Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

2,6-Dibromo-4-butylaniline

Liang Zhao* and Li-Ping Feng

Department of Chemical & Environmental Engineering, Anyang Institute of Technology, Anyang 455000, People's Republic of China
Correspondence e-mail: ayitzhao@yahoo.com.cn

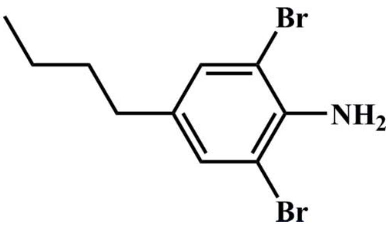
Received 12 November 2010; accepted 16 November 2010

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.009 Å; R factor = 0.069; wR factor = 0.187; data-to-parameter ratio = 22.3.

In the title compound, $C_{10}H_{13}Br_2N$, the amino N atom is essentially coplanar with the benzene ring, with an r.m.s. deviation of 0.004 Å. Weak intramolecular N—H···Br hydrogen bonds occur. In the crystal, molecules are linked into a zigzag chain parallel to the b axis by weak N—H···N hydrogen bonds.

Related literature

For related compounds, see: Fender *et al.* (2002); Grabowski (2005); Kryatova *et al.* (2004); Lehn (1995); Pedersen (1967); Scheiner (1997).



Experimental

Crystal data

$C_{10}H_{13}Br_2N$
M_r = 307.03
Monoclinic, $C2/c$
a = 17.566 (4) Å
b = 4.6083 (9) Å
c = 29.023 (6) Å
β = 98.93 (3)°
V = 2320.8 (8) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 6.94 mm^{-1}
T = 298 K
0.10 × 0.03 × 0.03 mm

Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.910, T_{max} = 1.000
9142 measured reflections
2633 independent reflections
1286 reflections with $I > 2\sigma(I)$
R_{int} = 0.117

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.187
S = 0.98
2633 reflections
118 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.80 e Å^{-3}
$\Delta\rho_{min}$ = −0.60 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···N1^{i}	0.86	2.53	3.181 (7)	134
N1—H1A···Br1	0.86	2.68	3.095 (5)	111
N1—H1B···Br2	0.86	2.64	3.074 (5)	113

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXTL*.

This work was supported by a School Start-up Grant to LZ.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2624).

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supporting information

Acta Cryst. (2010). E**66**, o3268   [https://doi.org/10.1107/S1600536810047410]

2,6-Dibromo-4-butylaniline

Liang Zhao and Li-Ping Feng

S1. Comment

In recent years there has been a rapidly increasing interest in the construction of various kinds of supramolecular systems for understanding molecular self-assembly principles and for designing molecular recognition devices (Fender *et al.*, 2002; Kryatova *et al.*, 2004; Pedersen, 1967). The supramolecular system generally refers to an assembly of molecules which are not covalently connected but assembled by other weak intermolecular interactions, such as hydrogen bonds (Grabowski, 2005; Lehn, 1995; Scheiner, 1997). We report here the crystal structure of the title compound, 2,6-dibromo-4-butylaniline.

In the title compound (Fig.1), the N atom of the amine group is essentially coplanar with the phenyl ring, with a r.m.s. deviation of 0.004 Å. This planar conformation might be resulting from weak intramolecular N-H···Br hydrogen bonds (Table 1). The butyl group is twisted with respect to the phenyl ring resulting in torsion angles of -179.1 (7)° for C9—C8—C7—C6 and -174.7 (7)° for C7—C8—C9—C10. Bond lengths and angles lie within normal ranges.

In the crystal structure, the organic molecules are linked to form a one-dimensional chain along *b* axis by N1—H···N1 hydrogen bonds (Table 1, Fig.2).

S2. Experimental

2,6-dibromo-4-butylaniline (3 mmol) was dissolved in ethanol (20 ml). The solution was allowed to evaporate to obtain colourless block-shaped crystals of the title compound.

