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N-(4-Bromophenyl)propionamide

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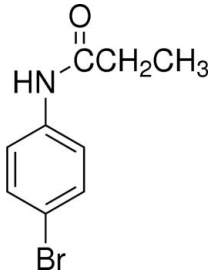
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.004 Å; R factor = 0.036; wR factor = 0.093; data-to-parameter ratio = 14.4.

In the title compound, $C_9H_{10}BrNO$, molecules are interconnected by a framework of intermolecular N—H···O hydrogen bonds. Infinite one-dimensional hydrogen-bonded chains extend along the *a* direction. These chains are aggregated into layers through weak inter-chain C—H···Br contacts along *c*.

Related literature

For structural studies on other amides, see: Knopfel *et al.* (2005); Guo (2004); Parvez *et al.* (2004). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_9H_{10}BrNO$
M_r = 228.09
Orthorhombic, *Pbca*
a = 9.3879 (19) Å
b = 9.2952 (19) Å
c = 20.721 (4) Å
V = 1808.2 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 4.50 mm^{-1}
T = 294 (2) K
0.08 × 0.08 × 0.04 mm

Data collection

Rigaku Saturn diffractometer
Absorption correction: multi-scan (Jacobson, 1998)
T_{min} = 0.712, T_{max} = 0.835
10043 measured reflections
1587 independent reflections
1375 reflections with $I > 2\sigma(I)$
R_{int} = 0.064

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.093
S = 1.10
1587 reflections
110 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.76 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9A···Br1^{i}	0.96	2.99	3.555 (3)	119
C2—H2···O1	0.93	2.32	2.880 (4)	118
N1—H1A···O1^{ii}	0.85	2.08	2.886 (3)	160

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

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXTL* (Bruker, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2337).

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supplementary materials

Acta Cryst. (2007). E**63**, o3884 [**doi:10.1107/S1600536807040950**]

N-(4-Bromophenyl)propionamide

C.-H. Guo, M.-L. Guo, H.-Y. Zhang and Y.-N. Ye

Comment

The amide moiety is an important constituent of many biologically significant compounds. Structural studies of amides are therefore of interest (Knopfel *et al.*, 2005; Guo, 2004; Parvez *et al.*, 2004). As part of a study of possible drugs, the crystal structure of the title compound (I) is reported herein, Fig. 1. Bond distances and angles are normal, within experimental error (Allen *et al.*, 1987).

In the structure of (I), the molecular skeleton is essentially planar with atoms O1, C7, C8 and C9 lying 0.6630, 0.2724, 0.0990 and 0.1530 Å, respectively, out of the N1/C1—C6/Br1 mean plane. Intermolecular N1—H1A···O1^{i} hydrogen bonds (see Table 1 for symmetry code) link the molecules into chains (Fig. 2). Further, short C—H···Br contacts (distance = 3.555 (3) Å) stabilize the packing in the structure.

Experimental

The title compound was prepared by slowly adding concentrated sulfuric acid (2.0 ml) dropwise to a mixture of *N*-phenylpropionamide (3.7 g, 0.025 mol), sodium bromide (2.6 g, 0.025 mol), 30% hydrogen peroxide (5.0 ml, 0.05 mol) and ethanol (20 ml). The mixture was stirred in air at room temperature for 30 min. The resulting product was separated by filtration (yield 5.3 g, 93%). Single crystals were obtained from a solution of 0.2 g of the product in 25 ml of distilled water by slow concentration over a period of 1 week at room temperature.

Refinement

All H-atoms were positioned geometrically and refined using a riding model with d(C—H) = 0.93 Å, U_{iso}=1.2U_{eq} (C) for aromatic, 0.97 Å, U_{iso} = 1.2U_{eq} (C) for CH_2, 0.96 Å, U_{iso} = 1.5U_{eq} (C) for CH_3 atoms and 0.86 Å, U_{iso} = 1.2U_{eq} (N) for the NH atom.

Figures

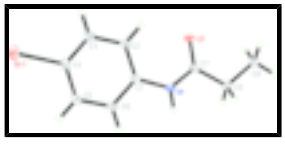

Fig. 1. A view of the structure of (I), showing the atom-numbering Scheme; displacement ellipsoids were drawn at the 30% probability level.

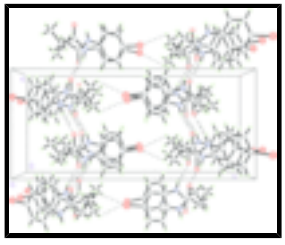

Fig. 2. The crystal packing of (I) viewed down the *b* axis with hydrogen bonds drawn as dashed lines.

