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4-Bromobenzamide oxime

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In the title compound, $C_7H_7BrN_2O$, which is a derivative of benzonitrile, an intramolecular N—H···O hydrogen bond occurs. Intermolecular N—H···O and O—H···N hydrogen bonds help to establish the crystal packing.

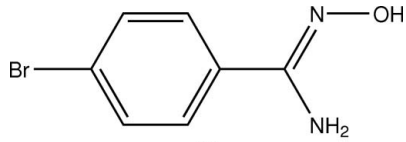
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.008 Å
R factor = 0.078
wR factor = 0.160
Data-to-parameter ratio = 15.8

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

Comment

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



(I)

The dihedral angle between the mean planes of the C1–C6 benzene ring and the C7/N1/N2/O grouping is 35.3 (2)°. An acute intramolecular N—H···O hydrogen bond occurs (Table 1) and an intermolecular O—H···N link leads to centrosymmetric dimers (Fig. 1). An intermolecular N—H···O bond also occurs.

Experimental

Three solutions were made up, namely 4-bromobenzonitrile (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 refluxed for 24 h. After cooling and filtering, the crude title compound was obtained; it was purified by crystallisation 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

$C_7H_7BrN_2O$
M_r = 215.05
Monoclinic, $P2_1/c$
a = 8.1347 (16) Å
b = 12.964 (3) Å
c = 7.6517 (15) Å
β = 90.41 (3)°
V = 806.9 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 5.04 mm^{-1}
T = 293 (2) K
0.40 × 0.20 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.299, T_{max} = 0.368
1699 measured reflections
1575 independent reflections
938 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.078$	100 parameters
$wR(F^2) = 0.160$	H-atom parameters constrained
$S = 1.26$	$\Delta\rho_{max} = 0.32$ e Å^{-3}
1575 reflections	$\Delta\rho_{min} = -0.26$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1^{i}	0.82	2.10	2.789 (9)	141
N2—H2A···O1	0.86	2.26	2.565 (7)	101
N2—H2B···O1^{ii}	0.86	2.48	3.174 (9)	138

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

All H atoms were positioned geometrically, with C—H = 0.93–0.97 Å, N—H = 0.86 Å and O—H = 0.82 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*.

References

Enraf–Nonius (1989). *CAD-4 Software*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.

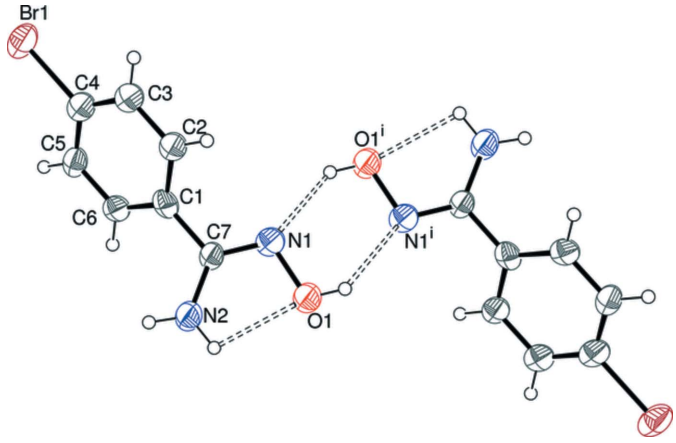


Figure 1
The structure of a dimer of (I), showing displacement ellipsoids at the 40% probability level (arbitrary spheres for H atoms). Dashed lines indicate the hydrogen bonds. [Symmetry code: (i) $1-x, 1-y, 2-z$.]

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