S3. Refinement

All H atoms attached to C and N atoms were calculated geometrically and treated as riding on their parent atoms with C–H = 0.93 Å (aromatic), 0.96 Å (methyl), 0.97 Å (methylene) and N-H = 0.86 Å, with $U_{iso}(H) = 1.2U_{eq}(C, N)$ or $U_{iso}(H) = 1.5U_{eq}(C_{methyl})$.

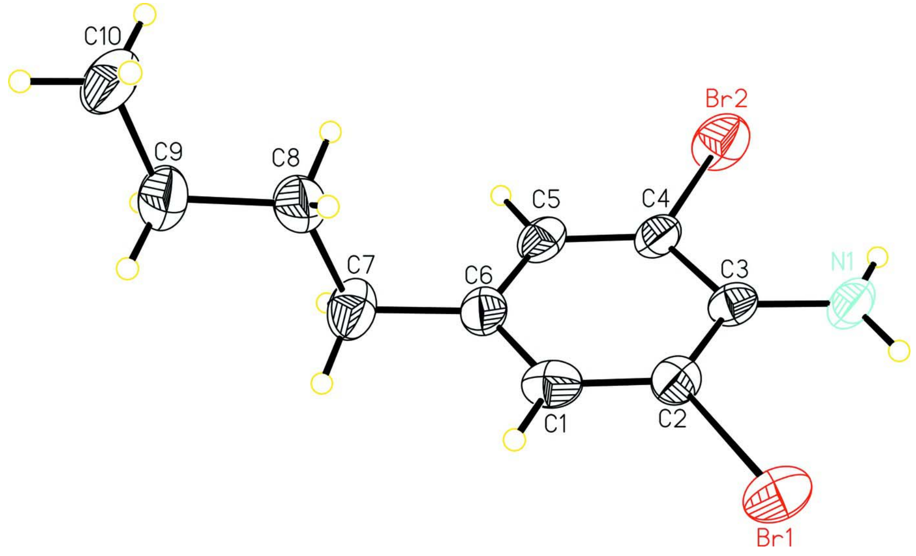

Figure 1

A view of the title compound with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.

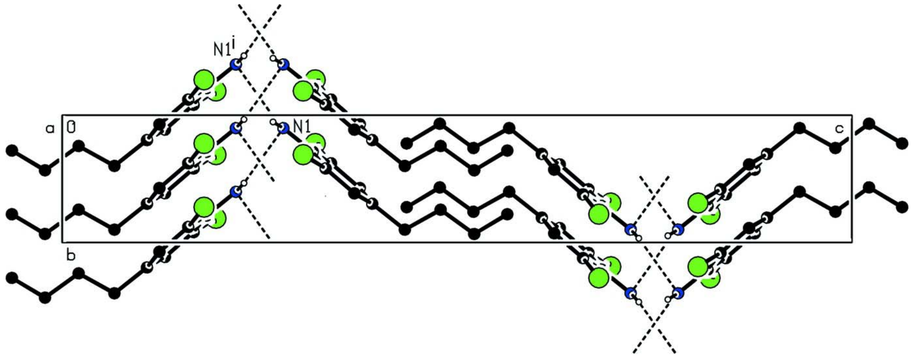

Figure 2

Partial packing view of the title compound along the a axis. H atoms not involved in hydrogen bonding (dashed lines) have been omitted for clarity. [Symmetry code: (i) -*x*+1/2, *y*-1/2, -*z*+1/2]

2,6-Dibromo-4-butylaniline

Crystal data

$C_{10}H_{13}Br_2N$
$M_r = 307.03$
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
$a = 17.566$ (4) Å
$b = 4.6083$ (9) Å
$c = 29.023$ (6) Å
$\beta = 98.93$ (3)°
$V = 2320.8$ (8) Å^3
$Z = 8$