N-(4-Bromophenyl)propionamide

Crystal data

$C_9H_{10}BrNO$	F_{000} = 912
M_r = 228.09	D_x = 1.676 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 3850 reflections
a = 9.3879 (19) Å	θ = 2.0–27.9º
b = 9.2952 (19) Å	μ = 4.50 mm^{-1}
c = 20.721 (4) Å	*T* = 294 (2) K
V = 1808.2 (6) Å^3	Plate, colorless
Z = 8	0.08 × 0.08 × 0.04 mm

Data collection

Rigaku Saturn diffractometer	1587 independent reflections
Radiation source: rotating anode	1375 reflections with $I > 2\sigma(I)$
Monochromator: confocal	R_{int} = 0.064
T = 294(2) K	θ_{max} = 25.0º
ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (Jacobson, 1998)	*h* = −11→7
T_{min} = 0.712, T_{max} = 0.835	*k* = −10→11
10043 measured reflections	*l* = −24→24

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.036	H-atom parameters constrained
$wR(F^2)$ = 0.093	$w = 1/[\sigma^2(F_o^2) + (0.0501P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.10	$(\Delta/\sigma)_{max}$ = 0.001
1587 reflections	$\Delta\rho_{max}$ = 0.59 e Å^{-3}
110 parameters	$\Delta\rho_{min}$ = −0.75 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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}
Br1	0.23826 (4)	0.03223 (3)	0.528300 (15)	0.03307 (18)
N1	0.3167 (3)	0.4370 (2)	0.30106 (11)	0.0211 (5)
H1A	0.4042	0.4501	0.2932	0.025*
O1	0.0960 (2)	0.45235 (19)	0.25674 (9)	0.0275 (5)
C1	0.2921 (3)	0.3403 (3)	0.35205 (13)	0.0195 (6)
C2	0.1577 (3)	0.3134 (3)	0.37778 (14)	0.0245 (7)
H2	0.0780	0.3580	0.3602	0.029*
C3	0.1428 (3)	0.2203 (3)	0.42943 (14)	0.0248 (7)
H3	0.0530	0.2016	0.4464	0.030*
C4	0.2612 (3)	0.1554 (3)	0.45556 (15)	0.0238 (7)
C5	0.3955 (3)	0.1803 (3)	0.43096 (14)	0.0280 (7)
H5	0.4746	0.1353	0.4489	0.034*
C6	0.4107 (3)	0.2730 (3)	0.37931 (14)	0.0251 (7)
H6	0.5009	0.2908	0.3625	0.030*
C7	0.2219 (3)	0.4876 (3)	0.25727 (16)	0.0209 (7)
C8	0.2844 (3)	0.5911 (3)	0.20894 (15)	0.0238 (7)
H8A	0.3453	0.5384	0.1794	0.029*
H8B	0.3432	0.6607	0.2315	0.029*
C9	0.1713 (3)	0.6702 (3)	0.17065 (15)	0.0294 (7)
H9A	0.1148	0.6021	0.1471	0.044*
H9B	0.2162	0.7353	0.1410	0.044*
H9C	0.1113	0.7234	0.1996	0.044*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0451 (3)	0.0296 (3)	0.0246 (3)	0.00330 (13)	0.00111 (13)	0.00321 (12)
N1	0.0113 (12)	0.0276 (12)	0.0244 (13)	−0.0007 (10)	0.0004 (11)	0.0004 (10)
O1	0.0147 (11)	0.0365 (11)	0.0314 (12)	−0.0016 (9)	−0.0024 (9)	0.0040 (9)
C1	0.0200 (15)	0.0187 (14)	0.0200 (15)	0.0013 (12)	−0.0006 (12)	−0.0058 (12)
C2	0.0153 (15)	0.0315 (15)	0.0267 (17)	−0.0013 (12)	−0.0021 (13)	−0.0026 (13)
C3	0.0210 (16)	0.0309 (15)	0.0224 (17)	−0.0044 (13)	−0.0007 (13)	−0.0025 (12)
C4	0.0333 (18)	0.0202 (15)	0.0177 (15)	0.0001 (12)	−0.0009 (13)	−0.0006 (14)
C5	0.0245 (17)	0.0319 (15)	0.0276 (17)	0.0077 (14)	−0.0042 (14)	−0.0024 (14)
C6	0.0180 (15)	0.0304 (15)	0.0269 (17)	0.0034 (12)	0.0007 (13)	−0.0014 (13)
C7	0.0168 (16)	0.0246 (14)	0.0212 (17)	0.0019 (12)	0.0012 (12)	−0.0060 (12)
C8	0.0202 (16)	0.0249 (15)	0.0263 (17)	−0.0023 (12)	0.0014 (12)	0.0032 (14)

