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Crystal structures of three *N*-aryl-2,2,2-tribromoacetamides

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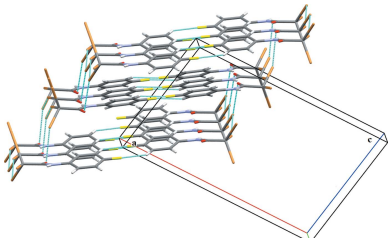
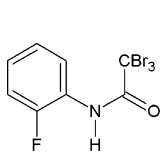
Three *N*-aryl-2,2,2-tribromoacetamides, namely, 2,2,2-tribromo-*N*-(2-fluorophenyl)acetamide, $C_8H_5Br_3FNO$, (I), 2,2,2-tribromo-*N*-[3-(trifluoromethyl)phenyl]acetamide, $C_9H_5Br_3F_3NO$, (II) and 2,2,2-tribromo-*N*-(4-fluorophenyl)acetamide, $C_8H_5Br_3FNO$, (III) were synthesized and their crystal structures were analysed. In the crystal structure of (I), C—Br···π_{aryl} interactions connect the molecules into dimers, which in turn are connected *via* Br···Br contacts [3.6519 (12) Å], leading to the formation of a one-dimensional ladder-type architecture. The crystal structure of (II) features chains linked by N—H···O and C—H···O hydrogen bonds. Two such chains are interlinked to form ribbons through Br···Br [3.6589 (1) Å] and Br···F [3.0290 (1) Å] interactions. C—Br···π_{aryl} and C—F···π_{aryl} interactions between the ribbons extend the supramolecular architecture of (II) from one dimension to two. In (III), the molecules are connected into $R_2^2(8)$ dimers *via* pairs of C—H···F interactions and these dimers form ribbons through Br···Br [3.5253 (1) Å] contacts. The ribbons are further interlinked into columns *via* C—Br···O=C contacts, forming a two-dimensional architecture.

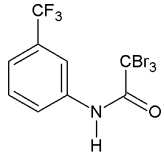
1. Chemical context

N-Aryl-haloamides show a broad spectrum of pharmacological properties, including antibacterial (Manojkumar *et al.*, 2013*a*), antitumor (Abdou *et al.*, 2004), anti-oxidant, analgesic and antiviral activity (Manojkumar *et al.*, 2013*b*). Keeping this in mind, and as a part of our ongoing efforts to understand the effect of the ring substituents on the molecular and crystal structures of *N*-aryl-2,2,2-tribromoacetamides Suchetan *et al.*, 2010) and also to study the role of different halogen interactions in solid-state structures, the crystal structures of three *N*-aryl-2,2,2-tribromoacetamides, namely, 2,2,2-tribromo-*N*-(2-fluorophenyl)acetamide, (I), 2,2,2-tribromo-*N*-[3-(trifluoromethyl)phenyl]acetamide, (II) and 2,2,2-tribromo-*N*-(4-fluorophenyl)acetamide, (III), are discussed here.

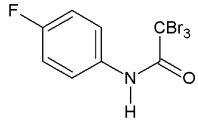




(I)



(II)



(III)

2. Structural commentary

The molecular structures of (I), (II) and (III) are shown in Figs. 1, 2 and 3, respectively.

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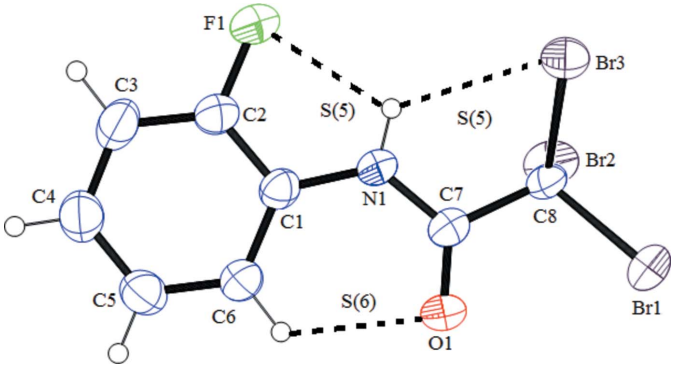

Figure 1
A view of (I), with displacement ellipsoids drawn at the 50% probability level.

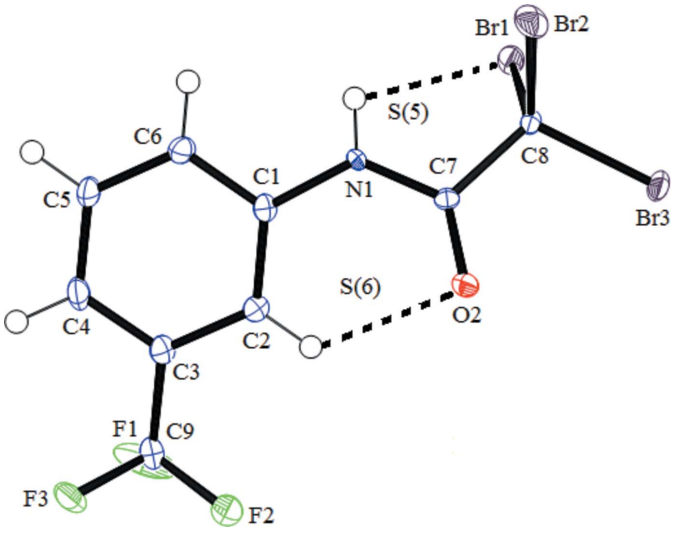

Figure 2
A view of (II), with displacement ellipsoids drawn at the 50% probability level.

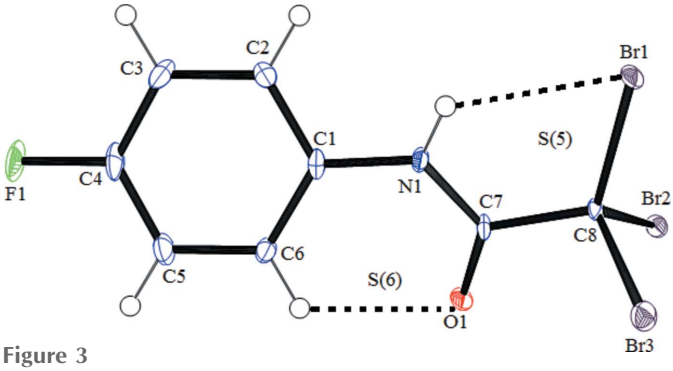

Figure 3
A view of (III), with displacement ellipsoids drawn at the 50% probability level.

