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N-Hydroxy-*N*-*o*-tolylacetamide

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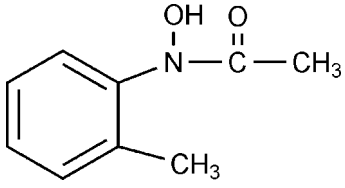
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.004 Å; R factor = 0.067; wR factor = 0.183; data-to-parameter ratio = 15.6.

In the molecule of the title compound, $C_9H_{11}NO_2$, the methyl C atom bonded to the ring and the N atom lie in the benzene ring plane. An intramolecular O—H···O hydrogen bond results in the formation of a five-membered planar ring, which is oriented at a dihedral angle of 81.37 (3)° with respect to the benzene ring. In the crystal structure, intermolecular O—H···O hydrogen bonds link the molecules stacked along the b axis. There are also π–π interactions between benzene rings with a face-to-face stacking distance of 3.434 Å.

Related literature

For related literature, see: Fu *et al.* (2000). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_9H_{11}NO_2$
M_r = 165.19
Monoclinic, $P2_1/c$
a = 7.7890 (16) Å
b = 7.1570 (14) Å
c = 15.613 (3) Å
β = 96.86 (3)°
V = 864.1 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 294 (2) K
0.40 × 0.30 × 0.30 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.965, T_{max} = 0.973
1821 measured reflections
1695 independent reflections
1187 reflections with $I > 2\sigma(I)$
R_{int} = 0.054
3 standard reflections
frequency: 120 min
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.182
S = 1.05
1695 reflections
109 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O2	0.82	2.19	2.608 (3)	112
O1—H1A···O2^{i}	0.82	1.97	2.719 (3)	152

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1985); 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: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2420).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Enraf–Nonius (1985). *CAD-4 Software*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.
Fu, S. Y., Zhan, H. Y. & Yu, H. S. (2000). *J. S. China Univ. Technol. (Nat. Sci. Ed.)*, **28**, 59–63.
Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

supporting information

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S1. Comment

The title compound, (I), contains hydroxy and formyl groups, which can react with different groups to prepare various function organic compounds. It is a kind of aromatic organic intermediate that can be used for many fields such as pesticide, paper making *etc*. (Fu *et al.*, 2000). We report herein its crystal structure.

In the molecule of (I), (Fig. 1), the bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. The atoms N and C1 lie in the benzene ring plane. The intramolecular O—H···O hydrogen bond (Table 1) results in the formation of a five-membered planar ring A (O1/H1A/O2/N/C8). The dihedral angle between five- and six-membered rings is 81.37 (3)°.

In the crystal structure, intermolecular O—H···O hydrogen bonds (Table 1) link the molecules stacked along the *b* axis (Fig. 2), in which they may be effective in the stabilization of the structure.

There are also the π-π interactions of benzene rings with a face-to-face stacking distance of 3.434 Å.

S2. Experimental

The title compound, (I), was prepared by the literature method (Fu *et al.*, 2000). Crystals suitable for X-ray analysis were obtained by dissolving (I) (0.5 g) in petroleum ether (20 ml) and evaporating the solvent slowly at room temperature for about 7 d.

S3. Refinement

H atoms were positioned geometrically, with O—H = 0.82 Å (for OH) and C—H = 0.93 and 0.96 Å for aromatic and methyl H, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C,*O*), where x = 1.2 for aromatic H, and x = 1.5 for all other H atoms.