C9	0.0282 (17)	0.0292 (15)	0.0308 (18)	0.0024 (14)	0.0007 (15)	0.0041 (14)

Geometric parameters (Å, °)

Br1—C4	1.905 (3)	C4—C5	1.380 (4)
N1—C7	1.355 (4)	C5—C6	1.382 (4)
N1—C1	1.406 (4)	C5—H5	0.9300
N1—H1A	0.8457	C6—H6	0.9300
O1—C7	1.226 (3)	C7—C8	1.508 (4)
C1—C2	1.392 (4)	C8—C9	1.516 (4)
C1—C6	1.397 (4)	C8—H8A	0.9700
C2—C3	1.383 (4)	C8—H8B	0.9700
C2—H2	0.9300	C9—H9A	0.9600
C3—C4	1.376 (4)	C9—H9B	0.9600
C3—H3	0.9300	C9—H9C	0.9600
C7—N1—C1	128.1 (3)	C5—C6—C1	120.7 (3)
C7—N1—H1A	117.3	C5—C6—H6	119.7
C1—N1—H1A	113.3	C1—C6—H6	119.7
C2—C1—C6	119.1 (3)	O1—C7—N1	123.1 (3)
C2—C1—N1	123.5 (3)	O1—C7—C8	122.6 (3)
C6—C1—N1	117.3 (3)	N1—C7—C8	114.2 (3)
C3—C2—C1	120.1 (3)	C7—C8—C9	112.6 (3)
C3—C2—H2	120.0	C7—C8—H8A	109.1
C1—C2—H2	120.0	C9—C8—H8A	109.1
C4—C3—C2	119.8 (3)	C7—C8—H8B	109.1
C4—C3—H3	120.1	C9—C8—H8B	109.1
C2—C3—H3	120.1	H8A—C8—H8B	107.8
C3—C4—C5	121.3 (3)	C8—C9—H9A	109.5
C3—C4—Br1	118.9 (2)	C8—C9—H9B	109.5
C5—C4—Br1	119.8 (2)	H9A—C9—H9B	109.5
C4—C5—C6	119.0 (3)	C8—C9—H9C	109.5
C4—C5—H5	120.5	H9A—C9—H9C	109.5
C6—C5—H5	120.5	H9B—C9—H9C	109.5

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9A···Br1^{i}	0.96	2.99	3.555 (3)	119
C2—H2···O1	0.93	2.32	2.880 (4)	118
N1—H1A···O1^{ii}	0.85	2.08	2.886 (3)	160

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

Fig. 1

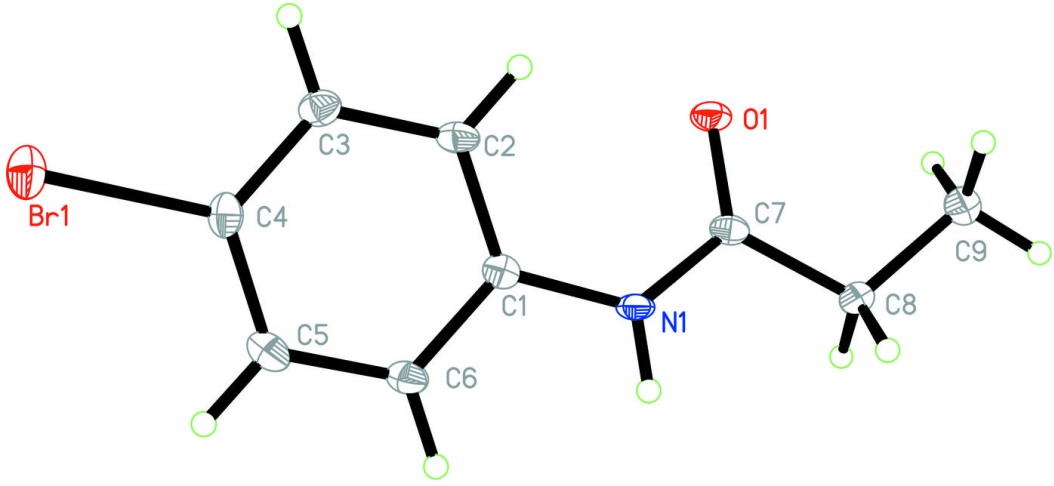

Fig. 2