In (I), the conformation of the N—H bond is *syn* to the 2-fluoro substituent in the benzene ring, similar to that observed in the crystal structures of other *ortho* substituted compounds (see database survey). Contrast to the above, in (II), the conformation of the N—H bond is *anti* to the 3-CF_3 substituent.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···Br3	0.86	2.56	3.056 (4)	118
N1—H1···F1	0.86	2.26	2.646 (6)	107
C6—H6···O1	0.93	2.32	2.896 (7)	120

Table 2
Hydrogen-bond geometry (Å, °) for (II).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···Br1	0.86	2.78	3.144 (4)	108
C2—H2···O2	0.93	2.34	2.893 (6)	118
N1—H1···O2^{i}	0.86	2.24	3.072 (5)	161
C6—H6···O2^{i}	0.93	2.58	3.357 (5)	142

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

Table 3
Hydrogen-bond geometry (Å, °) for (III).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···Br1	0.86	2.49	3.051 (5)	124
C2—H2···O1	0.93	2.35	2.912 (8)	118
C3—H3···F1^{i}	0.93	2.46	3.308 (8)	151

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

In (I), the dihedral angle between the benzene ring and the C1–N1–C7(O)–C8 segment is 4.2 (3)°, and, the various torsion angles defining the conformation between the benzene ring and the side chain have values closer to either 0 or 180°: C1—N1—C7—O1 = 0.2 (9), C1—N1—C7—C8 = 179.3 (5), C2—C1—N1—C7 = 175.8 (5) and C6—C1—N1—C7 = −4.0 (8)°. The molecule (excluding three bromine atoms) is close to planar, the r.m.s. deviation (excluding H and Br atoms) being 0.031 (1) Å. The planarity is consolidated by three kinds of intramolecular hydrogen bonds, namely, N1—H1···Br3, N1—H1···F1 and C6—H6···O1 (Fig. 1, Table 1).

The dihedral angle between the benzene ring and the C1–N1–C7(O)–C8 segment in (II) is 19.29 (1)°. The torsion angles are C1—N1—C7—O2 = −0.8 (7), C1—N1—C7—C8 = −177.3 (4), C2—C1—N1—C7 = −20.8 (7) and C6—C1—N1—C7 = 161.6 (4)°. These values deviate slightly from 0 or 180°, and thus molecular planarity (excluding three bromine atoms) is not observed, the r.m.s. deviation (excluding H and Br atoms) being 0.159 (1) Å. The structure of (II) features two intramolecular hydrogen bonds, namely, N1—H1···Br1 and C2—H2···O2 (Fig. 2, Table 2).

The dihedral angle between the benzene ring and the C1–N1–C7(O)–C8 segment in (III) is highest among the three compounds, it being 22.5 (3)°. Similar to (II), the molecular structure of (III) features two intramolecular hydrogen bonds, namely, N1—H1···Br1 and C2—H2···O1 (Fig. 3, Table 3). Further, the various torsion angles defining the conformation between the benzene ring and the side chain show that the two are not in a single plane: C1—N1—C7—O1 = 4.2 (9), C1—N1—C7—C8 = −172.4 (5), C2—C1—N1—C7 = 19.8 (9) and C6—C1—N1—C7 = −164.0 (6)°.

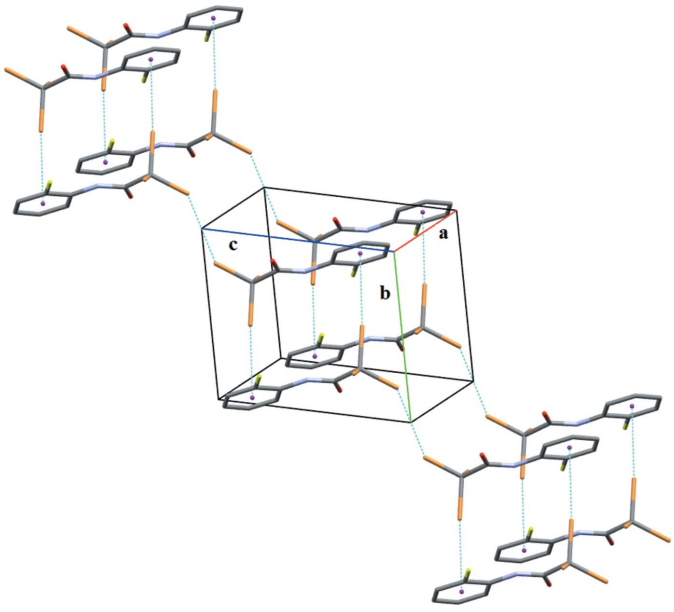

Figure 4
Crystal packing of (I), displaying C—Br···π and Br···Br contacts. H atoms are omitted for clarity.

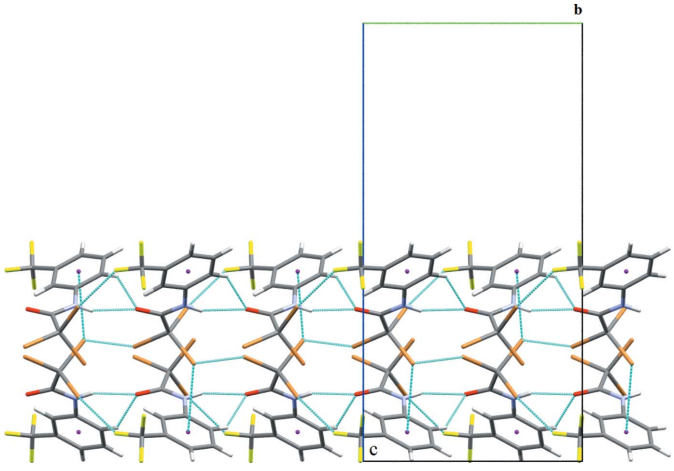

Figure 5
Crystal packing of (II), displaying various interactions of the types N—H···O, C—H···O, C—Br···π and Br···Br.

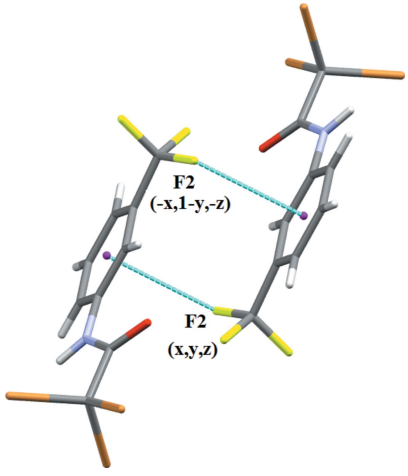

Figure 6
Crystal packing of (II), displaying C—F···π interactions.

