In the title compound, C₇H₇Br₂N, the C—C—C bond angles of the benzene ring are notably distorted and two short intramolecular N—H···Br contacts occur. In the crystal, the molecules are linked by N—H···N hydrogen bonds to generate C(2) chains propagating in the [001] direction.

Structure description

The solid-state structure of the title compound, C₇H₇Br₂N, was established by single-crystal X-ray diffraction analysis at 200 K and the molecular structure is illustrated in Fig. 1. The bromine atoms are slightly displaced from the mean plane of C₁–C₄/C₆/C₇ benzene ring, by 0.032 (1) and 0.065 (1) Å for Br₁ and Br₂, respectively. This can also be quantified by the C₄—C₃—C₂—Br₁ and C₄—C₆—C₇—Br₂ torsion angles, which are 179.7 (3) and 178.5 (3)°, respectively. The bond angles in the benzene ring are notably distorted from the ideal value of 120° with C₇—C₁—C₂ = 115.1 (4), C₁—C₂—C₃ = 122.8 (4) and C₁—C₇—C₆ = 123.0 (4)°. The amine group lying between the bromine atoms results in two short intramolecular N—H···Br contacts (Table 1).

In the crystal, the molecules are linked by weak N₁—H₁B···N₁ hydrogen bonds (Table 1) with N···N = 3.120 (7) Å to generate [001] C(2) chains with adjacent molecules related by the 2₁ screw axis. A similar hydrogen bond was observed in diamino-mesitylene (Brihi et al., 2016). The packing is illustrated in Fig. 2, which shows the topology of the chain is a zigzag, with an angle of inclination of the benzene ring to the a axis of 53.73 (14)°.
Synthesis and crystallization

The title compound is commercially available (Lancaster Synthesis). It was purified by recrystallization from a solution of 80% ethanol and 20% distilled water. The colorless single crystals obtained are in the form of needles, which grow along the $a$ axis.

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

| $D$—H—A | $D$—H | H—A | $D$···A | $D$—H···A |
|----------|--------|------|--------|----------|
| N1—H1A···Br1    | 0.86   | 2.65 | 3.077  | 4 (112)  |
| N1—H1B···Br2    | 0.86   | 2.64 | 3.072  | 4 (113)  |
| N1—H1B···N1'    | 0.86   | 2.38 | 3.120  | 7 (144)  |

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

Figure 1
The molecular structure of the title compound showing displacement ellipsoids at the 50% probability level.

Figure 2
Views along the (a) $b$ and (b) $c$ axes of the crystal packing of the title compound with hydrogen bonds shown as dotted lines.

Table 2
Experimental details.

| Crystal data                                                                 | Chemical formula C$_7$H$_7$Br$_2$N |
|------------------------------------------------------------------------------|------------------------------------|
| $M_r$                                                                        | 264.96                             |
| Crystal system, space group                                                  | Orthorhombic, $P2_12_12_1$         |
| Temperature (K)                                                              | 200                                |
| $a$, $b$, $c$ (Å)                                                            | 4.3773 (7), 13.585 (2), 14.057 (3) |
| $V$ (Å$^3$)                                                                  | 835.9 (2)                          |
| $Z$                                                                          | 4                                  |
| Radiation type                                                               | Mo Kα                              |
| $\mu$ (mm$^{-1}$)                                                            | 9.62                               |
| Crystal size (mm)                                                            | 0.12 × 0.05 × 0.04                 |
| Data collection                                                              | Bruker APEXII QUAZAR CCD           |
| Absorption correction                                                        | Multi-scan (SADABS; Bruker, 2016)   |
| $T_{\text{min}}$, $T_{\text{max}}$                                           | 0.396, 0.746                       |
| No. of measured, independent and observed $[I > 2\sigma(I)]$ reflections     | 7550, 1715, 1422                   |
| $R_{\text{int}}$, $wR_{\text{int}}$, $S$                                    | 0.061, 0.072, 0.91                 |
| No. of reflections                                                           | 1715                               |
| No. of parameters                                                            | 92                                 |
| H-atom treatment                                                             | H-atom parameters not refined      |
| $\Delta f_{\text{max}}$, $\Delta f_{\text{min}}$ (e Å$^{-3}$)               | 0.36, −0.38                        |
| Absolute structure                                                           | Flack (1983)                       |
| Absolute structure parameter                                                 | 0.02 (2)                           |

Computer programs: APEX2 and SAINT (Bruker, 2016), SIR92 (Altomare et al., 1994), SHELXL2013 (Sheldrick, 2015), ORTEP for Windows and WinGX publication routines (Farrugia, 2012).