$F(000) = 1200$
$D_x = 1.757$ Mg m^{-3}
Mo *Kα* radiation, $\lambda = 0.71073$ Å
Cell parameters from 2633 reflections
$\theta = 3.4$–27.5°
$\mu = 6.94$ mm^{-1}
$T = 298$ K
Block, colourless
0.10 × 0.03 × 0.03 mm

Data collection

Rigaku Mercury2 diffractometer	9142 measured reflections
Radiation source: fine-focus sealed tube	2633 independent reflections
Graphite monochromator	1286 reflections with $I > 2\sigma(I)$
Detector resolution: 13.6612 pixels mm^{-1}	$R_{\text{int}} = 0.117$
CCD profile fitting scans	$\theta_{\text{max}} = 27.5°$, $\theta_{\text{min}} = 3.4°$
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)	$h = -22 \rightarrow 22$
$T_{\text{min}} = 0.910$, $T_{\text{max}} = 1.000$	$k = -5 \rightarrow 5$
	$l = -37 \rightarrow 37$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.069$	H-atom parameters constrained
$wR(F^2) = 0.187$	$w = 1/[\sigma^2(F_o^2) + (0.063P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.98$	$(\Delta/\sigma)_{\text{max}} < 0.001$
2633 reflections	$\Delta\rho_{\text{max}} = 0.80$ e Å^{-3}
118 parameters	$\Delta\rho_{\text{min}} = -0.60$ e Å^{-3}
0 restraints	
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 > 2sigma(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	0.14631 (4)	0.22239 (18)	0.32043 (3)	0.0773 (4)
Br2	0.46385 (4)	0.3101 (2)	0.30522 (3)	0.0848 (4)
C3	0.3061 (3)	0.2877 (13)	0.31725 (18)	0.0482 (17)
C6	0.3272 (5)	0.6955 (13)	0.3926 (2)	0.0576 (18)
C2	0.2466 (3)	0.3776 (13)	0.3404 (2)	0.0512 (16)
C4	0.3781 (3)	0.4182 (15)	0.33358 (18)	0.0533 (16)
C5	0.3878 (4)	0.6137 (13)	0.36996 (19)	0.0544 (17)
H5	0.4363	0.6931	0.3796	0.065*
C1	0.2562 (4)	0.5724 (16)	0.3769 (2)	0.0596 (18)
H1	0.2141	0.6218	0.3912	0.072*
N1	0.2963 (3)	0.1017 (12)	0.28006 (16)	0.0621 (15)
H1A	0.2513	0.0335	0.2698	0.074*
H1B	0.3351	0.0530	0.2670	0.074*
C8	0.3747 (5)	0.7421 (14)	0.4792 (2)	0.076 (2)
H8A	0.3404	0.5851	0.4847	0.091*
H8B	0.4235	0.6566	0.4749	0.091*

C7	0.3402 (4)	0.8986 (16)	0.43391 (19)	0.072 (2)
H7A	0.2914	0.9862	0.4380	0.086*
H7B	0.3747	1.0530	0.4277	0.086*
C9	0.3877 (4)	0.9328 (19)	0.5218 (2)	0.086 (2)
H9A	0.4182	1.0995	0.5155	0.104*
H9B	0.3384	1.0034	0.5282	0.104*
C10	0.4278 (5)	0.7778 (17)	0.5637 (2)	0.102 (3)
H10A	0.4352	0.9084	0.5898	0.153*
H10B	0.4769	0.7094	0.5577	0.153*
H10C	0.3971	0.6160	0.5707	0.153*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0492 (5)	0.0947 (7)	0.0848 (6)	−0.0081 (4)	0.0005 (4)	0.0069 (4)
Br2	0.0537 (6)	0.1252 (9)	0.0770 (6)	−0.0047 (4)	0.0148 (4)	−0.0111 (4)
C3	0.046 (4)	0.059 (4)	0.039 (3)	0.001 (3)	0.004 (3)	0.008 (3)
C6	0.080 (5)	0.046 (4)	0.043 (4)	0.008 (4)	−0.004 (3)	0.005 (3)
C2	0.055 (4)	0.045 (4)	0.052 (4)	−0.004 (3)	0.002 (3)	0.008 (3)
C4	0.047 (4)	0.066 (5)	0.044 (3)	0.001 (3)	−0.003 (3)	0.000 (3)
C5	0.058 (4)	0.057 (4)	0.044 (4)	−0.004 (3)	−0.004 (3)	0.010 (3)
C1	0.054 (5)	0.076 (5)	0.051 (4)	0.011 (4)	0.014 (3)	0.017 (4)
N1	0.057 (3)	0.075 (4)	0.049 (3)	−0.005 (3)	−0.008 (2)	−0.008 (3)
C8	0.094 (6)	0.073 (5)	0.059 (4)	0.018 (4)	0.010 (4)	−0.004 (4)
C7	0.099 (6)	0.062 (5)	0.051 (4)	−0.009 (4)	0.002 (4)	0.000 (4)
C9	0.112 (6)	0.091 (6)	0.054 (4)	0.011 (5)	0.005 (4)	−0.014 (4)
C10	0.104 (7)	0.146 (9)	0.050 (4)	0.024 (5)	−0.008 (4)	−0.009 (5)