Table 4
Halogen contacts in (I).

Cg is the centroid of the C1–C6 aromatic ring.

C—*X*···*Y*	*X*···*Y*	C—*X*···*Y*
C8—Br2···Cg^{i}	3.426 (3)	174.52 (15)
C8—Br1···Br1^{ii}	3.6519 (12)	141.04 (14)

Symmetry codes: (i) $2-x, 1-y, 1-z$; $2-x, 2-y, -z$.

Table 5
Halogen contacts in (II).

Cg is the centroid of the C1–C6 aromatic ring.

C—*X*···*Y*	*X*···*Y*	C—*X*···*Y*
C8—Br1···Cg^{i}	3.7543 (18)	119.96 (13)
C9—F2···Cg^{ii}	3.195 (4)	109.5 (3)
C8—Br1···Br3^{iii}	3.6589 (6)	113.06 (2)
C8—Br2···F2^{iv}	3.0290 (6)	1769.9 (2)

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

Table 6
Halogen contacts in (III).

C—*X*···*Y*	*X*···*Y*	C—*X*···*Y*
C8—Br2···Br1^{i}	3.5254 (9)	158.87 (16)
C8—Br2···O1^{ii}	3.0623 (4)	160.06 (18)

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

3. Supramolecular features

In the crystal structure of (I), C8—Br2···π_{aryl} interactions (Table 4) connect the molecules into dimers and these dimers are in turn connected via Br1···Br1 contacts [3.6519 (12) Å] along the diagonal of the *bc* plane, leading to the formation of a one-dimensional ladder-type architecture (Fig. 4, Table 4). The Br1···Br1 contact has a type I *trans* geometry (Dikundwar *et al.*, 2012) with $\theta_1 = \theta_2 = 141.04\ (14)^\circ$. The crystal structure of (I) does not feature the strong N—H···O hydrogen bonds which are generally observed in amides.

The crystal structure of (II) features molecular chains along [010] formed by N1—H1···O2 and C6—H6···O2 hydrogen bonds (Fig. 5 and Table 2). Two such chains are interlinked to form ribbons through Br1···Br3 [3.6589 (1) Å] and Br2···F2 [3.0290 (1) Å] interactions (Fig. 6, Table 5). C8—Br1···π_{aryl} and C9—F2···π_{aryl} interactions between the ribbons extend the supramolecular architecture of (II) from one dimension to two (Fig. 6, Table 5). The Br···Br contact in (II) is close to a type II halogen···halogen contact (Dikundwar *et al.*, 2012), while, Br···F is a type I *cis* contact.

Quite different to the packing in (I) and (II), the molecules in (III) are connected *via* pairs of C3—H3···F1 interactions (Fig. 7 and Table 3), forming $R_2^2(8)$ dimers. Further, these dimers are connected through Br1···Br2 contacts [3.5253 (1) Å] along the *b* axis, forming ribbons. These ribbons are further interlinked into columns *via* C8—Br2···O1=C7 contacts (Table 6), forming a two-dimensional architecture

Table 7
Comparison of various parameters in the crystal structures of *N*-(aryl)-2,2,2-tribromoacetamides.

Parameters	H	2-F	2-Cl	2-CH_3	3-CF_3	3-Cl	3-CH_3	4-F	4-Cl	4-CH_3
Crystal system	orthorhombic	triclinic	orthorhombic	monoclinic	orthorhombic	orthorhombic	monoclinic	monoclinic	orthorhombic	monoclinic
Z′	1	1	1	2	1	1	2	1	1	2
Intramolecular hydrogen bonds	N—H···Br	N—H···Br, N—H···F, C—H···O	N—H···Br, N—H···Cl	N—H···Br	N—H···Br, C—H···O	N—H···Br	N—H···Br	N—H···Br, C—H···O	N—H···Br	N—H···Br
Orientation of the substituent to the N—H bond	-	*syn*	*syn*	*syn*	*anti*	*anti*	*anti*	-	-	-
Dihedral angle between the benzene ring and the central chain	38.1 (10)	4.2 (3)	40.5 (3)	67.7 (5), 87.2 (5)	19.29 (1)	32.0 (6)	36.2 (5), 52.9 (6)	22.5 (3)	35.1 (5)	22.5 (5), 48.4 (5)
Intermolecular interactions	N—H···O	Br···Br, C—Br···π	-	N—H···O	N—H···O, C—H···O, Br···Br, Br···F, C—Br···π, C—F···π	N—H···O	N—H···O	C—H···F, Br···Br, Br···O	N—H···O	N—H···O
Supramolecular architecture	1D chains	1D chains	0D	1D chains	2D	1D chains	1D chains	2D	1D chains	1D chains

(Fig. 8). The packing in (III) does not features conventional N—H···O hydrogen bonds, similar to (I).

4. Database survey

Seven *N*-aryl-2,2,2-tribromoacetamides, namely, 2,2,2-tribromo-*N*-phenylacetamide, 2,2,2-tribromo-*N*-(2/3/4-chlorophenyl)acetamides and 2,2,2-tribromo-*N*-(2/3/4-methylphenyl)acetamides have been previously reported. Comparison of the crystal systems of these series of compounds show that all the chloro-substituted compounds crystallize in the orthorhombic crystal system, while the methyl-substituted compounds crystallize in the monoclinic system (Table 7). However, such trends are not observed in fluoro-substituted compounds *i.e.* (I) and (III). Further, the asymmetric units of the fluoro- and chloro-substituted compounds contain one molecule, whereas the asymmetric units of the methyl-substituted tribromoacetamides contain two molecules.