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full crystallographic data

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2,6-Dibromo-4-methylaniline

Ouarda Brihi, Meriem Medjani, Hassiba Bougueria, Amel Djedouani, Michelle Francois, Solenne Fleutot and Ali Boudjada

2,6-Dibromo-4-methylaniline

Crystal data

C₇H₇Br₂N  
M_r = 264.96
Orthorhombic, P2₁2₁2₁  
Hall symbol: P 2ac 2ab
a = 4.3773 (7) Å  
b = 13.585 (2) Å  
c = 14.057 (3) Å  
V = 835.9 (2) Å³
Z = 4

F(000) = 504
D_x = 2.105 Mg m⁻³
Mo Kα radiation, λ = 0.71073 Å
Cell parameters from 7750 reflections
θ = 2.1–26.4°
µ = 9.62 mm⁻¹
T = 200 K
Needle, colorless
0.12 × 0.05 × 0.04 mm

Data collection

Bruker APEXI QUAZAR CCD  
diffractometer
Radiation source: ImuS
Graphite monochromator
Detector resolution: 8.02 pixels mm⁻¹
f and ω scans
Absorption correction: multi-scan
(SADABS; Bruker, 2016)
T_min = 0.396, T_max = 0.746
7550 measured reflections
1715 independent reflections
1422 reflections with I > 2σ(I)
R(int) = 0.061
θ_max = 26.4°, θ_min = 2.1°
h = −5→5
k = −15→16
l = −17→17

Refinement

Refinement on F²
Least-squares matrix: full
R(F²) = 0.030
wR(F²) = 0.072
S = 0.91
1715 reflections
92 parameters
0 restraints
0 constraints
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters not refined
\( w = 1/[(σ(F_c^2) + (0.0409P)^2)] \)
where P = (F_c^2 + 2F_S^2)/3
(Δσ)max = 0.001
Δρ_max = 0.36 e Å⁻³
Δρ_min = −0.38 e Å⁻³
Absolute structure: Flack (1983)
Absolute structure parameter: 0.02 (2)
Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su’s are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles.

Refinement. Refinement of F² against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F², conventional R-factors R are based on F, with F set to zero for negative F². The threshold expression of F² > 2σ(F²) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F² 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       | Uiso* / Ueq |
|-----|---------|---------|---------|-------------|
| Br1 | 0.69454 (12) | 0.51851 (3) | 0.40790 (4) | 0.0449 (2) |
| Br2 | 0.49325 (11)  | 0.11063 (3)  | 0.35184 (3)  | 0.0374 (2) |
| N1  | 0.4343 (8)     | 0.3124 (3)    | 0.4488 (2)    | 0.0340 (14) |
| C1  | 0.6072 (9)     | 0.3165 (3)    | 0.3674 (3)    | 0.0255 (14) |
| C2  | 0.7481 (9)     | 0.4015 (3)    | 0.3360 (3)    | 0.0277 (14) |
| C3  | 0.9295 (10)    | 0.4045 (3)    | 0.2553 (3)    | 0.0323 (17) |
| C4  | 0.9781 (10)    | 0.3217 (3)    | 0.2004 (3)    | 0.0313 (14) |
| C5  | 1.1658 (11)    | 0.3259 (3)    | 0.1108 (3)    | 0.0447 (17) |
| C6  | 0.8409 (10)    | 0.2336 (3)    | 0.2315 (3)    | 0.0317 (14) |
| C7  | 0.6636 (10)    | 0.2322 (3)    | 0.3118 (3)    | 0.0280 (12) |
| H1  | 1.33755       | 0.28238       | 0.11654       | 0.0669*      |
| H2  | 1.02080       | 0.46361       | 0.23780       | 0.0388*      |
| H3  | 0.87095       | 0.17585       | 0.19722       | 0.0378*      |
| H4  | 1.23699       | 0.39194       | 0.10090       | 0.0669*      |
| H5  | 1.04240       | 0.30603       | 0.05765       | 0.0669*      |

