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1-(3-Methoxyphenyl)-2-phenylethanone oxime

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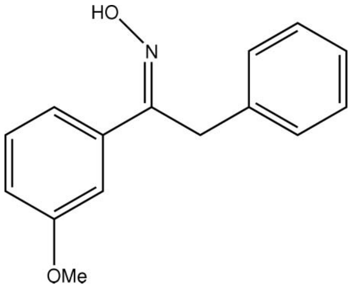
Key indicators: single-crystal X-ray study; *T* = 295 K; mean σ(C–C) = 0.003 Å; *R* factor = 0.052; *wR* factor = 0.118; data-to-parameter ratio = 15.1.

In the structure of the title compound, $C_{15}H_{15}NO_2$, the dihedral angle between the two benzene rings is 86.8 (1)°. An intramolecular methylene–oxime C—H⋯O hydrogen bond stabilizes the molecular structure. Intermolecular O—H⋯N hydrogen bonds between oxime subunits cluster the molecules into $R_2^2(6)$ dimers. Aromatic–aromatic stacking interactions are also observed in the packing [interplanar distance 3.344 Å, slippage 4.107 Å, centroid-to-centroid distance 5.297 (2) Å] and these, combined with the O—H⋯N hydrogen bonds, form a one-dimensional array of molecules along the *b* axis.

Related literature

For related background, see: Pati, Das, Ramirez-Erosa *et al.*, (2007); Pati, Das, Sharma *et al.*, (2007).



Experimental

Crystal data

$C_{15}H_{15}NO_2$
M_r = 241.28
Orthorhombic, *Pbca*
a = 9.7198 (9) Å
b = 12.139 (1) Å
c = 21.499 (2) Å
V = 2536.8 (4) Å^3
Z = 8
Mo *K*α radiation
μ = 0.08 mm^{-1}
T = 295 (2) K
0.22 × 0.16 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.901, T_{max} = 0.982
18438 measured reflections
2489 independent reflections
1358 reflections with $I > 2\sigma(I)$
R_{int} = 0.081

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.118
S = 1.01
2489 reflections
165 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.11 e Å^{-3}

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

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
C9—H9*B*⋯O1	0.97	2.27	2.676 (3)	104
O1—H1⋯N1^{i}	0.82	2.03	2.754 (3)	147

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

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT-Plus* (Bruker, 2003); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PLATON*.

RSR thanks the Science and Engineering Research Council (DST), Government of India, for a Fast-Track Scientist award, and the Bioinformatics Centre, School of Biotechnology, D. A. University, Indore, India, for the use of computational facilities.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2102).

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supplementary materials

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1-(3-Methoxyphenyl)-2-phenylethanone oxime

H. N. Pati, **B. K. Mishra**, **S. G. Hiriyanna**, **H. S. Yathirajan** and **R. S. Rathore**

Comment

As a part of our interest in the design of candidate cytotoxins, based on the α, β-unsaturated keto scaffold, a series of compounds have been synthesized. These molecules have been shown to alkylate thiols but not amino or hydroxyl substituents; the latter two functional groups are found in nucleic acids suggesting that enones may be devoid of unwanted genetic mutations causing genotoxic properties, that is common among a number of anticancer drugs currently in use (Pati *et al.*, 2007*a*) Pati *et al.*, 2007*b*). The title molecule, $C_{15}H_{15}NO_2$, (I), is one such compound, synthesized from structurally similar substituted desoxybenzoin precursor.

The three dimensional structure is composed of three planar subunits, namely, methoxyphenyl (O2/C1—C8), phenylethanone (C9—C15) and oxime (O1/N1/C1). The former two planes, on either side of oxime subunit make an angle of 87.9 (1)°, whereas the oxime subunit is oriented by 23.0 (2)° and 76.9 (1)° with respect to the first and second planes. Molecular structure is shown Fig. 1.

