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N-(3-Bromophenyl)acetamide

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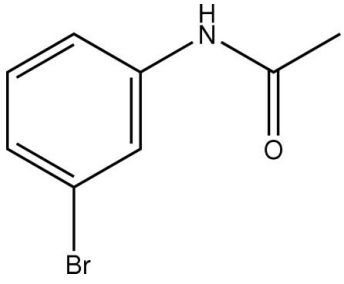
Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.007 Å; R factor = 0.045; wR factor = 0.093; data-to-parameter ratio = 17.2.

The conformation of the N—H bond in the structure of the title compound, C_8H_8BrNO, is *anti* to the C=O bond and to the *meta*-bromo substituent of the aromatic ring in both independent molecules comprising the asymmetric unit. Molecules are linked through N—H···O hydrogen bonding into supramolecular chains with a twisted topology.

Related literature

For the preparation of the compound, see: Gowda *et al.* (2006). For related structures, see: Gowda *et al.* (2007, 2008, 2009).



Experimental

Crystal data

C_8H_8BrNO
M_r = 214.06
Orthorhombic, $P2_12_12_1$
a = 4.7836 (6) Å
b = 18.765 (1) Å
c = 19.379 (2) Å
V = 1739.5 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 4.67 mm^{-1}
T = 299 K
0.44 × 0.10 × 0.08 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.226, T_{max} = 0.685
9612 measured reflections
3449 independent reflections
2043 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.093
S = 0.99
3449 reflections
201 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}
Absolute structure: Flack (1983), 1366 Friedel pairs
Flack parameter: −0.008 (13)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*···O2^{i}	0.86	2.05	2.887 (5)	166
N2—H2*N*···O1	0.86	2.10	2.953 (5)	169

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2004); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2417).

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supplementary materials

Acta Cryst. (2009). E**65**, o1039 [**doi:10.1107/S1600536809013294**]

N-(3-Bromophenyl)acetamide

B. T. Gowda, S. Foro, H. Terao and H. Fuess

Comment

As part of a study of the effect of ring and side-chain substitutions on the crystal structures of aromatic amides (Gowda *et al.*, 2007, 2008, 2009), in the present work, the structure of *N*-(3-bromophenyl)acetamide (I) has been determined. The conformation of the N—H bond in the structure is *anti* to the *meta*-bromo substituent of the aromatic ring (Fig. 1), in both independent molecules comprising the asymmetric unit, similar to that observed in *N*-(3-chlorophenyl)acetamide (Gowda *et al.*, 2008). Further, the conformation of the C=O bond is *anti* to the N—H bond. The two independent molecules in (I) are linked through intermolecular N—H···O hydrogen bonding into a supramolecular chains with a twisted topology (Table 1, Fig. 2).

Experimental

Compound (I) was prepared according to the literature method (Gowda *et al.*, 2006). Single crystals were obtained from an ethanolic solution of (I).

Refinement

The H atoms were positioned with idealized geometry using a riding model with C—H = 0.93–0.96 Å and N—H = 0.86 Å, and with U_{iso} set to 1.2 times U_{eq}(parent atom).

Figures

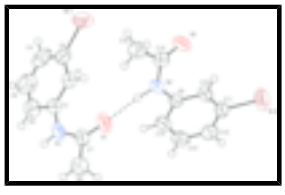

Fig. 1. Molecular structure of (I), showing the atom labeling scheme and displacement ellipsoids drawn at the 50% probability level. The intermolecular N-H···O hydrogen is shown as a dashed line.

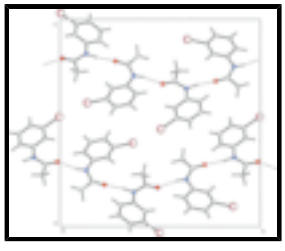

Fig. 2. Molecular packing of (I) viewed in projection down the a-axis highlighting the supramolecular chains mediated by hydrogen bonding (shown as dashed lines).

N-(3-Bromophenyl)acetamide

Crystal data

C_8H_8BrNO	F_{000} = 848
M_r = 214.06	D_x = 1.635 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 3601 reflections
a = 4.7836 (6) Å	θ = 2.4–27.6º
b = 18.765 (1) Å	μ = 4.67 mm^{-1}
c = 19.379 (2) Å	T = 299 K
V = 1739.5 (3) Å^3	Long needle, colourless
Z = 8	0.44 × 0.10 × 0.08 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector	3449 independent reflections
Radiation source: fine-focus sealed tube	2043 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.034
T = 299 K	θ_{max} = 26.4º
Rotation method data acquisition using ω and φ scans	θ_{min} = 2.4º
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007)	h = −5→5
T_{min} = 0.226, T_{max} = 0.685	k = −22→23
9612 measured reflections	l = −20→24

