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4-Methoxybenzamide oxime

Hai-Lin Li, Hai-Su Zeng, Si-Shun Kang and Hai-Bo Wang*

College of Science, Nanjing University of Technolgy, Xinmofan Road No. 5, Nanjing 210009, People's Republic of China
Correspondence e-mail: wanghaibo@njut.edu.cn

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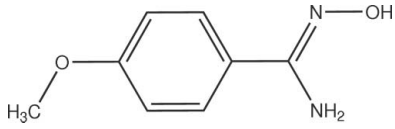
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.074; wR factor = 0.200; data-to-parameter ratio = 14.5.

In the title compound, $C_8H_{10}N_2O_2$, which is a derivative of benzonitrile, there are an intramolecular N—H···O hydrogen bond and intermolecular N—H···O and O—H···N hydrogen bonds.

Related literature

For related literature, see: Wang *et al.* (2007).



Experimental

Crystal data

$C_8H_{10}N_2O_2$
M_r = 166.18
Monoclinic, $P2_1/c$
a = 14.924 (3) Å
b = 5.0820 (10) Å
c = 10.784 (2) Å
β = 98.32 (3)°
V = 809.3 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 (2) K
0.40 × 0.30 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.961, T_{max} = 0.980
1581 measured reflections
1581 independent reflections
1139 reflections with $I > 2\sigma(I)$
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.074
$wR(F^2)$ = 0.200
S = 1.05
1581 reflections
109 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O2	0.86	2.22	2.541 (4)	102
N1—H1A···O2^{i}	0.86	2.30	3.056 (3)	146
O2—H2A···N2^{ii}	0.82	2.20	2.839 (4)	135

Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+\frac{5}{2}$; (ii) $-x+1, -y+1, -z+2$.

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: *PLATON* (Spek, 2003).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LW2044).

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supplementary materials

Acta Cryst. (2007). E**63**, o4763 [**doi:10.1107/S1600536807059429**]

4-Methoxybenzamide oxime

H.-L. Li, H.-S. Zeng, S.-S. Kang and H.-B. Wang

Comment

Some derivatives of benzonitrile is important chemical material (Wang *et al.*, 2007)·We report here the crystal structure of the title compound, (I).

The molecular structure of (I) is shown in Fig. 1.

Experimental

4-Methoxy-benzonitrile(20 mmol) was dissolved in ethanol (8 ml). Hydroxylamine hydrochloride(20 mmol) was dissolved in ethanol (6 ml). Potassium carbonate (10 mmol) was dissolved in water (10 ml). The three separate solutions were mixed and refluxed for 24 h. After cooling and filtrating, crude compound (I) was gained. Pure 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 ethyl acetate solution.

Refinement

All H atoms were placed geometrically (N—H = 0.86, C—H = 0.93–0.96 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(carrier) or 1.5U_{eq}(methyl carrier).

Figures

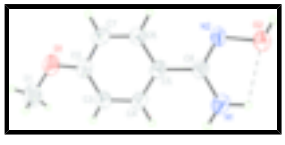

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. The dashed line indicates an N—H···O hydrogen bond.

4-Methoxybenzamide oxime

Crystal data

$C_8H_{10}N_2O_2$	F_{000} = 352
M_r = 166.18	D_x = 1.364 Mg m^{-3}
Monoclinic, $P2_1/C$	Melting point: 390 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 14.924 (3) Å	Cell parameters from 25 reflections
b = 5.0820 (10) Å	θ = 9–13°
c = 10.784 (2) Å	μ = 0.10 mm^{-1}

β = 98.32 (3)º	T = 293 (2) K
V = 809.3 (3) Å^3	Block, colorless
Z = 4	0.40 × 0.30 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.0000
Radiation source: fine-focus sealed tube	θ_{max} = 26.0º
Monochromator: graphite	θ_{min} = 1.4º
T = 293(2) K	h = −18→18
ω/2θ scans	k = 0→6
Absorption correction: ψ scan (North *et al.*, 1968)	l = 0→13
T_{min} = 0.961, T_{max} = 0.980	3 standard reflections
1581 measured reflections	every 200 reflections
1581 independent reflections	intensity decay: none
1139 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.060P)^2 + 1.850P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.074	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.200	$\Delta\rho_{max}$ = 0.29 e Å^{-3}
S = 1.05	$\Delta\rho_{min}$ = −0.31 e Å^{-3}
1581 reflections	Extinction correction: none
109 parameters	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