An intra-molecular C9B—H9B···O1 hydrogen bond stabilize the structure. O1 also participate in O1—H1···N1 hydrogen bond with another oxime subunit in the molecules related by $(-x, 1-y, 1-z)$ (Table 1). The O—H···N hydrogen bonds cluster molecules into $R^2_2(6)$ dimers. There is a good *Cg*2···*Cg*2 stacking interaction, with the second *Cg*2 at $(-x, 2-y, 1-z)$. The benzene rings are parallel to each other, 3.344 Å apart with a slippage of 4.107 Å. *Cg*2 is the centroid of the (C10—C15) ring. The center-to-center distance is 5.297 (2) Å. The intermolecular hydrogen bond and aromatic interactions interlink molecules into a one-dimensional array along *b* axis, as illustrated in Fig. 2. Two short contacts, *i.e.*, C8—H8A..*Cg*1 [H···*Cg* = 2.74 Å, C—H···*Cg* = 138°] C8—H8C···*Cg*2 [H···*Cg* = 2.90 Å, C—H···*Cg* = 144°] were also observed in the crystal, where *Cg*1 (centroid of C2—C7 ring) and *Cg*2 are situated in the molecule at the symmetry position $(1/2+x, y, 1/2-z)$. However, it is unlikely to have any structural significance, as methyl group is undergoing extremely rapid rotation about O2—C8.

Experimental

Desoxybenzoin (23.0 g, 0.102 mol) was dissolved in toluene (200 ml). In a separate 500 ml round-bottom flask equipped with a magnetic stirring bar, hydroxylamine hydrochloride (9.21 g, 0.132 mol) and potassium hydroxide (7.43 g, 0.132 mol) were suspended in absolute ethanol (50 ml) and stirred vigorously at room temperature for 30 min. The desoxybenzoin solution was added in one portion, and the yellow suspension was held at reflux, using a Dean-Stark trap to remove generated water, under a nitrogen blanket for 16 h. The suspension was cooled to room temperature and poured into water (200 ml). The system was extracted with ethyl acetate (2x150 ml), then the combined organic solution was washed with brine (200 ml), dried over sodium sulfate, and filtered. The solvents were evaporated under reduced pressure to yield a crude solid. The solid was recrystallized from hot ethanol and water, filtered and washed with water to yield, upon drying, desoxybenzoin keto-oxime (I) as white crystals (yield: 82%; m.p.: 389 K). IR(KBr): 3186, 2970, 2944, 1988, 1947, 1697, 1604, 1577, 1489, 1450, 1293, 1225, 1166, 1046, 965, 862, 721 cm-1; 1HNMR(CDCl3): 400Mz δ 3.77(s, 3H), 4.20(s, 2H), 6.87(m,1*H*), 7.16–7.26(m,8*H*); ESI(APCI)-MS: m/*z* 242(*M*+1).

Refinement

All the H atoms were placed at geometrically expected positions with riding options. The distances with H atoms are $C_{aromatic}$—H = 0.93 Å, $C_{methylene}$—H = 0.97 Å, C_{methyl}—H = 0.96 Å and O—H = 0.82 Å. The U_{iso}(H) was set to $1.2U_{eq}$ of parent atoms [$1.5U_{eq}$ for methyl atom].

Figures

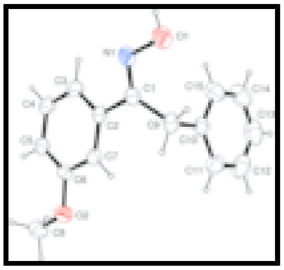

Fig. 1. A view of (I) with adopted numbering scheme. The displacement ellipsoids are drawn at 30% probability level.

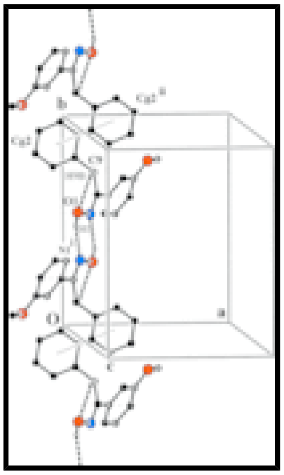

Fig. 2. Intermolecular hydrogen bonds and aromatic interactions cluster molecules into a linear array along *b* axis, shown in a view of crystal packing. *Cg*2 is the centroid of (C10—C15) ring. Symmetry codes: (i) $-x, 1-y, 1-z$, (ii) $-x, 2-y, 1-z$.

