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2-Methylbenzamidoxime

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.060
wR factor = 0.189
Data-to-parameter ratio = 16.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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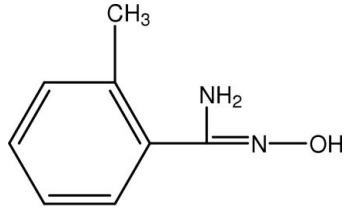
In the crystal structure of the title compound, $C_8H_{10}N_2O$, which is a benzonitrile derivative, an intramolecular N—H···O hydrogen bond and intermolecular N—H···O and O—H···N hydrogen bonds are present.

Comment

As part of our ongoing studies of benzonitrile derivatives, we report here the crystal structure of the title compound, (I).



(I)

The geometrical parameters for (I) are normal; its molecular structure is shown in Fig. 1. The dihedral angle between the mean planes of the C2–C7 benzene ring and the C7/C8/N1/N2/O group is 81.68 (11)°. A combination of intramolecular and intermolecular hydrogen bonds (Table 2) helps to establish the crystal packing.

Experimental

Three solutions were prepared: 2-methylbenzonitrile (20 mmol) in ethanol (8 ml), hydroxylamine hydrochloride (20 mmol) in ethanol (6 ml) and potassium carbonate (10 mmol) in water (10 ml). The three solutions were mixed and the resulting mixture was refluxed for

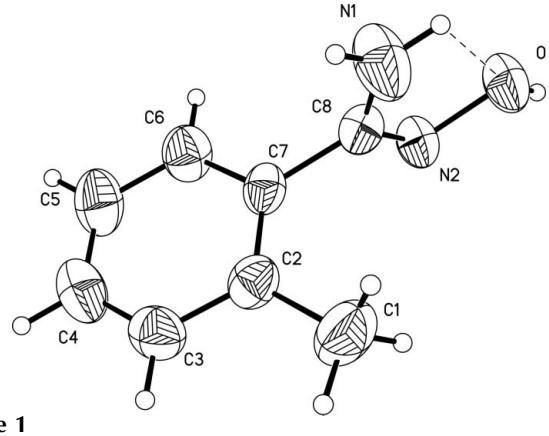


Figure 1
The molecular structure of (I), showing displacement ellipsoids drawn at the 30% probability level (arbitrary spheres for the H atoms). The dashed line indicates the intramolecular N—H···O hydrogen bond.

24 h. After cooling and filtration, crude compound (I) was obtained. Pure compound (I) was obtained by crystallization from a mixture of ethanol (6 ml) and water (2 ml). Yellow crystals of (I) suitable for X-ray diffraction were obstained by slow evaporation of an ethanol solution.

Crystal data

$C_8H_{10}N_2O$
M_r = 150.18
Monoclinic, $P2_1/n$
a = 9.751 (2) Å
b = 7.0880 (14) Å
c = 11.982 (2) Å
β = 98.60 (3)°
V = 818.8 (3) Å^3
Z = 4
D_x = 1.218 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
Block, yellow
0.40 × 0.20 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.968, T_{max} = 0.984
1694 measured reflections
1600 independent reflections
1124 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 26.0°
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.189
S = 1.08
1600 reflections
100 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1125P)^2 + 0.0887P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1B···O^{i}	0.86	2.44	3.267 (3)	163
N1—H1A···O	0.86	2.22	2.542 (3)	102
O—H1w···N2^{ii}	0.82	2.08	2.787 (3)	145

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

All H atoms were positioned gemoetrically (C—H = 0.93–0.97, O—H = 0.82, N—H = 0.86 Å) and refined as riding with U_{iso}(H) = 1.2 or 1.5U_{eq} of the carrier atom.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXL97*.

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