles are within normal ranges . The phenyl ring A (C1-C6) is oriented with respect to the planar (O1/N1/C1/C7/C8) moiety at a dihedral angle of 5.46 (3)°. N2 atom is -0.014 (3) Å away from the phenyl plane.

In the crystal structure, intermolecular O-H···N and N-H···O hydrogen bonds (Table 1) link the molecules to form a supramolecular structure (Fig. 2), in which they may be effective in the stabilization of the structure.

Experimental

For the preparation of the title compound, a solution of 1-(4-aminophenyl)- ethanone (1.35 g, 10 mmol) in methanol (15 ml) was added to a mixture of hydroxylamine sulfate (1.31 g, 10 mmol) and sodium acetate (2.0 g, 25 mmol). The reaction mass was refluxed for 4-5 h, until the reaction completed. The solvent was evaporated under vacuo and demineralized water (40 ml) was added, cooled to 268-265 K and filtered to obtain crystalline solid (yield; 1.11 g, 75%; m.p. 401-402 K).

Refinement

H atoms (for OH and NH_2) were located in difference syntheses and refined isotropically [O-H = 0.92 (2) Å; U_{iso}(H) = 0.049 (5) Å^2 and N-H = 0.916 (18) and 0.929 (19) Å; U_{iso}(H) = 0.035 (4) and 0.039 (4) Å^2]. The remaining H atoms were positioned geometrically, with C-H = 0.95 and 0.98 Å for aromatic and methyl H, respectively, and constrained to ride on their parent atoms with U_{iso}(H) = xU_{eq}(C), where x = 1.5 for methyl H and x = 1.2 for aromatic H atoms.

Figures

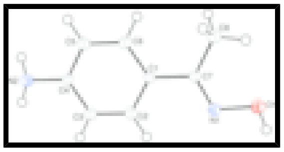

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

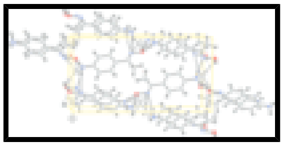

Fig. 2. A partial packing diagram. Hydrogen bonds are shown as dashed lines.

(*E*)-1-(4-Aminophenyl)ethanone oxime

Crystal data

$C_8H_{10}N_2O$

$M_r = 150.18$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 4.8641$ (2) Å

$b = 9.2016$ (3) Å

$c = 17.1447$ (7) Å

$\beta = 95.535$ (2)°

$V = 763.78$ (5) Å^3

$Z = 4$

$F_{000} = 320$

$D_x = 1.306$ Mg m^{-3}

Melting point: 401(1) K

Mo *K*α radiation
λ = 0.71073 Å

Cell parameters from 3781 reflections

θ = 1.0–30.0°

μ = 0.09 mm^{-1}

$T = 100$ (2) K

Block, pale yellow

0.34 × 0.28 × 0.26 mm

Data collection

Enraf–Nonius KappaCCD diffractometer

Radiation source: fine-focus sealed tube

Monochromator: horizontally mounted graphite crystal

Detector resolution: 9 pixels mm^{-1}

$T = 100(2)$ K

φ and ω scans

Absorption correction: multi-scan
(DENZO; Otwinowski & Minor, 1997)

$T_{min} = 0.972$, $T_{max} = 0.979$

6132 measured reflections

1761 independent reflections

1483 reflections with $I > 2\sigma(I)$

$R_{int} = 0.026$

$\theta_{max} = 27.5$°

$\theta_{min} = 4.2$°

$h = -6 \rightarrow 6$

$k = -11 \rightarrow 11$

$l = -22 \rightarrow 22$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.040$

$wR(F^2) = 0.108$

$S = 1.04$

1761 reflections

113 parameters

Secondary atom site location: difference Fourier map

Hydrogen site location: mixed

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0554P)^2 + 0.2855P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.24$ e Å^{-3}