1-(3-Methoxyphenyl)-2-phenylethanone oxime

Crystal data

$C_{15}H_{15}NO_2$

$M_r = 241.28$

Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

$a = 9.7198 (9)$ Å

$b = 12.139 (1)$ Å

$c = 21.499 (2)$ Å

$V = 2536.8 (4)$ Å^3

$Z = 8$

$F_{000} = 1024$

$D_x = 1.264$ Mg m^{-3}

Melting point: 389 K

Mo *K*α radiation
$\lambda = 0.71073$ Å

Cell parameters from 1558 reflections

$\theta = 2.8–17.9°$

$\mu = 0.08$ mm^{-1}

$T = 295 (2)$ K

Cube, white

0.22 × 0.16 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer	2489 independent reflections
Radiation source: fine-focus sealed tube	1358 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.081$
$T = 295(2)$ K	$\theta_{\text{max}} = 26.0^\circ$
ω and φ scans	$\theta_{\text{min}} = 1.9^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -11\rightarrow11$
$T_{\text{min}} = 0.901$, $T_{\text{max}} = 0.982$	$k = -14\rightarrow14$
18438 measured reflections	$l = -26\rightarrow25$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.052$	H-atom parameters constrained
$wR(F^2) = 0.118$	$w = 1/[\sigma^2(F_o^2) + (0.0397P)^2 + 0.4359P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{\text{max}} < 0.001$
2489 reflections	$\Delta\rho_{\text{max}} = 0.16$ e Å^{-3}
165 parameters	$\Delta\rho_{\text{min}} = -0.11$ 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.

#=== Weighted least-squares planes through the starred atoms (Nardelli, Musatti, Domiano & Andreetti Ric·Sci.(1965),15(II—A),807). Equation of the plane: m1**X*+m2*Y+m3**Z*=d

Plane 1 m1 = −0.71737(0.00029) m2 = 0.45861(0.00059) m3 = −0.52445(0.00048) D = −1.78586(0.00828) Atom d s d/s (d/s)**2 C1 * 0.0203 0.0022 9.396 88.292 C2 * 0.0014 0.0020 0.707 0.500 C3 * 0.0132 0.0023 5.852 34.248 C4 * −0.0039 0.0024 − 1.610 2.593 C5 * −0.0236 0.0023 − 10.094 101.887 C6 * −0.0159 0.0021 − 7.557 57.105 C7 * −0.0085 0.0020 − 4.143 17.162 C8 * 0.0884 0.0026 33.687 1134.810 O2 * −0.0229 0.0016 − 14.783 218.527 N1 − 0.3852 0.0019 − 198.121 39252.105 O1 − 0.2706 0.0018 − 151.577 22975.512 ============ Sum((d/s)**2) for starred atoms 1655.122 Chi-squared at 95% for 6 degrees of freedom: 12.60 The group of atoms deviates significantly from planarity

Plane 2 m1 = 0.34347(0.00083) m2 = −0.37088(0.00093) m3 = −0.86283(0.00035) D = −12.13015(0.00796) Atom d s d/s (d/s)**2 C9 * −0.0197 0.0022 − 9.077 82.396 C10 * 0.0154 0.0022 6.965 48.507 C11 * 0.0122 0.0025 4.953 24.530 C12 * −0.0012 0.0030 − 0.401 0.161 C13 * −0.0267 0.0031 − 8.604 74.026 C14 * −0.0083 0.0031 − 2.662 7.086 C15 * 0.0187 0.0026 7.232 52.303

============ Sum((d/s)**2) for starred atoms 289.009 Chi-squared at 95% for 4 degrees of freedom: 9.49 The group of atoms deviates significantly from planarity

Plane 3 m1 = 0.78942(0.00088) m2 = −0.07504(0.00299) m3 = 0.60924(0.00133) D = 5.86175(0.03322) Atom d s d/s (d/s)**2 O1 * 0.0000 0.0018 0.000 0.000 N1 * 0.0000 0.0019 0.000 0.000 C1 * 0.0000 0.0021 0.000 0.000 C9 0.0489 0.0022 22.155 490.826 C2 − 0.0912 0.0020 − 45.470 2067.499 ============ Sum((d/s)**2) for starred atoms 0.000 Dihedral angles formed by LSQ-planes Plane - plane angle (s.u.) angle (s.u.) 1 2 87.94 (0.05) 92.06 (0.05) 1 3 23.04 (0.17) 156.96 (0.17) 2 3 76.90 (0.10) 103.10 (0.10) #==

