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4-Nitrobenzamidoxime

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.073
wR factor = 0.200
Data-to-parameter ratio = 13.6

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

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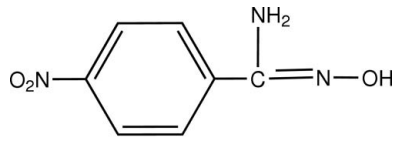
In the title compound, $C_7H_7N_3O_3$, which is a derivative of benzonitrile, the molecular conformation is stabilized by an intramolecular N—H···O hydrogen bond.

Comment

As part of our ongoing studies of benzonitrile derivatives (Wang *et al.*, 2007), we report here the crystal structure of the title compound, (I).



(I)

The dihedral angle between the mean planes of the C1–C6 benzene ring and the C6/C7/N2/N3/O3 grouping is 41.0 (2)°. In the related 2-methylbenzamidoxime the equivalent dihedral angle is 81.68 (11)° (Wang *et al.*, 2007).

The molecular structure of (I) is shown in Fig. 1. Its conformation is stabilized by an intramolecular N2—H2*A*···O3 hydrogen bond. The same H atom also participates in an intermolecular interaction (Table 1). Further intermolecular hydrogen bonds result in a three-dimensional network.

Experimental

4-Nitrobenzonitrile (20 mmol) was dissolved in ethanol (8 ml), hydroxylamine hydrochloride (20 mmol) was dissolved in ethanol (6 ml) and potassium carbonate (10 mmol) was dissolved in water (10 ml); the three separate solutions were mixed. The resulting

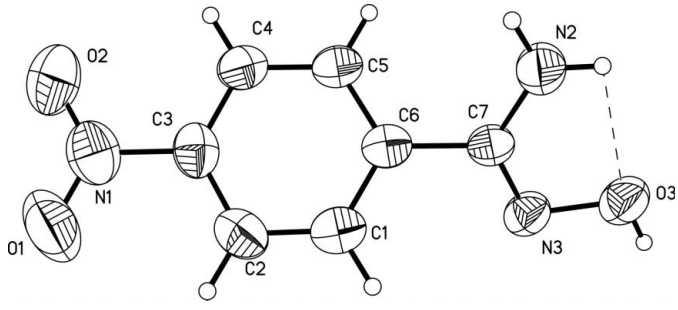


Figure 1
A view of the molecular structure of (I), showing displacement ellipsoids at the 50% probability level (arbitrary spheres for the H atoms). The dashed line indicates the intramolecular N—H···O hydrogen bond.

mixture was refluxed for 24 h. After cooling and filtering, crude compound (I) was obtained by crystallizing from a mixture of ethanol (6 ml) and water (2 ml). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

Crystal data

$C_7H_7N_3O_3$
M_r = 181.16
Orthorhombic, *Pbca*
a = 11.320 (2) Å
b = 7.7760 (16) Å
c = 18.802 (4) Å
V = 1655.0 (6) Å^3
Z = 8
D_x = 1.454 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 293 (2) K
Needle, yellow
0.20 × 0.10 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.977, T_{max} = 0.988
1609 measured reflections
1609 independent reflections
671 reflections with $I > 2\sigma(I)$
θ_{max} = 26.0°
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.073
$wR(F^2)$ = 0.200
S = 0.98
1609 reflections
118 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0689P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: none

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O3	0.86	2.23	2.544 (5)	102
N2—H2A···O2^{i}	0.86	2.45	3.071 (5)	130
N2—H2B···O3^{ii}	0.86	2.27	3.102 (6)	163
O3—H3A···N3^{iii}	0.82	2.11	2.758 (5)	136

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

The H atoms were positioned geometrically (C—H = 0.93 Å, O—H = 0.82 Å, N—H = 0.86 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C,N) or 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*.

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