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.045	$w = 1/[\sigma^2(F_o^2) + (0.0455P)^2 + 0.0252P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.093	$(\Delta/\sigma)_{max}$ = 0.001
S = 0.99	$\Delta\rho_{max}$ = 0.31 e Å^{-3}
3449 reflections	$\Delta\rho_{min}$ = −0.49 e Å^{-3}
201 parameters	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 1366 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: −0.008 (13)

Special details

Experimental. Absorption correction: CrysAlis RED, Oxford Diffraction Ltd. (2007). Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

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 $F^2 > \sigma(F^2)$ 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	0.64658 (17)	0.36438 (3)	0.40336 (3)	0.0961 (3)
O1	1.0611 (8)	0.22271 (18)	0.20168 (19)	0.0786 (12)
N1	0.9531 (7)	0.13129 (19)	0.27225 (19)	0.0531 (10)
H1N	0.9782	0.0863	0.2779	0.064*
C1	0.7804 (10)	0.1647 (2)	0.3206 (2)	0.0492 (12)
C2	0.7903 (10)	0.2377 (2)	0.3338 (2)	0.0524 (12)
H2	0.9111	0.2670	0.3092	0.063*
C3	0.6192 (12)	0.2656 (3)	0.3838 (2)	0.0606 (14)
C4	0.4398 (12)	0.2247 (4)	0.4216 (3)	0.0740 (17)
H4	0.3269	0.2450	0.4553	0.089*
C5	0.4300 (12)	0.1519 (3)	0.4084 (3)	0.0848 (18)
H5	0.3068	0.1234	0.4331	0.102*
C6	0.6000 (11)	0.1215 (3)	0.3592 (3)	0.0691 (15)
H6	0.5951	0.0726	0.3516	0.083*
C7	1.0850 (10)	0.1608 (3)	0.2180 (2)	0.0546 (13)
C8	1.2664 (11)	0.1102 (2)	0.1767 (2)	0.0726 (17)
H8A	1.2240	0.0620	0.1895	0.087*
H8B	1.4597	0.1199	0.1861	0.087*
H8C	1.2303	0.1166	0.1284	0.087*
Br2	0.30944 (16)	0.49664 (3)	−0.03009 (3)	0.0919 (3)
O2	0.9050 (8)	0.48750 (17)	0.18809 (18)	0.0709 (10)
N2	0.8933 (8)	0.36972 (18)	0.16644 (18)	0.0475 (9)
H2N	0.9634	0.3294	0.1785	0.057*
C9	0.6865 (9)	0.3675 (2)	0.11456 (19)	0.0397 (10)
C10	0.6162 (10)	0.4252 (2)	0.0737 (2)	0.0464 (11)
H10	0.7039	0.4690	0.0799	0.056*
C11	0.4147 (10)	0.4168 (2)	0.0239 (2)	0.0499 (12)
C12	0.2819 (9)	0.3533 (3)	0.0127 (2)	0.0528 (12)
H12	0.1476	0.3489	−0.0218	0.063*
C13	0.3519 (12)	0.2959 (3)	0.0536 (2)	0.0576 (13)
H13	0.2619	0.2525	0.0473	0.069*
C14	0.5532 (9)	0.3025 (2)	0.1035 (2)	0.0490 (12)
H14	0.6013	0.2632	0.1302	0.059*
C15	0.9939 (9)	0.4277 (3)	0.1993 (2)	0.0490 (12)
C16	1.2135 (10)	0.4133 (3)	0.2521 (3)	0.0652 (14)