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 $F^2 > 2\text{sigma}(F^2)$ 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_{iso}*/U_{eq}
N1	0.0384 (2)	0.60399 (16)	0.46703 (9)	0.0594 (6)
O1	−0.04754 (19)	0.62133 (14)	0.51858 (8)	0.0760 (6)
H1	−0.0654	0.5620	0.5349	0.114*
O2	0.43137 (16)	0.82951 (13)	0.30324 (7)	0.0659 (5)
C1	0.0879 (2)	0.6926 (2)	0.44421 (10)	0.0489 (6)
C2	0.1715 (2)	0.67863 (18)	0.38728 (9)	0.0445 (5)
C3	0.1560 (2)	0.58610 (18)	0.35011 (10)	0.0544 (6)
H3	0.0926	0.5320	0.3609	0.065*
C4	0.2344 (3)	0.57431 (19)	0.29738 (11)	0.0615 (7)
H4	0.2235	0.5116	0.2730	0.074*
C5	0.3289 (2)	0.65320 (19)	0.27962 (11)	0.0557 (6)
H5	0.3818	0.6439	0.2439	0.067*
C6	0.3429 (2)	0.74521 (18)	0.31568 (10)	0.0467 (6)
C7	0.2653 (2)	0.75760 (18)	0.36914 (9)	0.0478 (6)
H7	0.2766	0.8204	0.3933	0.057*
C8	0.5054 (3)	0.8267 (2)	0.24622 (12)	0.0779 (8)
H8A	0.5637	0.7629	0.2454	0.117*
H8B	0.5607	0.8920	0.2426	0.117*
H8C	0.4417	0.8234	0.2121	0.117*
C9	0.0622 (2)	0.80492 (18)	0.47080 (10)	0.0550 (6)
H9A	0.1481	0.8456	0.4715	0.066*
H9B	0.0305	0.7973	0.5134	0.066*
C10	−0.0429 (2)	0.8697 (2)	0.43428 (10)	0.0521 (6)
C11	−0.0157 (3)	0.9746 (2)	0.41389 (11)	0.0675 (7)
H11	0.0702	1.0057	0.4214	0.081*
C12	−0.1143 (4)	1.0343 (2)	0.38237 (13)	0.0865 (9)
H12	−0.0945	1.1050	0.3683	0.104*
C13	−0.2407 (4)	0.9894 (3)	0.37188 (13)	0.0948 (11)
H13	−0.3081	1.0301	0.3515	0.114*
C14	−0.2683 (3)	0.8851 (3)	0.39125 (14)	0.0893 (9)
H14	−0.3541	0.8542	0.3836	0.107*
C15	−0.1697 (3)	0.8255 (2)	0.42201 (12)	0.0712 (8)

H15	−0.1892	0.7540	0.4347	0.085*

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0648 (13)	0.0630 (15)	0.0505 (12)	0.0077 (11)	0.0185 (11)	0.0045 (10)
O1	0.0870 (13)	0.0768 (13)	0.0642 (11)	0.0126 (11)	0.0319 (10)	0.0082 (10)
O2	0.0643 (10)	0.0621 (11)	0.0713 (11)	−0.0145 (9)	0.0174 (9)	−0.0095 (9)
C1	0.0479 (13)	0.0545 (16)	0.0444 (13)	0.0064 (12)	−0.0006 (11)	−0.0007 (12)
C2	0.0459 (12)	0.0463 (14)	0.0412 (12)	0.0052 (11)	−0.0018 (11)	−0.0023 (11)
C3	0.0598 (15)	0.0489 (15)	0.0545 (15)	−0.0042 (12)	0.0095 (12)	−0.0043 (12)
C4	0.0719 (17)	0.0482 (15)	0.0642 (17)	−0.0046 (13)	0.0103 (14)	−0.0183 (13)
C5	0.0572 (15)	0.0560 (16)	0.0537 (14)	0.0020 (12)	0.0122 (12)	−0.0116 (13)
C6	0.0426 (12)	0.0456 (14)	0.0520 (14)	−0.0016 (12)	−0.0013 (11)	−0.0006 (12)
C7	0.0502 (13)	0.0470 (14)	0.0461 (14)	0.0005 (12)	−0.0011 (11)	−0.0108 (11)
C8	0.0775 (19)	0.0750 (19)	0.0812 (19)	−0.0119 (15)	0.0259 (16)	0.0026 (16)
C9	0.0608 (15)	0.0595 (16)	0.0447 (13)	0.0058 (13)	0.0042 (12)	−0.0085 (12)
C10	0.0578 (15)	0.0558 (16)	0.0427 (13)	0.0064 (12)	0.0098 (12)	−0.0042 (12)
C11	0.0804 (18)	0.0583 (18)	0.0639 (17)	0.0016 (15)	0.0080 (14)	−0.0041 (14)
C12	0.117 (3)	0.069 (2)	0.074 (2)	0.026 (2)	0.0136 (19)	0.0142 (16)
C13	0.092 (2)	0.120 (3)	0.072 (2)	0.045 (2)	0.0088 (19)	0.022 (2)
C14	0.0583 (18)	0.123 (3)	0.087 (2)	0.0066 (19)	−0.0025 (16)	0.020 (2)
C15	0.0594 (16)	0.083 (2)	0.0710 (17)	0.0007 (16)	0.0043 (15)	0.0148 (15)