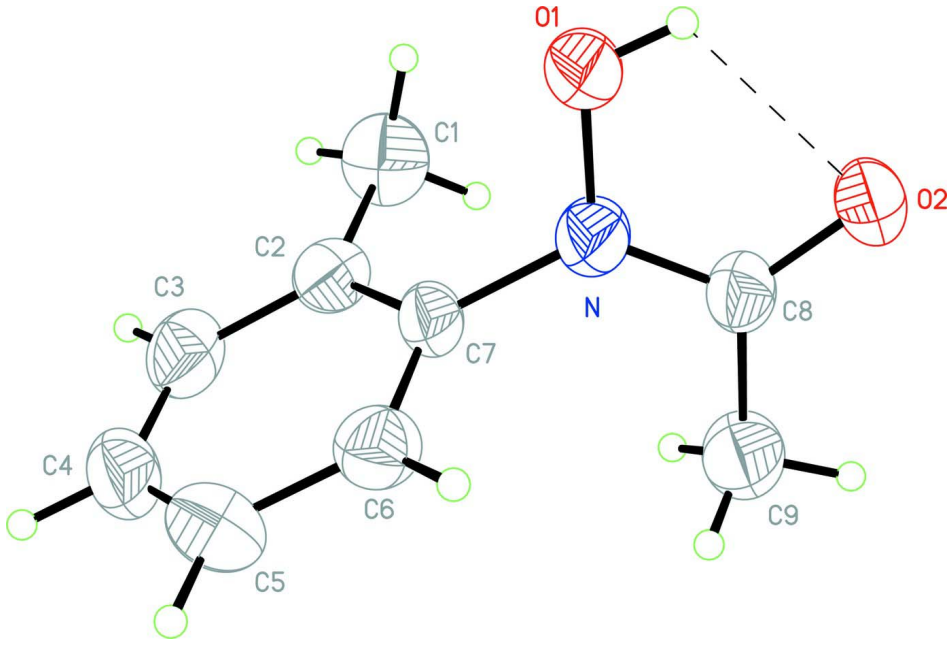

Figure 1

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

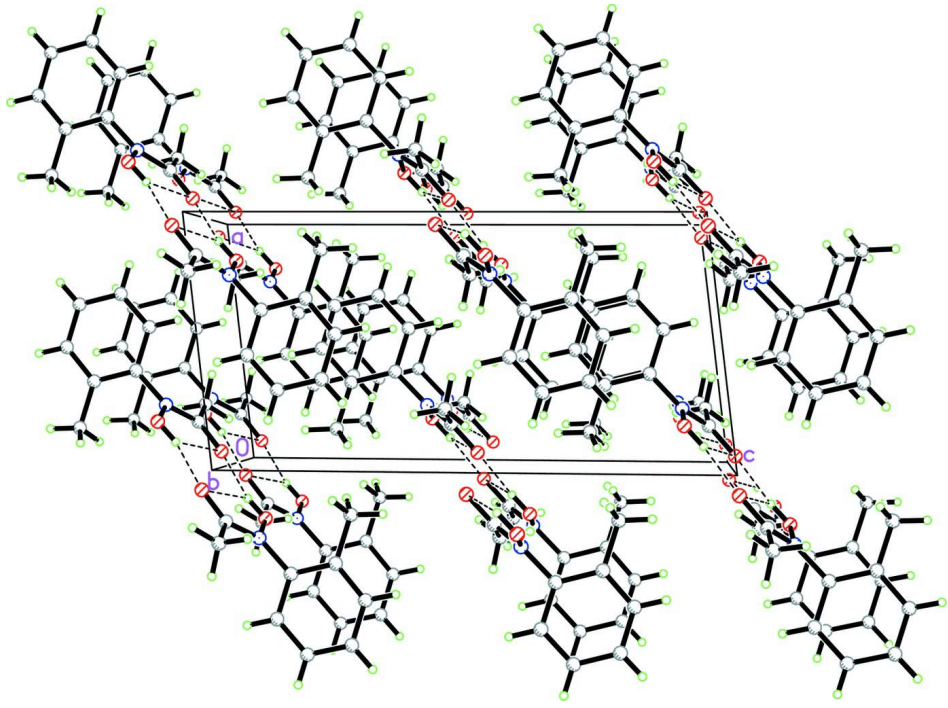

Figure 2

A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

N-Hydroxy-*N*-*o*-tolylacetamide

Crystal data

$C_9H_{11}NO_2$
$M_r = 165.19$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.7890$ (16) Å
$b = 7.1570$ (14) Å
$c = 15.613$ (3) Å
$\beta = 96.86$ (3)°
$V = 864.1$ (3) Å^3
$Z = 4$
$F(000) = 352$
$D_x = 1.270$ Mg m^{-3}
Melting point: 350 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 10$–13°
$\mu = 0.09$ mm^{-1}
$T = 294$ K
Block, colorless
0.40 × 0.30 × 0.30 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.965$, $T_{max} = 0.973$
1821 measured reflections
1695 independent reflections
1187 reflections with $I > 2\sigma(I)$
$R_{int} = 0.054$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.6°$
$h = -9\rightarrow9$
$k = 0\rightarrow8$
$l = 0\rightarrow19$
3 standard reflections every 120 min
intensity decay: none

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.067$
$wR(F^2) = 0.182$
$S = 1.05$
1695 reflections
109 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
$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 1.5P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N	0.7518 (4)	0.1297 (4)	0.08788 (17)	0.0451 (7)
O1	0.8117 (3)	−0.0536 (3)	0.08895 (15)	0.0554 (7)
H1A	0.8888	−0.0624	0.0577	0.083*

O2	0.9365 (3)	0.2046 (3)	−0.00399 (16)	0.0573 (7)
C1	0.8476 (4)	0.1834 (6)	0.2703 (2)	0.0593 (10)
H1B	0.8527	0.2003	0.3316	0.089*
H1C	0.9065	0.2848	0.2461	0.089*