$\Delta\rho_{min} = -0.28$ e Å^{-3}

Primary atom site location: structure-invariant direct methods

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 (Å^2)

	x	y	z	$U_{\rm iso}$*/$U_{\rm eq}$
O1	0.42570 (18)	0.21270 (10)	0.47528 (5)	0.0203 (2)
H1O	0.273 (4)	0.158 (2)	0.4589 (11)	0.049 (5)*
N1	0.38949 (19)	0.23108 (10)	0.55574 (5)	0.0168 (2)
N2	0.4407 (2)	0.42572 (11)	0.91465 (6)	0.0186 (2)
H2N	0.288 (4)	0.3807 (18)	0.9308 (10)	0.035 (4)*
H2M	0.440 (4)	0.525 (2)	0.9257 (10)	0.039 (4)*
C1	0.5281 (2)	0.34967 (12)	0.67458 (6)	0.0147 (2)
C2	0.3462 (2)	0.26638 (12)	0.71490 (7)	0.0179 (3)
H2	0.2421	0.1914	0.6878	0.021*
C3	0.3148 (2)	0.29074 (13)	0.79324 (7)	0.0177 (3)
H3	0.1903	0.2327	0.8192	0.021*
C4	0.4655 (2)	0.40050 (12)	0.83408 (6)	0.0156 (2)
C5	0.6512 (2)	0.48187 (13)	0.79535 (7)	0.0187 (3)
H5	0.7588	0.5550	0.8230	0.022*
C6	0.6810 (2)	0.45726 (13)	0.71660 (7)	0.0178 (3)
H6	0.8075	0.5146	0.6910	0.021*
C7	0.5571 (2)	0.32441 (12)	0.59009 (6)	0.0149 (2)
C8	0.7713 (2)	0.40782 (13)	0.55104 (7)	0.0195 (3)
H8A	0.7606	0.3815	0.4954	0.029*
H8B	0.9553	0.3841	0.5762	0.029*
H8C	0.7377	0.5123	0.5560	0.029*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0222 (5)	0.0272 (5)	0.0121 (4)	−0.0020 (4)	0.0043 (3)	−0.0033 (3)
N1	0.0190 (5)	0.0200 (5)	0.0118 (5)	0.0020 (4)	0.0038 (4)	−0.0010 (4)
N2	0.0230 (5)	0.0190 (5)	0.0141 (5)	0.0005 (4)	0.0032 (4)	−0.0012 (4)
C1	0.0144 (5)	0.0144 (5)	0.0156 (5)	0.0029 (4)	0.0024 (4)	0.0005 (4)
C2	0.0191 (6)	0.0168 (5)	0.0178 (5)	−0.0026 (4)	0.0018 (4)	−0.0015 (4)
C3	0.0172 (5)	0.0182 (6)	0.0181 (6)	−0.0017 (4)	0.0042 (4)	0.0018 (4)

C4	0.0168 (5)	0.0160 (5)	0.0138 (5)	0.0042 (4)	0.0012 (4)	0.0003 (4)
C5	0.0200 (6)	0.0173 (6)	0.0187 (6)	−0.0025 (4)	0.0017 (4)	−0.0036 (4)
C6	0.0179 (5)	0.0176 (5)	0.0185 (6)	−0.0017 (4)	0.0041 (4)	0.0006 (4)
C7	0.0139 (5)	0.0158 (5)	0.0153 (5)	0.0039 (4)	0.0027 (4)	0.0019 (4)
C8	0.0177 (5)	0.0231 (6)	0.0182 (5)	−0.0019 (4)	0.0045 (4)	0.0010 (4)

Geometric parameters (Å, °)