H16A	1.2663	0.3640	0.2502	0.078*
H16B	1.1416	0.4242	0.2971	0.078*
H16C	1.3739	0.4426	0.2429	0.078*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.1400 (6)	0.0715 (4)	0.0768 (4)	0.0319 (4)	−0.0121 (4)	−0.0259 (3)
O1	0.110 (3)	0.046 (2)	0.080 (2)	0.013 (2)	0.022 (2)	0.0251 (19)
N1	0.067 (3)	0.035 (2)	0.057 (2)	0.0055 (19)	0.003 (2)	0.012 (2)
C1	0.058 (3)	0.045 (3)	0.044 (3)	0.005 (2)	−0.005 (2)	0.006 (2)
C2	0.065 (3)	0.045 (3)	0.047 (2)	0.004 (2)	−0.003 (3)	0.003 (2)
C3	0.075 (4)	0.064 (3)	0.043 (3)	0.021 (3)	−0.007 (3)	−0.006 (3)
C4	0.068 (4)	0.108 (5)	0.046 (3)	0.021 (3)	0.008 (3)	−0.009 (3)
C5	0.089 (5)	0.096 (5)	0.070 (4)	−0.020 (3)	0.014 (4)	0.002 (4)
C6	0.083 (4)	0.059 (3)	0.065 (3)	−0.009 (3)	0.003 (3)	0.009 (3)
C7	0.067 (4)	0.045 (3)	0.052 (3)	0.007 (2)	0.002 (3)	0.008 (2)
C8	0.086 (5)	0.065 (3)	0.066 (3)	0.005 (3)	0.012 (3)	0.002 (3)
Br2	0.1222 (5)	0.0670 (4)	0.0866 (4)	0.0074 (4)	−0.0273 (4)	0.0277 (3)
O2	0.091 (3)	0.0351 (18)	0.086 (2)	0.0039 (19)	−0.014 (2)	−0.0108 (17)
N2	0.058 (3)	0.0299 (19)	0.054 (2)	0.0034 (19)	0.000 (2)	0.0001 (18)
C9	0.044 (3)	0.035 (2)	0.040 (2)	0.000 (2)	0.004 (2)	−0.003 (2)
C10	0.051 (3)	0.035 (2)	0.053 (3)	−0.002 (2)	−0.001 (3)	0.005 (2)
C11	0.059 (3)	0.044 (3)	0.047 (3)	0.008 (2)	0.003 (3)	0.007 (2)
C12	0.048 (3)	0.058 (3)	0.052 (3)	−0.002 (2)	−0.003 (2)	−0.006 (2)
C13	0.056 (3)	0.051 (3)	0.066 (3)	−0.002 (3)	−0.007 (3)	−0.011 (3)
C14	0.053 (3)	0.035 (3)	0.058 (3)	0.000 (2)	0.006 (3)	−0.002 (2)
C15	0.050 (3)	0.047 (3)	0.050 (3)	−0.001 (3)	−0.001 (3)	−0.007 (3)
C16	0.065 (4)	0.062 (3)	0.069 (3)	−0.009 (3)	−0.007 (3)	−0.012 (3)

Geometric parameters (Å, °)

Br1—C3	1.897 (5)	Br2—C11	1.895 (4)
O1—C7	1.209 (5)	O2—C15	1.220 (5)
N1—C7	1.346 (5)	N2—C15	1.349 (5)
N1—C1	1.398 (5)	N2—C9	1.411 (5)
N1—H1N	0.8600	N2—H2N	0.8600
C1—C2	1.394 (6)	C9—C10	1.383 (5)
C1—C6	1.400 (6)	C9—C14	1.392 (6)
C2—C3	1.372 (6)	C10—C11	1.374 (6)
C2—H2	0.9300	C10—H10	0.9300
C3—C4	1.364 (7)	C11—C12	1.369 (6)
C4—C5	1.390 (7)	C12—C13	1.377 (6)
C4—H4	0.9300	C12—H12	0.9300
C5—C6	1.377 (7)	C13—C14	1.371 (6)
C5—H5	0.9300	C13—H13	0.9300
C6—H6	0.9300	C14—H14	0.9300
C7—C8	1.514 (6)	C15—C16	1.490 (6)
C8—H8A	0.9600	C16—H16A	0.9600