In (I), the conformation of the N—H bond is *syn* to the 2-fluoro substituent in the benzene ring, similar to that observed in the crystal structures of 2,2,2-tribromo-*N*-(2-chlorophenyl)acetamide (I*a*) (Gowda *et al.*, 2010*a*) and 2,2,2-tribromo-*N*-(2-methylphenyl)acetamide (I*b*) (Gowda *et al.*, 2010*b*). In contrast to the above, in (II) the conformation of the N—H bond is *anti* to the 3-CF_3 substituent, as observed in the other *meta*-substituted compounds *i.e.* 2,2,2-tribromo-*N*-(3-chlorophenyl)acetamide (I*a*) (Suchetan *et al.*, 2010) and 2,2,2-tribromo-*N*-(3-methylphenyl)acetamide (I*b*) (Gowda *et al.*, 2009*c*). Further, it can be observed that the molecular structure of each of the compounds features intramolecular N—H···Br hydrogen bonds, while the 2-fluoro and 2-chloro derivatives feature additional N—H···*X* (*X* = F or Cl) intramolecular hydrogen bonds. Further, compounds (I), (II) and (III) exhibit C—H···O intramolecular hydrogen bonds which are not displayed in the structures reported in the literature.

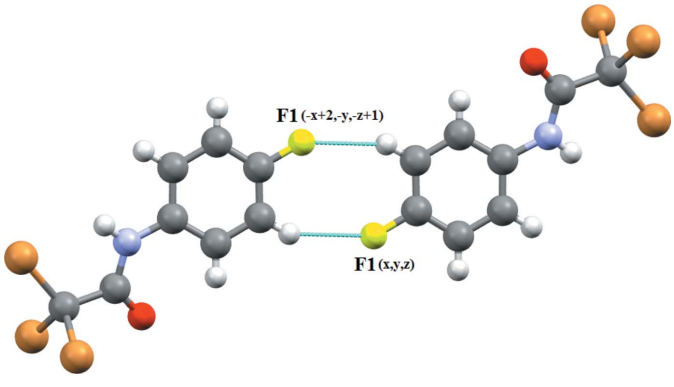

Figure 7
Formation of $R_2^2(8)$ dimers *via* C—H···F interactions in (III).

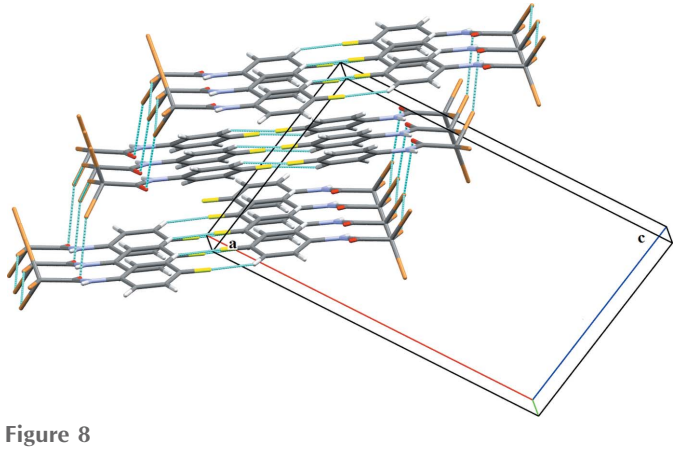

Figure 8
Column-like architecture displayed in (III) *via* Br···Br and Br···O contacts.

Table 8
Experimental details.

	(I)	(II)	(III)
Crystal data			
Chemical formula	$C_8H_5Br_3FNO$	$C_9H_5Br_3F_3NO$	$C_8H_5Br_3FNO$
M_r	389.86	439.87	389.86
Crystal system, space group	Triclinic, $P\overline{1}$	Orthorhombic, *Pbca*	Monoclinic, $P2_1/c$
Temperature (K)	296	100	100
a, b, c (Å)	6.1825 (13), 8.929 (2), 9.971 (2)	11.3441 (6), 10.3047 (6), 20.6397 (11)	16.9830 (9), 6.1095 (3), 10.1508 (6)
α, β, γ (°)	85.858 (8), 87.966 (8), 78.919 (8)	90, 90, 90	90, 100.485 (1), 90
V (Å^3)	538.6 (2)	2412.7 (2)	1035.64 (10)
Z	2	8	4
Radiation type	Cu $K\alpha$	Cu $K\alpha$	Cu $K\alpha$
μ (mm^{-1})	13.77	12.66	14.33
Crystal size (mm)	0.28 × 0.24 × 0.22	0.30 × 0.27 × 0.25	0.31 × 0.26 × 0.22
Data collection			
Diffractometer	Bruker APEXII	Bruker APEXII	Bruker APEXII
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)	Multi-scan (*SADABS*; Bruker, 2009)	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.048, 0.053	0.116, 0.144	0.029, 0.043
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	4683, 1549, 1485	11524, 1978, 1967	6934, 1674, 1664
R_{int}	0.051	0.054	0.054
θ_{max} (°)	60.0	64.5	64.3
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.562	0.585	0.584
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.045, 0.120, 1.10	0.040, 0.102, 1.22	0.047, 0.128, 1.19
No. of reflections	1549	1978	1674
No. of parameters	128	154	127
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.96, −0.60	0.96, −0.81	1.48, −1.01

Computer programs: *APEX2*, *SAINT-Plus* and *XPREP* (Bruker, 2009), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2008).

A comparison of the dihedral angle between the benzene ring and the C1–N1–C7(O)–C8 segment in all of the compounds shows that the dihedral angles in the fluoro-substituted compounds are smaller than those observed in chloro-substituted ones, which in turn have smaller values than the methyl-substituted tribromoacetamides (Table 7). The dihedral angle in the parent (*i.e.* unsubstituted) compound is closer to those of chloro-substituted ones, thus the order is F < Cl(═H) < CH_3.

The crystal structures of all of the seven compounds [except (I*a*)] reported in the literature feature strong N—H···O hydrogen bonds leading into *C*(4) chains forming a one-dimensional architecture. Compound (I*a*) (2-chloro derivative) does not exhibit any conventional intermolecular interactions and therefore exhibits a zero-dimensional supramolecular architecture. However, the packing of molecules in the three structures reported here are very different and are controlled by interactions mainly involving the halogen atoms.

5. Synthesis and crystallization

All three compounds were prepared according to a literature method (Gowda *et al.*, 2003). The purity of the compounds was checked by determining the melting points. Single crystals of all the compounds used for X-ray diffraction studies were obtained by slow evaporation of an ethanolic solutions of the compound at room temperature.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 8. H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 Å and N—H = 0.86 Å, and with U_{iso}(H) = 1.2U_{eq}(C,N).

