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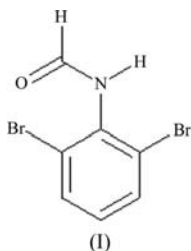
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In the crystal structure of the title compound, $C_7H_5Br_2NO$, molecules related by translation are linked through $N-H\cdots O$ hydrogen bonds to form chains in the crystallographic a direction, with the aryl rings stacked parallel to each other along the chain. Besides the $N-H\cdots O$ hydrogen bonds, $Br\cdots O$ and $Br\cdots Br$ intermolecular interactions complete the packing of molecules in the crystal structure.

Comment

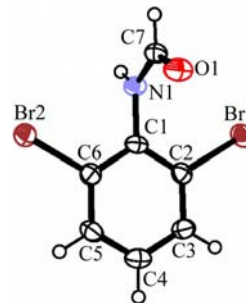
The title compound, (I) (Fig. 1), is of interest as part of a study on polymorphism and phase transformations in 2,6-disubstituted *N*-phenylformamides. Previous reports showed the effect of different interactions ($N-H\cdots O$ hydrogen bonds and $C-H\cdots O$, $Cl\cdots Cl$ and $\pi-\pi$ intermolecular interactions) on the phase transitions of 2-chloro-6-methyl-*N*-phenylformamide (Omondi *et al.*, 2005). 2,6-Dibromo-*N*-phenylformamide is only the second among the 2,6-disubstituted *N*-phenylformamides that has a chiral crystal structure. Another example of an *N*-phenylformamide which is chiral in the crystalline state is 4-bromo-2,6-difluoro-*N*-phenylformamide [Cambridge Structural Database (Allen, 2002) refcode SEDGAJ; Ferguson *et al.*, 1998]. In this paper, $N-H\cdots O$, $Br\cdots Br$ and $Br\cdots O$ intermolecular interactions are discussed.



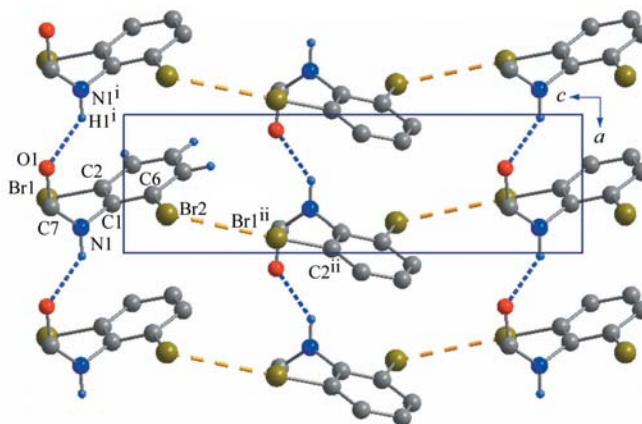
Molecules of compound (I) are linked through $N-H\cdots O$ hydrogen bonds, forming chains that run along the crystallographic a direction. The molecules in the chains are related by translation, with the aryl rings along the chain stacked

parallel to each other. Connecting pairs of adjacent $N-H\cdots O$ hydrogen-bonded chains separated by a one-half unit-cell translation in the crystallographic b direction are $Br\cdots O$ interactions [Kubicki, 2004, and references therein; $Br2\cdots O1(x + \frac{1}{2}, -y + \frac{3}{2}, -z + 2) = 3.100(3) \text{ \AA}$] between molecules related by a 2_1 screw axis along the a axis, and in the crystallographic c direction, intermolecular $Br\cdots Br$ interactions [$Br2\cdots Br1(-x + \frac{3}{2}, -y + 1, z - \frac{1}{2}) = 3.5268(7) \text{ \AA}$] (Fig. 2), also between molecules related by a 2_1 screw axis, along the c axis. Two $Br\cdots O$ intermolecular interactions and the $N-H\cdots O$ hydrogen bond form a ring between adjacent hydrogen-bonded chains described by graph-set motif $R_3^2(12)$ (Etter, 1990; Bernstein *et al.*, 1995).

Atom Br2 is involved in two intermolecular interactions (Fig. 3). It has been reported that the Br atom is frequently involved in such contacts as a result of its nonspherical shape (Lieberman *et al.*, 2000; Lommerse *et al.*, 1996; Beyer *et al.*, 2001). Atom Br2 of (I) interacts with atom O1 in the molecule at $(x + \frac{1}{2}, -y + \frac{3}{2}, -z + 2)$ head-on and with atom Br1 in the molecule at $(-x + \frac{3}{2}, -y + 1, z - \frac{1}{2})$ side-on (O being a nucleophile and Br an electrophile). Similar interactions were

**Figure 1**

A view of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

**Figure 2**

$N1-H1\cdots O1$ hydrogen-bonded chains (short-dashed lines) in (I), showing the stacking relationship in each chain. Molecules along the chain are related by a unit-cell translation. Long-dashed lines show intermolecular $Br1\cdots Br2$ interactions that link up the hydrogen-bonded chains. [Symmetry codes: (i) $-1 + x, y, z$; (ii) $\frac{3}{2} - x, 1 - y, -\frac{1}{2} + z$.]