O1—N1	1.4175 (11)	C3—C4	1.3961 (16)
O1—H1O	0.92 (2)	C3—H3	0.9500
N1—C7	1.2869 (15)	C4—C5	1.3905 (16)
N2—C4	1.4173 (14)	C5—C6	1.3903 (15)
N2—H2N	0.916 (18)	C5—H5	0.9500
N2—H2M	0.929 (19)	C6—H6	0.9500
C1—C6	1.3961 (16)	C7—C8	1.5026 (15)
C1—C2	1.4020 (16)	C8—H8A	0.9800
C1—C7	1.4872 (14)	C8—H8B	0.9800
C2—C3	1.3846 (15)	C8—H8C	0.9800
C2—H2	0.9500		
N1—O1—H1O	100.9 (11)	C3—C4—N2	121.15 (10)
C7—N1—O1	113.10 (9)	C6—C5—C4	120.63 (10)
C4—N2—H2N	111.6 (10)	C6—C5—H5	119.7
C4—N2—H2M	111.1 (11)	C4—C5—H5	119.7
H2N—N2—H2M	111.2 (15)	C5—C6—C1	121.09 (10)
C6—C1—C2	117.60 (10)	C5—C6—H6	119.5
C6—C1—C7	121.17 (10)	C1—C6—H6	119.5
C2—C1—C7	121.23 (10)	N1—C7—C1	115.76 (9)
C3—C2—C1	121.59 (11)	N1—C7—C8	124.95 (10)
C3—C2—H2	119.2	C1—C7—C8	119.29 (10)
C1—C2—H2	119.2	C7—C8—H8A	109.5
C2—C3—C4	120.12 (10)	C7—C8—H8B	109.5
C2—C3—H3	119.9	H8A—C8—H8B	109.5
C4—C3—H3	119.9	C7—C8—H8C	109.5
C5—C4—C3	118.94 (10)	H8A—C8—H8C	109.5
C5—C4—N2	119.85 (10)	H8B—C8—H8C	109.5

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1O···N2^{i}	0.92 (2)	1.88 (2)	2.7919 (14)	169.8 (18)
N2—H2N···O1^{ii}	0.916 (18)	2.165 (18)	3.0790 (13)	175.7 (15)
N2—H2M···N1^{iii}	0.929 (19)	2.525 (19)	3.3000 (14)	141.0 (14)

Symmetry codes: (i) $x-1/2, -y+1/2, z-1/2$; (ii) $x-1/2, -y+1/2, z+1/2$; (iii) $-x+1/2, y+1/2, -z+3/2$.

Fig. 1

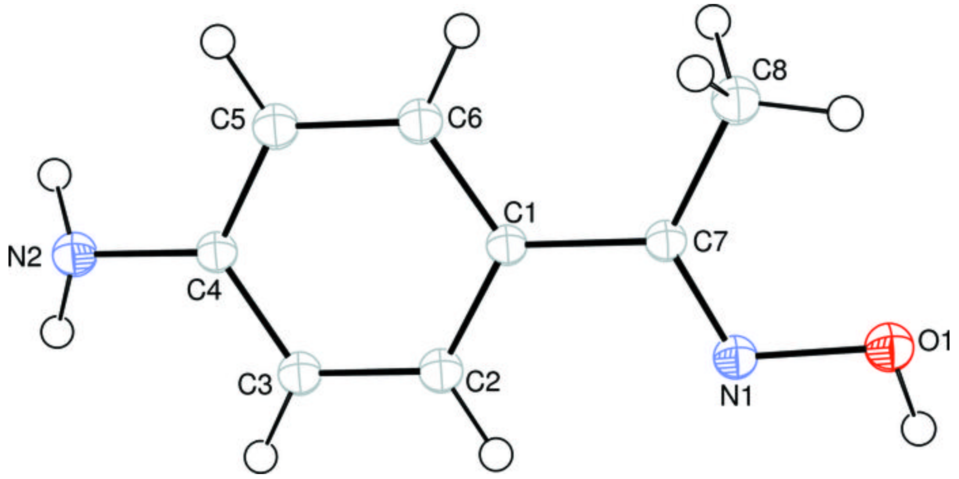

Fig. 2