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supporting information

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Crystal structures of three *N*-aryl-2,2,2-tribromoacetamides

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Computing details

For all compounds, data collection: *APEX2* (Bruker, 2009); cell refinement: *APEX2* and *SAINT-Plus* (Bruker, 2009); data reduction: *SAINT-Plus* and *XPREP* (Bruker, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

(I) 2,2,2-Tribromo-*N*-(2-fluorophenyl)acetamide

Crystal data

$C_8H_5Br_3FNO$
M_r = 389.86
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 6.1825 (13) Å
b = 8.929 (2) Å
c = 9.971 (2) Å
α = 85.858 (8)°
β = 87.966 (8)°
γ = 78.919 (8)°
V = 538.6 (2) Å^3
Z = 2
$F(000)$ = 364
Prism
D_x = 2.404 Mg m^{-3}
Melting point: 403 K
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 123 reflections
θ = 7.3–60.0°
μ = 13.77 mm^{-1}
T = 296 K
Prism, colourless
0.28 × 0.24 × 0.22 mm

Data collection

Bruker APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and φ scans
Absorption correction: multi-scan (SADABS; Bruker, 2009)
T_{min} = 0.048, T_{max} = 0.053
4683 measured reflections
1549 independent reflections
1485 reflections with $I > 2\sigma(I)$
R_{int} = 0.051
θ_{max} = 60.0°, θ_{min} = 7.3°
h = −6→6
k = −10→10
l = −11→10
1 standard reflections every 1 reflections
intensity decay: 0.1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.120
S = 1.10
1549 reflections
128 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.073P)^2 + 0.4735P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.96$ e Å^{-3}
$\Delta\rho_{min} = -0.60$ e Å^{-3}
Extinction correction: SHELXL, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0074 (12)

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
F1	0.3498 (7)	0.6456 (4)	0.5450 (4)	0.0760 (11)
C2	0.4528 (10)	0.7432 (6)	0.6065 (5)	0.0501 (12)
C1	0.6308 (9)	0.7870 (5)	0.5395 (5)	0.0429 (11)
C6	0.7390 (10)	0.8852 (6)	0.6027 (5)	0.0536 (13)
H6	0.8603	0.9181	0.5613	0.064*
C5	0.6636 (11)	0.9331 (6)	0.7277 (5)	0.0569 (14)
H5	0.7358	0.9984	0.7698	0.068*
C4	0.4852 (11)	0.8866 (7)	0.7908 (6)	0.0607 (14)
H4	0.4378	0.9204	0.8748	0.073*
C3	0.3764 (11)	0.7905 (7)	0.7305 (6)	0.0614 (15)
H3	0.2547	0.7583	0.7722	0.074*
N1	0.6900 (8)	0.7303 (5)	0.4129 (4)	0.0487 (10)
H1	0.6157	0.6658	0.3871	0.058*
C7	0.8475 (8)	0.7644 (5)	0.3276 (5)	0.0430 (11)
O1	0.9690 (8)	0.8512 (5)	0.3453 (4)	0.0735 (14)
C8	0.8737 (8)	0.6801 (5)	0.1956 (5)	0.0410 (11)
Br1	0.99546 (11)	0.80114 (7)	0.05528 (5)	0.0602 (3)
Br2	1.07967 (10)	0.48905 (6)	0.23436 (7)	0.0669 (3)
Br3	0.60118 (10)	0.63535 (7)	0.13471 (6)	0.0600 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.073 (2)	0.089 (2)	0.081 (2)	−0.049 (2)	0.0223 (19)	−0.0244 (19)
C2	0.054 (3)	0.045 (3)	0.055 (3)	−0.019 (2)	0.003 (2)	−0.003 (2)
C1	0.047 (3)	0.041 (2)	0.040 (2)	−0.010 (2)	0.001 (2)	0.0047 (19)
C6	0.065 (4)	0.053 (3)	0.047 (3)	−0.023 (3)	0.004 (2)	0.001 (2)
C5	0.070 (4)	0.053 (3)	0.050 (3)	−0.018 (3)	−0.008 (3)	−0.005 (2)
C4	0.073 (4)	0.057 (3)	0.051 (3)	−0.011 (3)	0.009 (3)	−0.005 (2)
C3	0.063 (4)	0.058 (3)	0.061 (3)	−0.012 (3)	0.023 (3)	−0.003 (3)

N1	0.057 (3)	0.048 (2)	0.048 (2)	−0.026 (2)	0.009 (2)	−0.0048 (17)
C7	0.041 (3)	0.042 (3)	0.046 (2)	−0.012 (2)	0.000 (2)	0.0031 (19)
O1	0.078 (3)	0.096 (3)	0.064 (2)	−0.060 (3)	0.017 (2)	−0.022 (2)
C8	0.033 (2)	0.046 (3)	0.046 (2)	−0.0129 (19)	0.0032 (19)	−0.001 (2)
Br1	0.0689 (5)	0.0687 (5)	0.0477 (4)	−0.0297 (3)	0.0123 (3)	0.0032 (3)
Br2	0.0537 (5)	0.0484 (5)	0.0950 (6)	−0.0024 (3)	−0.0021 (3)	−0.0005 (3)
Br3	0.0455 (5)	0.0839 (5)	0.0573 (5)	−0.0263 (3)	−0.0035 (3)	−0.0095 (3)

Geometric parameters (Å, º)