H1D	0.9022	0.0675	0.2585	0.089*
C2	0.6626 (4)	0.1799 (4)	0.23108 (19)	0.0406 (7)
C3	0.5278 (5)	0.2025 (5)	0.2806 (2)	0.0508 (9)
H3A	0.5533	0.2200	0.3398	0.061*
C4	0.3579 (5)	0.1999 (5)	0.2453 (2)	0.0536 (9)
H4A	0.2706	0.2150	0.2805	0.064*
C5	0.3164 (4)	0.1750 (5)	0.1577 (2)	0.0572 (9)
H5A	0.2013	0.1721	0.1337	0.069*
C6	0.4465 (4)	0.1545 (5)	0.1062 (2)	0.0454 (8)
H6A	0.4194	0.1392	0.0470	0.054*
C7	0.6189 (4)	0.1567 (4)	0.14250 (18)	0.0370 (7)
C8	0.8214 (4)	0.2543 (5)	0.03929 (18)	0.0411 (7)
C9	0.7578 (5)	0.4524 (5)	0.0400 (3)	0.0586 (10)
H9A	0.8186	0.5270	0.0023	0.088*
H9B	0.7779	0.5013	0.0975	0.088*
H9C	0.6362	0.4555	0.0205	0.088*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N	0.0584 (17)	0.0377 (14)	0.0420 (14)	0.0072 (12)	0.0179 (12)	0.0028 (12)
O1	0.0735 (16)	0.0420 (13)	0.0570 (15)	0.0174 (11)	0.0338 (12)	0.0085 (11)
O2	0.0654 (15)	0.0530 (15)	0.0599 (15)	0.0118 (12)	0.0343 (13)	0.0102 (12)
C1	0.054 (2)	0.066 (2)	0.057 (2)	−0.0089 (18)	0.0002 (16)	−0.0039 (18)
C2	0.0504 (18)	0.0360 (16)	0.0352 (16)	0.0026 (14)	0.0045 (13)	−0.0034 (12)
C3	0.073 (2)	0.0481 (19)	0.0339 (16)	0.0030 (17)	0.0155 (15)	−0.0029 (14)
C4	0.057 (2)	0.050 (2)	0.059 (2)	0.0045 (16)	0.0285 (17)	0.0015 (17)
C5	0.0411 (18)	0.064 (2)	0.066 (2)	0.0057 (17)	0.0044 (16)	−0.0010 (19)
C6	0.0486 (18)	0.0471 (19)	0.0401 (17)	0.0052 (15)	0.0043 (14)	0.0001 (14)
C7	0.0423 (16)	0.0363 (16)	0.0349 (15)	0.0036 (13)	0.0150 (12)	0.0012 (12)
C8	0.0440 (16)	0.0482 (18)	0.0318 (15)	0.0009 (14)	0.0076 (12)	0.0017 (13)
C9	0.069 (2)	0.044 (2)	0.066 (2)	0.0046 (17)	0.0243 (19)	0.0052 (17)

