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4-Methylbenzamide oxime

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.059
wR factor = 0.186
Data-to-parameter ratio = 15.7

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

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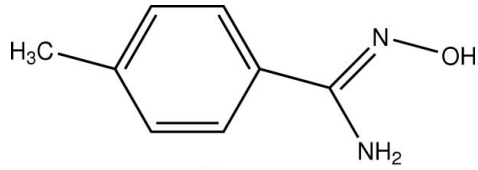
The title compound, $C_8H_{10}N_2O$, is a derivative of benzonitrile. It crystallizes with two molecules per asymmetric unit. There are intramolecular N—H···O hydrogen bonds, as well as intermolecular N—H···O and O—H···N hydrogen-bond interactions.

Comment

Some derivatives of benzonitrile are important chemical materials as they are intermediates of oxadiazoles We report here the crystal structure of one such derivative, (I), which crystallizes in space group $P\overline{1}$ with two independent molecules in the asymmetric unit.



(I)

The molecular structure of (I) is shown in Fig. 1, where the dashed lines indicate N—H···O intramolecular hydrogen bonds (Table 1). Each of the independent molecules is hydrogen bonded to two of its symmetry-related neighbors, around inversion centers, by one N—H···O bond and one O—H···N bond (Table 1). There are no interactions between the independent molecules.

Experimental

4-Methylbenzonitrile (20 mmol) and hydroxylamine hydrochloride (20 mmol) in ethanol (20 ml) were mixed with potassium carbonate (10 mmol) in water (10 ml) and refluxed for 24 h, cooled and then filtered to obtain crude compound (I). Pure compound (I) was obtained by recrystallization from a mixture of ethanol (6 ml) and water (2 ml). Crystals of (I) suitable for X-ray diffraction were grown by slow evaporation of an ethanol solution.

Crystal data

$C_8H_{10}N_2O$
M_r = 150.18
Triclinic, $P\overline{1}$
a = 6.4220 (13) Å
b = 7.4720 (15) Å
c = 17.181 (3) Å
α = 79.48 (3)°
β = 82.16 (3)°
γ = 85.45 (3)°
V = 801.7 (3) Å^3
Z = 4
D_x = 1.244 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
Block, colorless
0.30 × 0.30 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.975, T_{max} = 0.992
3446 measured reflections
3147 independent reflections
2216 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 26.0°
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.186
S = 1.05
3147 reflections
200 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.09P)^2 + 0.27P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.083 (11)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···N2^{i}	0.82	2.01	2.728 (3)	146
N1—H1E···O1	0.86	2.21	2.530 (3)	102
N1—H1E···O1^{ii}	0.86	2.27	3.043 (3)	150
O2—H2A···N3^{iii}	0.82	2.03	2.721 (2)	142
N4—H4A···O2	0.86	2.20	2.527 (3)	102
N4—H4A···O2^{iv}	0.86	2.27	3.039 (3)	148

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

All H atoms bonded to the C atoms were positioned geometrically at distances of 0.93–0.97 Å and included in the refinement in riding-model approximation with U_{iso}(H) = 1.2 or 1.5U_{eq}(carrier atom). The O—H and N—H distances were constrained to 0.82 and 0.86 Å and these H atoms were refined as riding, with U_{iso}(H) = 1.2U_{eq}(N) and 1.5U_{eq}(O).

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*.

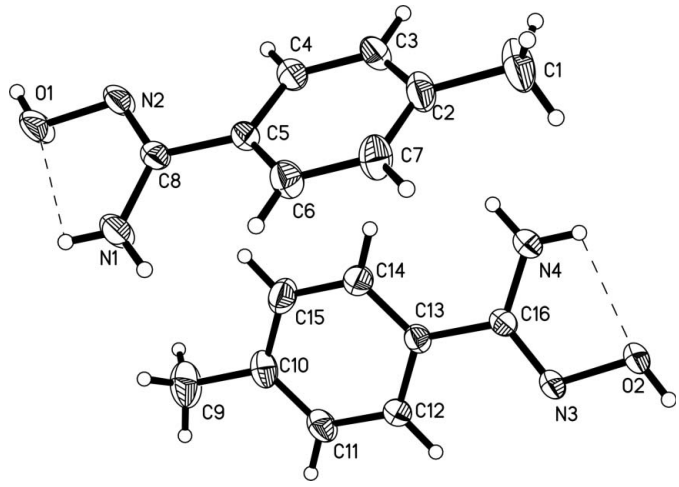


Figure 1
A view of the molecular structure of (I), showing both molecules in the asymmetric unit, with displacement ellipsoids drawn at the 30% probability level. Dashed lines indicate the intramolecular N—H···O hydrogen bonds.

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