F1—C2	1.363 (6)	C4—H4	0.9300
C2—C3	1.374 (8)	C3—H3	0.9300
C2—C1	1.373 (8)	N1—C7	1.334 (6)
C1—C6	1.396 (7)	N1—H1	0.8600
C1—N1	1.405 (6)	C7—O1	1.204 (6)
C6—C5	1.382 (8)	C7—C8	1.551 (7)
C6—H6	0.9300	C8—Br1	1.927 (4)
C5—C4	1.369 (9)	C8—Br3	1.932 (5)
C5—H5	0.9300	C8—Br2	1.946 (5)
C4—C3	1.370 (9)		
F1—C2—C3	119.2 (5)	C2—C3—C4	117.8 (6)
F1—C2—C1	116.9 (5)	C2—C3—H3	121.1
C3—C2—C1	123.9 (5)	C4—C3—H3	121.1
C2—C1—C6	117.3 (5)	C7—N1—C1	127.9 (4)
C2—C1—N1	117.8 (5)	C7—N1—H1	116.1
C6—C1—N1	124.9 (5)	C1—N1—H1	116.1
C5—C6—C1	119.2 (5)	O1—C7—N1	126.1 (5)
C5—C6—H6	120.4	O1—C7—C8	118.7 (4)
C1—C6—H6	120.4	N1—C7—C8	115.3 (4)
C4—C5—C6	121.5 (5)	C7—C8—Br1	109.6 (3)
C4—C5—H5	119.2	C7—C8—Br3	113.7 (3)
C6—C5—H5	119.2	Br1—C8—Br3	108.8 (2)
C5—C4—C3	120.2 (5)	C7—C8—Br2	105.9 (3)
C5—C4—H4	119.9	Br1—C8—Br2	109.6 (2)
C3—C4—H4	119.9	Br3—C8—Br2	109.1 (2)
F1—C2—C1—C6	−179.1 (5)	C2—C1—N1—C7	175.8 (5)
C3—C2—C1—C6	0.1 (8)	C6—C1—N1—C7	−4.0 (8)
F1—C2—C1—N1	1.0 (7)	C1—N1—C7—O1	0.2 (9)
C3—C2—C1—N1	−179.7 (5)	C1—N1—C7—C8	179.3 (5)
C2—C1—C6—C5	0.0 (8)	O1—C7—C8—Br1	−27.4 (6)
N1—C1—C6—C5	179.8 (5)	N1—C7—C8—Br1	153.5 (4)
C1—C6—C5—C4	−0.1 (9)	O1—C7—C8—Br3	−149.4 (5)
C6—C5—C4—C3	0.0 (9)	N1—C7—C8—Br3	31.5 (5)
F1—C2—C3—C4	179.0 (6)	O1—C7—C8—Br2	90.8 (5)
C1—C2—C3—C4	−0.2 (9)	N1—C7—C8—Br2	−88.3 (4)
C5—C4—C3—C2	0.2 (9)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···Br3	0.86	2.56	3.056 (4)	118
N1—H1···F1	0.86	2.26	2.646 (6)	107
C6—H6···O1	0.93	2.32	2.896 (7)	120

(II) 2,2,2-Tribromo-*N*-[3-(trifluoromethyl)phenyl]acetamide

Crystal data

$C_9H_5Br_3F_3NO$
M_r = 439.87
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
a = 11.3441 (6) Å
b = 10.3047 (6) Å
c = 20.6397 (11) Å
V = 2412.7 (2) Å^3
Z = 8
F(000) = 1648
Prism
D_x = 2.422 Mg m^{-3}
Melting point: 425 K
Cu *Kα* radiation, λ = 1.54178 Å
Cell parameters from 145 reflections
θ = 5.8–64.5°
μ = 12.66 mm^{-1}
T = 100 K
Prism, colourless
0.30 × 0.27 × 0.25 mm

Data collection

Bruker APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and φ scans
Absorption correction: multi-scan (SADABS; Bruker, 2009)
T_{min} = 0.116, T_{max} = 0.144
11524 measured reflections
1978 independent reflections
1967 reflections with $I > 2\sigma(I)$
R_{int} = 0.054
θ_{max} = 64.5°, θ_{min} = 5.8°
h = −13→13
k = −11→6
l = −23→24
1 standard reflections every 1 reflections
intensity decay: 0.1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.102
S = 1.22
1978 reflections
154 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0569P)^2 + 5.8187P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.96 e Å^{-3}
$\Delta\rho_{min}$ = −0.81 e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.82269 (4)	0.22572 (4)	0.72340 (2)	0.01621 (19)
Br2	0.97513 (4)	0.19720 (5)	0.85195 (2)	0.0197 (2)
Br3	0.93377 (4)	−0.04340 (4)	0.76175 (2)	0.0208 (2)
F1	0.2435 (3)	−0.0016 (4)	0.89656 (15)	0.0418 (9)
F2	0.3744 (3)	−0.1282 (3)	0.93617 (17)	0.0340 (8)
F3	0.2658 (2)	−0.0138 (3)	0.99878 (14)	0.0237 (6)
N1	0.6923 (3)	0.1851 (4)	0.85629 (17)	0.0120 (8)
H1	0.7205	0.2589	0.8445	0.014*
O2	0.7243 (3)	−0.0319 (3)	0.84716 (15)	0.0149 (7)
C4	0.3873 (4)	0.2127 (4)	0.9709 (2)	0.0172 (10)
H4	0.3194	0.2210	0.9959	0.021*
C3	0.4123 (4)	0.0974 (4)	0.9396 (2)	0.0131 (9)
C2	0.5142 (4)	0.0835 (4)	0.9018 (2)	0.0118 (8)
H2	0.5306	0.0054	0.8811	0.014*
C1	0.5903 (4)	0.1887 (4)	0.8958 (2)	0.0113 (8)
C7	0.7500 (4)	0.0795 (4)	0.83513 (19)	0.0102 (8)
C8	0.8624 (4)	0.1125 (4)	0.7951 (2)	0.0120 (8)
C9	0.3251 (4)	−0.0103 (5)	0.9422 (2)	0.0160 (9)
C5	0.4656 (4)	0.3166 (5)	0.9645 (2)	0.0169 (9)
H5	0.4501	0.3945	0.9856	0.020*
C6	0.5654 (4)	0.3043 (4)	0.9272 (2)	0.0150 (9)
H6	0.6167	0.3742	0.9231	0.018*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0198 (3)	0.0158 (3)	0.0130 (3)	0.00137 (17)	0.00429 (17)	0.00239 (17)
Br2	0.0118 (3)	0.0246 (3)	0.0226 (3)	−0.00234 (18)	−0.00244 (17)	−0.00310 (19)
Br3	0.0237 (3)	0.0121 (3)	0.0265 (3)	0.00441 (18)	0.0140 (2)	−0.00061 (18)
F1	0.0314 (17)	0.062 (2)	0.0323 (17)	−0.0301 (16)	−0.0199 (14)	0.0239 (17)
F2	0.0258 (16)	0.0208 (16)	0.055 (2)	−0.0061 (12)	0.0192 (14)	−0.0077 (14)
F3	0.0226 (14)	0.0253 (15)	0.0230 (14)	−0.0085 (12)	0.0105 (12)	−0.0016 (11)
N1	0.0119 (18)	0.0095 (18)	0.0147 (18)	−0.0009 (14)	0.0072 (14)	−0.0002 (14)
O2	0.0131 (16)	0.0123 (17)	0.0194 (15)	−0.0004 (12)	0.0038 (12)	0.0026 (12)
C4	0.015 (2)	0.019 (2)	0.018 (2)	0.0045 (18)	0.0053 (18)	−0.0009 (18)
C3	0.011 (2)	0.015 (2)	0.014 (2)	0.0036 (17)	−0.0014 (16)	0.0017 (17)
C2	0.011 (2)	0.012 (2)	0.013 (2)	0.0016 (16)	−0.0032 (16)	0.0004 (17)
C1	0.0088 (19)	0.013 (2)	0.012 (2)	0.0034 (16)	−0.0024 (17)	0.0012 (16)
C7	0.010 (2)	0.010 (2)	0.0104 (19)	−0.0016 (16)	−0.0014 (16)	−0.0004 (16)
C8	0.013 (2)	0.009 (2)	0.0146 (19)	0.0019 (17)	0.0038 (17)	0.0000 (17)
C9	0.015 (2)	0.019 (2)	0.015 (2)	0.0023 (18)	0.0028 (17)	−0.0012 (18)
C5	0.013 (2)	0.015 (2)	0.023 (2)	0.0031 (18)	0.0032 (18)	−0.0044 (19)
C6	0.013 (2)	0.012 (2)	0.020 (2)	0.0017 (16)	0.0001 (18)	0.0004 (18)