Geometric parameters (Å, °)

N1—C1	1.276 (3)	C8—H8A	0.9600
N1—O1	1.404 (2)	C8—H8B	0.9600
O1—H1	0.8200	C8—H8C	0.9600
O2—C6	1.363 (2)	C9—C10	1.509 (3)
O2—C8	1.422 (3)	C9—H9A	0.9700
C1—C2	1.479 (3)	C9—H9B	0.9700
C1—C9	1.500 (3)	C10—C15	1.370 (3)
C2—C7	1.379 (3)	C10—C11	1.372 (3)
C2—C3	1.387 (3)	C11—C12	1.380 (4)
C3—C4	1.373 (3)	C11—H11	0.9300
C3—H3	0.9300	C12—C13	1.363 (4)
C4—C5	1.381 (3)	C12—H12	0.9300
C4—H4	0.9300	C13—C14	1.360 (4)
C5—C6	1.366 (3)	C13—H13	0.9300
C5—H5	0.9300	C14—C15	1.371 (4)
C6—C7	1.383 (3)	C14—H14	0.9300
C7—H7	0.9300	C15—H15	0.9300
C1—N1—O1	113.68 (18)	O2—C8—H8C	109.5
N1—O1—H1	109.5	H8A—C8—H8C	109.5
C6—O2—C8	118.06 (18)	H8B—C8—H8C	109.5
N1—C1—C2	115.4 (2)	C1—C9—C10	112.84 (18)
N1—C1—C9	123.9 (2)	C1—C9—H9A	109.0

C2—C1—C9	120.7 (2)	C10—C9—H9A	109.0
C7—C2—C3	118.1 (2)	C1—C9—H9B	109.0
C7—C2—C1	121.2 (2)	C10—C9—H9B	109.0
C3—C2—C1	120.7 (2)	H9A—C9—H9B	107.8
C4—C3—C2	120.0 (2)	C15—C10—C11	118.4 (2)
C4—C3—H3	120.0	C15—C10—C9	120.3 (2)
C2—C3—H3	120.0	C11—C10—C9	121.3 (2)
C3—C4—C5	121.7 (2)	C10—C11—C12	120.7 (3)
C3—C4—H4	119.2	C10—C11—H11	119.6
C5—C4—H4	119.2	C12—C11—H11	119.6
C6—C5—C4	118.5 (2)	C13—C12—C11	119.8 (3)
C6—C5—H5	120.8	C13—C12—H12	120.1
C4—C5—H5	120.8	C11—C12—H12	120.1
O2—C6—C5	124.4 (2)	C14—C13—C12	119.9 (3)
O2—C6—C7	115.17 (19)	C14—C13—H13	120.0
C5—C6—C7	120.4 (2)	C12—C13—H13	120.0
C2—C7—C6	121.3 (2)	C13—C14—C15	120.1 (3)
C2—C7—H7	119.3	C13—C14—H14	119.9
C6—C7—H7	119.3	C15—C14—H14	119.9
O2—C8—H8A	109.5	C10—C15—C14	121.0 (3)
O2—C8—H8B	109.5	C10—C15—H15	119.5
H8A—C8—H8B	109.5	C14—C15—H15	119.5