Geometric parameters (Å, º)

N—C8	1.328 (4)	C3—H3A	0.9300
N—O1	1.392 (3)	C4—C5	1.378 (5)
N—C7	1.431 (4)	C4—H4A	0.9300
O1—H1A	0.8200	C5—C6	1.375 (5)
C1—C2	1.497 (5)	C5—H5A	0.9300
C1—H1B	0.9600	C6—C7	1.394 (4)
C1—H1C	0.9600	C6—H6A	0.9300
C1—H1D	0.9600	C8—C9	1.502 (5)
O2—C8	1.238 (3)	C9—H9A	0.9600

C2—C3	1.386 (4)	C9—H9B	0.9600
C2—C7	1.394 (4)	C9—H9C	0.9600
C3—C4	1.371 (5)		

C8—N—O1	118.8 (2)	C6—C5—C4	119.5 (3)
C8—N—C7	128.6 (3)	C6—C5—H5A	120.3
O1—N—C7	112.7 (2)	C4—C5—H5A	120.3
N—O1—H1A	109.5	C5—C6—C7	120.2 (3)
C2—C1—H1B	109.5	C5—C6—H6A	119.9
C2—C1—H1C	109.5	C7—C6—H6A	119.9
H1B—C1—H1C	109.5	C6—C7—C2	120.9 (3)
C2—C1—H1D	109.5	C6—C7—N	119.1 (3)
H1B—C1—H1D	109.5	C2—C7—N	119.9 (3)
H1C—C1—H1D	109.5	O2—C8—N	119.4 (3)
C3—C2—C7	117.1 (3)	O2—C8—C9	122.4 (3)
C3—C2—C1	121.7 (3)	N—C8—C9	118.2 (3)
C7—C2—C1	121.1 (3)	C8—C9—H9A	109.5
C4—C3—C2	122.2 (3)	C8—C9—H9B	109.5
C4—C3—H3A	118.9	H9A—C9—H9B	109.5
C2—C3—H3A	118.9	C8—C9—H9C	109.5
C3—C4—C5	120.1 (3)	H9A—C9—H9C	109.5
C3—C4—H4A	119.9	H9B—C9—H9C	109.5
C5—C4—H4A	119.9		

C7—C2—C3—C4	0.9 (5)	C1—C2—C7—N	2.0 (4)
C1—C2—C3—C4	179.9 (3)	C8—N—C7—C6	82.5 (4)
C2—C3—C4—C5	−0.3 (5)	O1—N—C7—C6	−98.0 (3)
C3—C4—C5—C6	−0.6 (6)	C8—N—C7—C2	−99.2 (4)
C4—C5—C6—C7	0.8 (5)	O1—N—C7—C2	80.4 (3)
C5—C6—C7—C2	−0.1 (5)	O1—N—C8—O2	0.4 (5)
C5—C6—C7—N	178.2 (3)	C7—N—C8—O2	179.9 (3)
C3—C2—C7—C6	−0.7 (4)	O1—N—C8—C9	−178.9 (3)
C1—C2—C7—C6	−179.7 (3)	C7—N—C8—C9	0.6 (5)
C3—C2—C7—N	−179.0 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···O2	0.82	2.19	2.608 (3)	112
O1—H1*A*···O2^{i}	0.82	1.97	2.719 (3)	152

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