Atomic displacement parameters (Å²)

|     | U¹¹     | U¹²     | U¹³     | U¹²     | U¹³     | U¹³     |
|-----|---------|---------|---------|---------|---------|---------|
| Br1 | 0.0576 (3) | 0.0274 (2) | 0.0497 (3) | −0.0005 (2) | 0.0057 (3) | −0.0016 (2) |
| Br2 | 0.0373 (3) | 0.0279 (2) | 0.0471 (3) | −0.0053 (2) | −0.0027 (3) | 0.0002 (2) |
| N1  | 0.038 (3)  | 0.031 (2)  | 0.033 (2)  | −0.0013 (18)| 0.0070 (18)| 0.0005 (17) |
| C1  | 0.0174 (19)| 0.028 (2)  | 0.031 (3)  | 0.0015 (17)| −0.0052 (19)| 0.007 (2) |
| C2  | 0.023 (2)  | 0.027 (2)  | 0.033 (3)  | 0.0023 (18)| −0.0039 (19)| 0.0002 (19) |
| C3  | 0.027 (3)  | 0.029 (3)  | 0.041 (3)  | 0.0011 (19)| 0.001 (2)  | 0.006 (2) |
| C4  | 0.021 (2)  | 0.041 (3)  | 0.032 (2)  | 0.005 (2)  | 0.000 (2)  | 0.007 (2) |
| C5  | 0.036 (3)  | 0.057 (3)  | 0.041 (3)  | 0.009 (3)  | 0.005 (3)  | 0.008 (3) |
| C6  | 0.030 (2)  | 0.038 (3)  | 0.027 (2)  | 0.004 (2)  | −0.004 (2) | −0.002 (2) |
| C7  | 0.024 (2)  | 0.028 (2)  | 0.032 (2)  | 0.001 (2)  | −0.006 (2) | −0.0010 (19)|

Geometric parameters (Å, °)

|        |        |        |        |        |        |        |
|--------|--------|--------|--------|--------|--------|--------|
| Br1—C2 | 1.898 (4) | C4—C5 | 1.505 (6) |
| Br2—C7 | 1.898 (4) | C4—C6 | 1.409 (6) |
N1—C1 1.373 (5)  C6—C7 1.370 (6)
N1—H1A 0.8600  C3—H2 0.9300
N1—H1B 0.8600  C5—H5 0.9600
C1—C7 1.408 (6)  C5—H4 0.9600
C1—C2 1.382 (6)  C6—H3 0.9300
C2—C3 1.385 (6)
C3—C4 1.381 (6)
C1—N1—H1B 120.00 Br2—C7—C1 118.3 (3)
H1A—N1—H1B 120.00 Br2—C7—C6 118.6 (3)
C1—N1—H1A 120.00 C1—C7—C6 123.0 (4)
C2—C1—C7 115.2 (4) C2—C3—H2 119.00
N1—C1—C7 121.8 (4) C4—C3—H2 119.00
N1—C1—C2 123.1 (4) C1—C7—C6 123.0 (4)
Br1—C2—C1 118.3 (3) C2—C3—C4 121.5 (4)
Br1—C2—C3 118.8 (3) H1—C5—H4 109.00
C1—C2—C3 122.8 (4) H1—C5—H5 109.00
C2—C3—C4 121.5 (4) H1—C5—H4 109.00
C5—C4—C6 121.7 (4) C4—C6—H3 120.00
C3—C4—C5 121.4 (4) C7—C6—H3 120.00
C3—C4—C6 116.9 (4) C4—C6—C7 179.7 (3)
C4—C6—C7 120.6 (4)
N1—C1—C2—Br1 −1.0 (5) Br1—C2—C3—C4 179.7 (3)
N1—C1—C2—C3 178.1 (4) C1—C2—C3—C4 0.6 (7)
C7—C1—C2—Br1 −178.5 (3) C2—C3—C4—C5 177.7 (4)
C7—C1—C2—C3 0.6 (6) C2—C3—C4—C6 −1.5 (6)
N1—C1—C7—Br2 0.1 (6) C3—C4—C6—C7 −1.2 (6)
N1—C1—C7—C6 −178.5 (4) C5—C4—C6—C7 178.1 (4)
C2—C1—C7—Br2 177.6 (3) C4—C6—C7—Br2 −178.5 (3)
C2—C1—C7—C6 −1.0 (6) C4—C6—C7—C1 0.1 (7)

Hydrogen-bond geometry (Å, °)

| D—H···A | D—H | H···A | D···A | D—H···A |
|---------|-----|------|-------|---------|
| N1—H1A···Br1 | 0.86 | 2.65 | 3.077 (4) | 112 |
| N1—H1B···Br2 | 0.86 | 2.64 | 3.072 (4) | 113 |
| N1—H1B···N1i | 0.86 | 2.38 | 3.120 (7) | 144 |

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