O1—N1—C1—C2	−176.09 (17)	C1—C2—C7—C6	−179.50 (19)
O1—N1—C1—C9	2.3 (3)	O2—C6—C7—C2	179.88 (18)
N1—C1—C2—C7	−159.0 (2)	C5—C6—C7—C2	−0.5 (3)
C9—C1—C2—C7	22.6 (3)	N1—C1—C9—C10	−102.7 (3)
N1—C1—C2—C3	22.0 (3)	C2—C1—C9—C10	75.6 (3)
C9—C1—C2—C3	−156.4 (2)	C1—C9—C10—C15	53.3 (3)
C7—C2—C3—C4	0.9 (3)	C1—C9—C10—C11	−128.3 (2)
C1—C2—C3—C4	180.0 (2)	C15—C10—C11—C12	0.7 (4)
C2—C3—C4—C5	−0.5 (4)	C9—C10—C11—C12	−177.8 (2)
C3—C4—C5—C6	−0.5 (4)	C10—C11—C12—C13	0.7 (4)
C8—O2—C6—C5	5.8 (3)	C11—C12—C13—C14	−1.5 (5)
C8—O2—C6—C7	−174.5 (2)	C12—C13—C14—C15	0.8 (5)
C4—C5—C6—O2	−179.5 (2)	C11—C10—C15—C14	−1.3 (4)
C4—C5—C6—C7	0.9 (3)	C9—C10—C15—C14	177.1 (2)
C3—C2—C7—C6	−0.4 (3)	C13—C14—C15—C10	0.6 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9B···O1	0.97	2.27	2.676 (3)	104
O1—H1···N1^{i}	0.82	2.03	2.754 (3)	147

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

Fig. 1

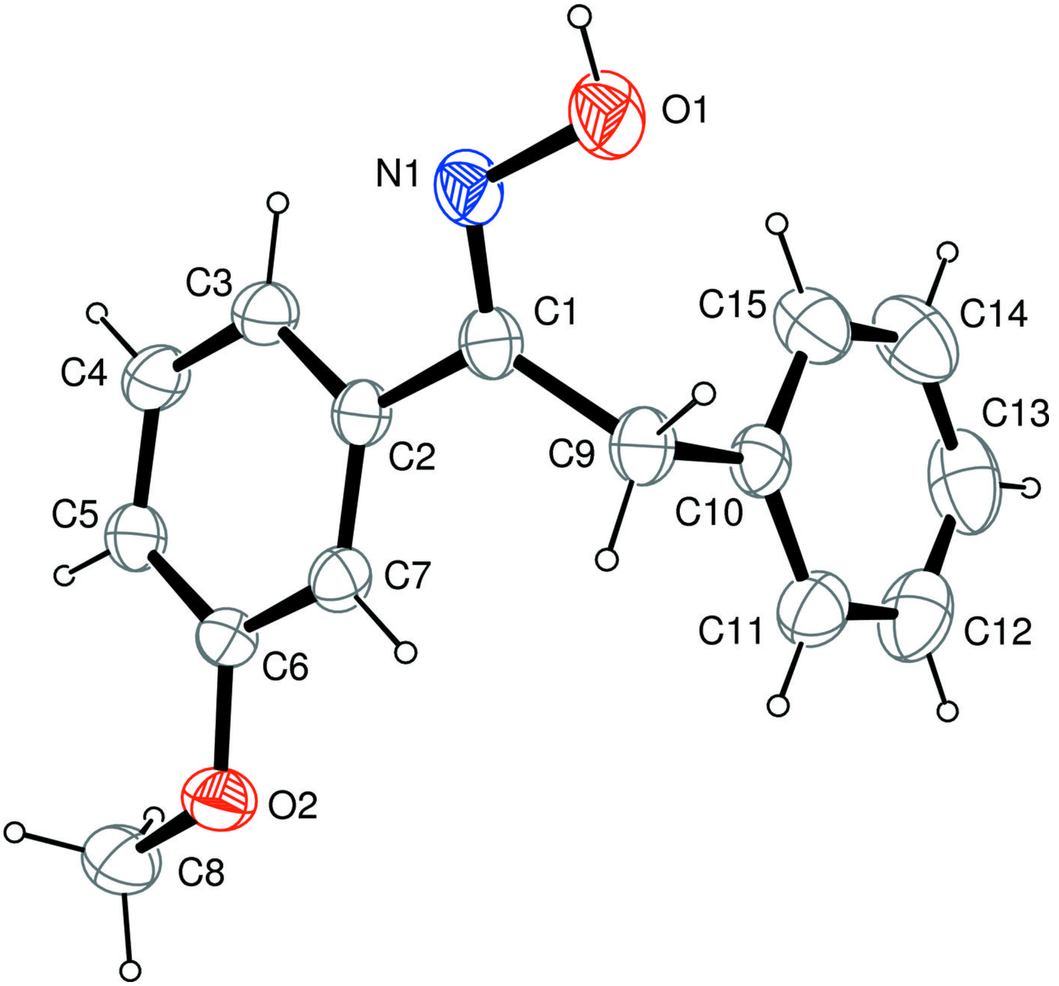

Fig. 2