Geometric parameters (Å, º)

Br1—C8	1.938 (4)	C4—C5	1.397 (7)
Br2—C8	1.943 (4)	C4—H4	0.9300
Br3—C8	1.926 (4)	C3—C2	1.402 (6)
F1—C9	1.324 (5)	C3—C9	1.488 (7)
F2—C9	1.343 (6)	C2—C1	1.391 (6)
F3—C9	1.348 (5)	C2—H2	0.9300
N1—C7	1.343 (6)	C1—C6	1.386 (6)
N1—C1	1.416 (6)	C7—C8	1.557 (6)
N1—H1	0.8600	C5—C6	1.376 (7)
O2—C7	1.211 (5)	C5—H5	0.9300
C4—C3	1.383 (7)	C6—H6	0.9300
C7—N1—C1	127.3 (4)	C7—C8—Br3	110.6 (3)
C7—N1—H1	116.3	C7—C8—Br1	110.2 (3)
C1—N1—H1	116.3	Br3—C8—Br1	109.1 (2)
C3—C4—C5	118.9 (4)	C7—C8—Br2	108.5 (3)
C3—C4—H4	120.5	Br3—C8—Br2	108.3 (2)
C5—C4—H4	120.5	Br1—C8—Br2	110.1 (2)
C4—C3—C2	121.2 (4)	F1—C9—F2	106.6 (4)
C4—C3—C9	119.2 (4)	F1—C9—F3	105.6 (3)
C2—C3—C9	119.5 (4)	F2—C9—F3	105.3 (4)
C1—C2—C3	118.8 (4)	F1—C9—C3	112.8 (4)
C1—C2—H2	120.6	F2—C9—C3	113.2 (4)
C3—C2—H2	120.6	F3—C9—C3	112.5 (4)
C6—C1—C2	120.1 (4)	C6—C5—C4	120.4 (4)
C6—C1—N1	117.3 (4)	C6—C5—H5	119.8
C2—C1—N1	122.6 (4)	C4—C5—H5	119.8
O2—C7—N1	125.8 (4)	C5—C6—C1	120.6 (4)
O2—C7—C8	120.8 (4)	C5—C6—H6	119.7
N1—C7—C8	113.3 (4)	C1—C6—H6	119.7
C5—C4—C3—C2	−0.1 (7)	N1—C7—C8—Br1	−55.4 (4)
C5—C4—C3—C9	−175.5 (4)	O2—C7—C8—Br2	−111.5 (4)
C4—C3—C2—C1	−0.4 (6)	N1—C7—C8—Br2	65.2 (4)
C9—C3—C2—C1	175.1 (4)	C4—C3—C9—F1	85.9 (5)
C3—C2—C1—C6	0.5 (6)	C2—C3—C9—F1	−89.7 (5)
C3—C2—C1—N1	−177.1 (4)	C4—C3—C9—F2	−152.9 (4)
C7—N1—C1—C6	161.6 (4)	C2—C3—C9—F2	31.6 (6)
C7—N1—C1—C2	−20.8 (7)	C4—C3—C9—F3	−33.6 (6)
C1—N1—C7—O2	−0.8 (7)	C2—C3—C9—F3	150.9 (4)
C1—N1—C7—C8	−177.3 (4)	C3—C4—C5—C6	0.5 (7)
O2—C7—C8—Br3	7.2 (5)	C4—C5—C6—C1	−0.4 (7)
N1—C7—C8—Br3	−176.1 (3)	C2—C1—C6—C5	−0.1 (7)
O2—C7—C8—Br1	127.9 (4)	N1—C1—C6—C5	177.6 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···Br1	0.86	2.78	3.144 (4)	108
C2—H2···O2	0.93	2.34	2.893 (6)	118
N1—H1···O2^{i}	0.86	2.24	3.072 (5)	161
C6—H6···O2^{i}	0.93	2.58	3.357 (5)	142

Symmetry code: (i) −*x*+3/2, *y*+1/2, *z*.

(III) 2,2,2-Tribromo-*N*-(4-fluorophenyl)acetamide

Crystal data

$C_8H_5Br_3FNO$
M_r = 389.86
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 16.9830 (9) Å
b = 6.1095 (3) Å
c = 10.1508 (6) Å
β = 100.485 (1)°
V = 1035.64 (10) Å^3
Z = 4
F(000) = 728

Prism
D_x = 2.500 Mg m^{-3}
Melting point: 434 K
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 133 reflections
θ = 5.3–64.3°
μ = 14.33 mm^{-1}
T = 100 K
Prism, colourless
0.31 × 0.26 × 0.22 mm

Data collection

Bruker APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and φ scans
Absorption correction: multi-scan (SADABS; Bruker, 2009)
T_{min} = 0.029, T_{max} = 0.043
6934 measured reflections