C8—H8B	0.9600	C16—H16B	0.9600
C8—H8C	0.9600	C16—H16C	0.9600
C7—N1—C1	128.1 (4)	C15—N2—C9	127.6 (4)
C7—N1—H1N	116.0	C15—N2—H2N	116.2
C1—N1—H1N	116.0	C9—N2—H2N	116.2
C2—C1—N1	123.0 (4)	C10—C9—C14	119.1 (4)
C2—C1—C6	119.5 (5)	C10—C9—N2	123.7 (4)
N1—C1—C6	117.5 (4)	C14—C9—N2	117.2 (4)
C3—C2—C1	119.0 (5)	C11—C10—C9	118.9 (4)
C3—C2—H2	120.5	C11—C10—H10	120.5
C1—C2—H2	120.5	C9—C10—H10	120.5
C4—C3—C2	122.7 (5)	C12—C11—C10	122.5 (4)
C4—C3—Br1	119.1 (4)	C12—C11—Br2	118.5 (4)
C2—C3—Br1	118.2 (4)	C10—C11—Br2	119.0 (3)
C3—C4—C5	118.3 (5)	C11—C12—C13	118.4 (4)
C3—C4—H4	120.8	C11—C12—H12	120.8
C5—C4—H4	120.8	C13—C12—H12	120.8
C6—C5—C4	121.0 (5)	C14—C13—C12	120.4 (4)
C6—C5—H5	119.5	C14—C13—H13	119.8
C4—C5—H5	119.5	C12—C13—H13	119.8
C5—C6—C1	119.6 (5)	C13—C14—C9	120.6 (4)
C5—C6—H6	120.2	C13—C14—H14	119.7
C1—C6—H6	120.2	C9—C14—H14	119.7
O1—C7—N1	123.7 (4)	O2—C15—N2	122.2 (4)
O1—C7—C8	121.3 (4)	O2—C15—C16	122.3 (4)
N1—C7—C8	115.0 (4)	N2—C15—C16	115.5 (4)
C7—C8—H8A	109.5	C15—C16—H16A	109.5
C7—C8—H8B	109.5	C15—C16—H16B	109.5
H8A—C8—H8B	109.5	H16A—C16—H16B	109.5
C7—C8—H8C	109.5	C15—C16—H16C	109.5
H8A—C8—H8C	109.5	H16A—C16—H16C	109.5
H8B—C8—H8C	109.5	H16B—C16—H16C	109.5
C7—N1—C1—C2	−22.3 (7)	C15—N2—C9—C10	21.5 (6)
C7—N1—C1—C6	160.8 (4)	C15—N2—C9—C14	−160.2 (4)
N1—C1—C2—C3	−177.9 (4)	C14—C9—C10—C11	0.7 (6)
C6—C1—C2—C3	−1.0 (7)	N2—C9—C10—C11	178.9 (4)
C1—C2—C3—C4	0.4 (7)	C9—C10—C11—C12	−0.5 (7)
C1—C2—C3—Br1	177.6 (3)	C9—C10—C11—Br2	178.0 (3)
C2—C3—C4—C5	−0.4 (8)	C10—C11—C12—C13	0.7 (7)
Br1—C3—C4—C5	−177.6 (4)	Br2—C11—C12—C13	−177.8 (4)
C3—C4—C5—C6	1.0 (8)	C11—C12—C13—C14	−1.1 (7)
C4—C5—C6—C1	−1.7 (8)	C12—C13—C14—C9	1.2 (7)
C2—C1—C6—C5	1.7 (7)	C10—C9—C14—C13	−1.0 (6)
N1—C1—C6—C5	178.7 (4)	N2—C9—C14—C13	−179.4 (4)
C1—N1—C7—O1	−3.1 (8)	C9—N2—C15—O2	2.2 (7)
C1—N1—C7—C8	177.9 (4)	C9—N2—C15—C16	−179.9 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1N···O2^{i}	0.86	2.05	2.887 (5)	166
N2—H2N···O1	0.86	2.10	2.953 (5)	169

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

Fig. 1

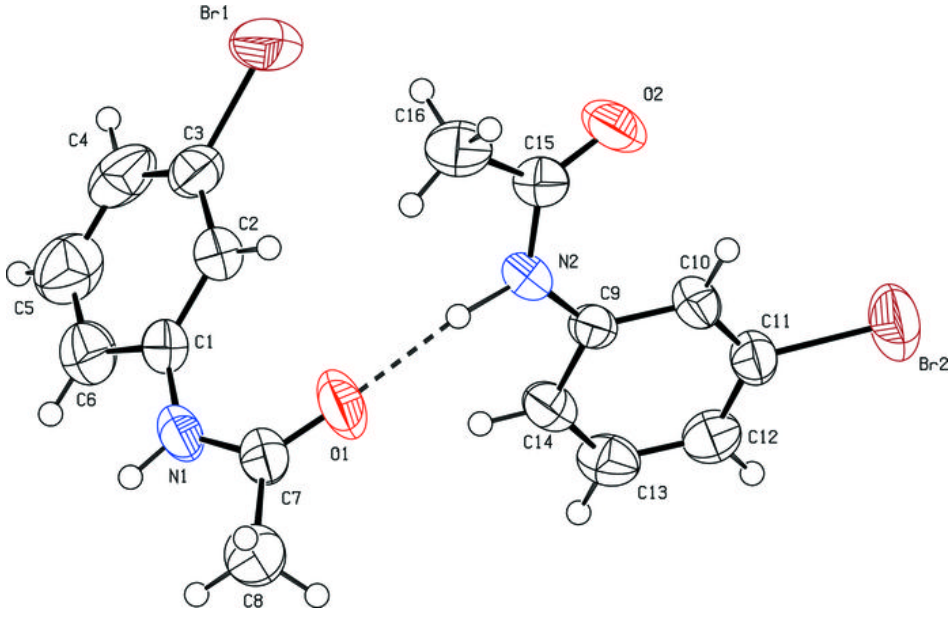
Br1
C4
C3
C2
C5
C1
C6
N1
C7
C8
O1
C16
C15
O2
N2
C9
C10
C11
Br2
C14
C12
C13

Fig. 2