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 $F^2 > 2\text{sigma}(F^2)$ 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}
O1	0.09171 (17)	1.0551 (6)	0.6300 (2)	0.0584 (8)
N1	0.39977 (19)	1.0978 (6)	1.1139 (2)	0.0447 (7)
H1A	0.4421	1.0689	1.1754	0.054*
H1B	0.3695	1.2422	1.1106	0.054*
C1	0.0286 (3)	1.2658 (10)	0.6303 (4)	0.0706 (12)
H1C	−0.0166	1.2530	0.5576	0.106*
H1D	0.0599	1.4307	0.6291	0.106*
H1E	0.0001	1.2556	0.7045	0.106*
O2	0.49656 (15)	0.6850 (5)	1.1236 (2)	0.0471 (7)
H2A	0.5230	0.5436	1.1234	0.071*
N2	0.42404 (17)	0.6930 (6)	1.0210 (2)	0.0396 (7)
C2	0.1603 (2)	1.0373 (7)	0.7280 (3)	0.0420 (8)
C3	0.1666 (2)	1.1836 (8)	0.8375 (3)	0.0502 (9)
H3A	0.1225	1.3079	0.8476	0.060*
C4	0.2388 (2)	1.1439 (8)	0.9315 (3)	0.0490 (9)
H4A	0.2429	1.2456	1.0039	0.059*
C5	0.3045 (2)	0.9588 (6)	0.9215 (3)	0.0369 (7)
C6	0.2972 (2)	0.8165 (8)	0.8104 (3)	0.0487 (9)
H6A	0.3419	0.6947	0.7994	0.058*
C7	0.2257 (3)	0.8512 (8)	0.7167 (3)	0.0533 (10)
H7A	0.2214	0.7482	0.6448	0.064*
C8	0.3808 (2)	0.9153 (7)	1.0217 (3)	0.0370 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0535 (15)	0.0737 (19)	0.0432 (13)	0.0074 (14)	−0.0094 (11)	0.0004 (13)
N1	0.0510 (16)	0.0471 (17)	0.0338 (13)	0.0011 (14)	−0.0012 (12)	−0.0030 (13)
C1	0.066 (3)	0.075 (3)	0.063 (3)	0.008 (2)	−0.015 (2)	0.010 (2)
O2	0.0469 (13)	0.0515 (15)	0.0397 (12)	0.0117 (12)	−0.0045 (10)	0.0020 (11)
N2	0.0407 (14)	0.0426 (16)	0.0325 (13)	0.0038 (13)	−0.0046 (11)	0.0042 (12)
C2	0.0394 (17)	0.049 (2)	0.0364 (16)	−0.0018 (15)	0.0018 (13)	0.0046 (15)
C3	0.051 (2)	0.052 (2)	0.0442 (18)	0.0150 (17)	−0.0037 (15)	−0.0046 (17)
C4	0.055 (2)	0.054 (2)	0.0353 (17)	0.0099 (18)	−0.0031 (15)	−0.0088 (16)
C5	0.0405 (16)	0.0398 (18)	0.0300 (15)	−0.0036 (14)	0.0033 (12)	0.0033 (13)
C6	0.0469 (19)	0.057 (2)	0.0399 (17)	0.0169 (17)	−0.0021 (14)	−0.0095 (16)
C7	0.060 (2)	0.061 (2)	0.0377 (17)	0.0098 (19)	0.0030 (16)	−0.0087 (17)
C8	0.0408 (16)	0.0417 (18)	0.0286 (14)	0.0012 (14)	0.0049 (12)	0.0034 (13)

Geometric parameters (Å, °)

O1—C2	1.364 (4)	C2—C7	1.377 (5)
O1—C1	1.426 (5)	C2—C3	1.387 (5)
N1—C8	1.359 (4)	C3—C4	1.384 (5)
N1—H1A	0.8600	C3—H3A	0.9300

N1—H1B	0.8600	C4—C5	1.375 (5)
C1—H1C	0.9600	C4—H4A	0.9300
C1—H1D	0.9600	C5—C6	1.390 (5)
C1—H1E	0.9600	C5—C8	1.469 (4)
O2—N2	1.432 (3)	C6—C7	1.370 (5)
O2—H2A	0.8200	C6—H6A	0.9300
N2—C8	1.302 (4)	C7—H7A	0.9300
C2—O1—C1	118.1 (3)	C2—C3—H3A	120.2
C8—N1—H1A	120.0	C5—C4—C3	122.1 (3)
C8—N1—H1B	120.0	C5—C4—H4A	119.0
H1A—N1—H1B	120.0	C3—C4—H4A	119.0
O1—C1—H1C	109.5	C4—C5—C6	117.1 (3)
O1—C1—H1D	109.5	C4—C5—C8	122.1 (3)
H1C—C1—H1D	109.5	C6—C5—C8	120.8 (3)
O1—C1—H1E	109.5	C7—C6—C5	121.6 (3)
H1C—C1—H1E	109.5	C7—C6—H6A	119.2
H1D—C1—H1E	109.5	C5—C6—H6A	119.2
N2—O2—H2A	109.5	C6—C7—C2	120.6 (3)
C8—N2—O2	109.9 (3)	C6—C7—H7A	119.7
O1—C2—C7	116.1 (3)	C2—C7—H7A	119.7
O1—C2—C3	125.0 (3)	N2—C8—N1	123.1 (3)
C7—C2—C3	118.8 (3)	N2—C8—C5	117.3 (3)
C4—C3—C2	119.7 (3)	N1—C8—C5	119.5 (3)
C4—C3—H3A	120.2		
C1—O1—C2—C7	−172.4 (4)	C5—C6—C7—C2	2.6 (6)
C1—O1—C2—C3	10.1 (5)	O1—C2—C7—C6	−179.6 (4)
O1—C2—C3—C4	178.7 (3)	C3—C2—C7—C6	−1.9 (6)
C7—C2—C3—C4	1.2 (6)	O2—N2—C8—N1	−4.7 (4)
C2—C3—C4—C5	−1.3 (6)	O2—N2—C8—C5	179.3 (2)
C3—C4—C5—C6	1.9 (6)	C4—C5—C8—N2	160.8 (3)
C3—C4—C5—C8	−179.6 (3)	C6—C5—C8—N2	−20.7 (5)
C4—C5—C6—C7	−2.5 (6)	C4—C5—C8—N1	−15.4 (5)
C8—C5—C6—C7	178.9 (3)	C6—C5—C8—N1	163.1 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O2	0.86	2.22	2.541 (4)	102
N1—H1A···O2^{i}	0.86	2.30	3.056 (3)	146
O2—H2A···N2^{ii}	0.82	2.20	2.839 (4)	135

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+5/2; (ii) −*x*+1, −*y*+1, −*z*+2.

Fig. 1