1674 independent reflections
1664 reflections with $I > 2\sigma(I)$
R_{int} = 0.054
θ_{max} = 64.3°, θ_{min} = 5.3°
h = −19→19
k = −4→7
l = −11→11
1 standard reflections every 1 reflections
intensity decay: 0.1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.128
S = 1.19
1674 reflections
127 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0755P)^2 + 4.744P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.48 e Å^{-3}
$\Delta\rho_{min}$ = −1.01 e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.8156 (3)	0.2042 (11)	0.7648 (6)	0.0142 (12)
C2	0.8352 (4)	0.0287 (10)	0.6916 (6)	0.0152 (12)
H2	0.8084	−0.1037	0.6933	0.018*
C3	0.8953 (4)	0.0494 (11)	0.6151 (7)	0.0219 (14)
H3	0.9094	−0.0684	0.5662	0.026*
C4	0.9331 (4)	0.2482 (12)	0.6135 (6)	0.0218 (14)
C5	0.9147 (4)	0.4249 (11)	0.6834 (7)	0.0199 (14)
H5	0.9414	0.5570	0.6801	0.024*
C6	0.8548 (4)	0.4041 (11)	0.7601 (6)	0.0174 (13)
H6	0.8409	0.5233	0.8081	0.021*
C7	0.7195 (3)	0.0190 (10)	0.8844 (6)	0.0127 (12)
C8	0.6445 (3)	0.0612 (9)	0.9497 (6)	0.0116 (12)
N1	0.7536 (3)	0.1979 (9)	0.8401 (5)	0.0138 (10)
H1	0.7353	0.3224	0.8602	0.017*
O1	0.7404 (3)	−0.1693 (7)	0.8719 (4)	0.0183 (9)
F1	0.9926 (2)	0.2668 (7)	0.5404 (4)	0.0319 (10)
Br1	0.62345 (4)	0.36497 (10)	0.98592 (6)	0.0175 (3)
Br2	0.65806 (4)	−0.10117 (10)	1.11533 (6)	0.0141 (3)
Br3	0.55374 (3)	−0.05639 (11)	0.82576 (6)	0.0182 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.010 (3)	0.022 (3)	0.012 (3)	0.001 (2)	0.005 (2)	0.003 (3)
C2	0.014 (3)	0.011 (3)	0.022 (3)	0.001 (2)	0.009 (2)	0.003 (3)
C3	0.023 (3)	0.021 (4)	0.026 (3)	0.004 (3)	0.016 (3)	0.001 (3)
C4	0.015 (3)	0.028 (4)	0.027 (3)	0.007 (3)	0.014 (3)	0.008 (3)
C5	0.016 (3)	0.017 (3)	0.029 (4)	−0.003 (2)	0.008 (3)	0.006 (3)
C6	0.017 (3)	0.019 (3)	0.018 (3)	−0.002 (2)	0.007 (2)	−0.005 (2)
C7	0.010 (3)	0.016 (3)	0.014 (3)	0.000 (2)	0.008 (2)	0.001 (2)
C8	0.009 (3)	0.008 (3)	0.020 (3)	0.003 (2)	0.008 (2)	0.001 (2)
N1	0.014 (2)	0.010 (3)	0.021 (3)	0.0011 (19)	0.011 (2)	0.003 (2)
O1	0.022 (2)	0.008 (2)	0.029 (2)	0.0023 (17)	0.0151 (18)	−0.0017 (18)
F1	0.027 (2)	0.032 (2)	0.045 (2)	0.0015 (17)	0.0296 (18)	0.008 (2)
Br1	0.0218 (4)	0.0085 (4)	0.0261 (4)	0.0034 (2)	0.0147 (3)	0.0002 (2)
Br2	0.0184 (4)	0.0110 (4)	0.0144 (4)	0.0008 (2)	0.0073 (3)	0.0016 (2)
Br3	0.0118 (4)	0.0235 (4)	0.0193 (4)	0.0000 (2)	0.0027 (3)	−0.0035 (3)

Geometric parameters (Å, º)

C1—C2	1.379 (9)	C5—H5	0.9300
C1—C6	1.396 (9)	C6—H6	0.9300
C1—N1	1.410 (7)	C7—O1	1.218 (8)
C2—C3	1.397 (9)	C7—N1	1.352 (8)
C2—H2	0.9300	C7—C8	1.560 (7)
C3—C4	1.375 (10)	C8—Br2	1.929 (6)
C3—H3	0.9300	C8—Br1	1.938 (6)
C4—C5	1.359 (10)	C8—Br3	1.942 (6)
C4—F1	1.363 (7)	N1—H1	0.8600
C5—C6	1.395 (9)		
C2—C1—C6	119.9 (5)	C5—C6—C1	119.9 (6)
C2—C1—N1	123.3 (6)	C5—C6—H6	120.0
C6—C1—N1	116.7 (5)	C1—C6—H6	120.0
C1—C2—C3	120.1 (6)	O1—C7—N1	125.4 (5)
C1—C2—H2	119.9	O1—C7—C8	118.5 (5)
C3—C2—H2	119.9	N1—C7—C8	116.1 (5)
C4—C3—C2	118.4 (6)	C7—C8—Br2	107.9 (4)
C4—C3—H3	120.8	C7—C8—Br1	115.6 (4)
C2—C3—H3	120.8	Br2—C8—Br1	108.9 (3)
C5—C4—F1	118.8 (6)	C7—C8—Br3	106.1 (4)
C5—C4—C3	122.9 (6)	Br2—C8—Br3	109.2 (3)
F1—C4—C3	118.3 (6)	Br1—C8—Br3	109.0 (3)
C4—C5—C6	118.7 (6)	C7—N1—C1	127.6 (5)
C4—C5—H5	120.7	C7—N1—H1	116.2
C6—C5—H5	120.7	C1—N1—H1	116.2
C6—C1—C2—C3	1.3 (9)	O1—C7—C8—Br2	50.5 (6)
N1—C1—C2—C3	177.4 (6)	N1—C7—C8—Br2	−132.8 (4)
C1—C2—C3—C4	−0.8 (10)	O1—C7—C8—Br1	172.6 (4)
C2—C3—C4—C5	0.1 (10)	N1—C7—C8—Br1	−10.6 (7)
C2—C3—C4—F1	179.0 (6)	O1—C7—C8—Br3	−66.5 (6)
F1—C4—C5—C6	−178.8 (6)	N1—C7—C8—Br3	110.3 (5)
C3—C4—C5—C6	0.0 (10)	O1—C7—N1—C1	4.2 (9)
C4—C5—C6—C1	0.5 (10)	C8—C7—N1—C1	−172.4 (5)
C2—C1—C6—C5	−1.2 (9)	C2—C1—N1—C7	19.8 (9)
N1—C1—C6—C5	−177.5 (6)	C6—C1—N1—C7	−164.0 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···Br1	0.86	2.49	3.051 (5)	124
C2—H2···O1	0.93	2.35	2.912 (8)	118
C3—H3···F1^{i}	0.93	2.46	3.308 (8)	151

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