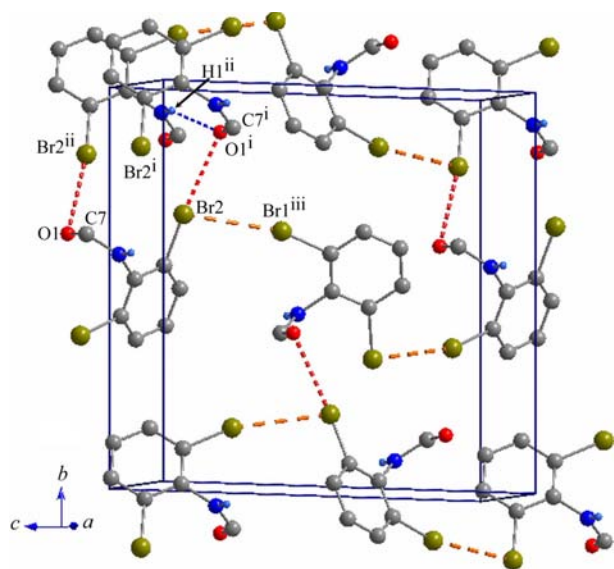


Figure 3

A perspective view of compound (I), showing intermolecular Br1...O interactions as short-dashed lines and intermolecular Br1...Br2 interactions as long-dashed lines. The Br...O interactions, together with N—H...O interactions, form an R_3^3 ring. [Symmetry codes: (i) $\frac{1}{2} + x, \frac{3}{2} - y, 2 - z$; (ii) $-\frac{1}{2} + x, \frac{3}{2} - y, 2 - z$; (iii) $\frac{3}{2} - x, 1 - y, -\frac{1}{2} + z$.]

observed in the crystal structures of 2,3,6,7-tetrabromonaphthalene (space group $P2_1/c$) and the cocrystal of 2,3,6,7-tetrabromonaphthalene and bromobenzene (Navon *et al.*, 1997).

Although compound (I) has the same hydrogen-bonded chains as the high-temperature forms of 2,6-dichloro-*N*-phenylformamide and 2-chloro-6-methyl-*N*-phenylformamide, and of 2,6-dimethyl-*N*-phenylformamide (Omondi *et al.*, 2005), in which they all have one short axis of about 4 Å along which the formamide molecules are stacked along the N—H...O hydrogen-bonded chain (Fig. 2), the packing in (I) is similar only to that in 2,6-dichloro-*N*-phenylformamide, where the N—H...O hydrogen-bonded chains in the high-temperature form are connected through Cl...Cl contacts forming (010) sheets.

Using the *OPIX* suite of programs (Gavezzotti, 2003), the lattice energy of (I) was calculated to be $-90.5 \text{ kJ mol}^{-1}$. These calculations permitted estimation of the contributions to this energy of the intermolecular N—H...O, Br...O and Br...Br interactions as -40 , -9.5 and -8.1 kJ mol^{-1} , respectively. This energy pattern resembles that for the high-temperature forms of 2,6-dichloro-*N*-phenylformamide and 2-chloro-6-methyl-*N*-phenylformamide, and that of 2,6-dimethyl-*N*-phenylformamide (Omondi *et al.*, 2005), in which there is one strong stabilizing interaction (along the N—H...O hydrogen-bonded chain), while the second and third stabilizing interactions are significantly weaker.

Experimental

2,6-Dibromo-*N*-phenylformamide was synthesized following a known procedure (Ugi *et al.*, 1965). Commercially available 2,6-dibromo-*N*-

phenylaniline (5 g, 0.02 mol; Aldrich, purity >95%) was heated in a tenfold excess of formic acid for a period of 15 h at 363 K. The excess formic acid was then removed under reduced pressure to give a white solid, which was treated with dilute hydrochloric acid (0.1 M HCl, 10 ml) and ethyl acetate (60 ml). The organic layer was separated from the aqueous layer, dried over magnesium sulfate and filtered. Colourless needle-shaped crystals of (I) were grown from the filtrate. The purity of the compound was confirmed by NMR analysis. It was found to exist in solution (C_6D_6) as a mixture of *cis* and *trans* isomers in a 2:1 ratio.

Crystal data

$\text{C}_7\text{H}_5\text{Br}_2\text{NO}$	$V = 849.40 (18) \text{ \AA}^3$
$M_r = 278.94$	$Z = 4$
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
$a = 4.2946 (5) \text{ \AA}$	$\mu = 9.48 \text{ mm}^{-1}$
$b = 13.8755 (16) \text{ \AA}$	$T = 173 \text{ K}$
$c = 14.2541 (19) \text{ \AA}$	$0.56 \times 0.08 \times 0.08 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer	5541 measured reflections
Absorption correction: multi-scan (<i>SADABS</i> ; Bruker, 2004)	2100 independent reflections
$T_{\min} = 0.069$, $T_{\max} = 0.466$	1841 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.030$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.027$	$\Delta\rho_{\text{max}} = 0.63 \text{ e \AA}^{-3}$
$wR(F^2) = 0.060$	$\Delta\rho_{\text{min}} = -0.34 \text{ e \AA}^{-3}$
$S = 1.03$	Absolute structure: Flack (1983), with 840 Friedel pairs
2100 reflections	Flack parameter: 0.055 (18)
100 parameters	
H-atom parameters constrained	

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1-H1}\cdots\text{O1}^i$	0.88	2.08	2.793 (4)	138

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

H atoms were located in difference maps and then treated as riding, with $\text{C-H} = 0.95 \text{ \AA}$ and $\text{N-H} = 0.88 \text{ \AA}$, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C,N})$.

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINTE* (Bruker, 2004); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997), *PLATON* (Spek, 2009) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: GD3278). Services for accessing these data are described at the back of the journal.

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