Geometric parameters (Å, º)

Br1—C2	1.906 (6)	N1—H1B	0.8600
Br2—C4	1.891 (6)	C8—C9	1.504 (9)
C3—N1	1.368 (7)	C8—C7	1.539 (9)
C3—C2	1.392 (8)	C8—H8A	0.9700
C3—C4	1.414 (8)	C8—H8B	0.9700
C6—C1	1.382 (9)	C7—H7A	0.9700
C6—C5	1.387 (9)	C7—H7B	0.9700
C6—C7	1.510 (9)	C9—C10	1.491 (10)
C2—C1	1.379 (8)	C9—H9A	0.9700
C4—C5	1.378 (8)	C9—H9B	0.9700
C5—H5	0.9300	C10—H10A	0.9600
C1—H1	0.9300	C10—H10B	0.9600
N1—H1A	0.8600	C10—H10C	0.9600

N1—C3—C2	123.7 (5)	C7—C8—H8A	108.6
N1—C3—C4	121.9 (5)	C9—C8—H8B	108.6
C2—C3—C4	114.3 (5)	C7—C8—H8B	108.6
C1—C6—C5	116.9 (6)	H8A—C8—H8B	107.6

C1—C6—C7	122.2 (7)	C6—C7—C8	112.2 (6)
C5—C6—C7	120.9 (6)	C6—C7—H7A	109.2
C1—C2—C3	123.6 (6)	C8—C7—H7A	109.2
C1—C2—Br1	118.3 (5)	C6—C7—H7B	109.2
C3—C2—Br1	118.0 (5)	C8—C7—H7B	109.2
C5—C4—C3	122.1 (6)	H7A—C7—H7B	107.9
C5—C4—Br2	119.6 (5)	C10—C9—C8	112.6 (7)
C3—C4—Br2	118.2 (4)	C10—C9—H9A	109.1
C4—C5—C6	121.9 (6)	C8—C9—H9A	109.1
C4—C5—H5	119.0	C10—C9—H9B	109.1
C6—C5—H5	119.0	C8—C9—H9B	109.1
C2—C1—C6	121.1 (6)	H9A—C9—H9B	107.8
C2—C1—H1	119.4	C9—C10—H10A	109.5
C6—C1—H1	119.4	C9—C10—H10B	109.5
C3—N1—H1A	120.0	H10A—C10—H10B	109.5
C3—N1—H1B	120.0	C9—C10—H10C	109.5
H1A—N1—H1B	120.0	H10A—C10—H10C	109.5
C9—C8—C7	114.7 (6)	H10B—C10—H10C	109.5
C9—C8—H8A	108.6		

N1—C3—C2—C1	−177.8 (6)	C1—C6—C5—C4	−0.2 (9)
C4—C3—C2—C1	−1.3 (8)	C7—C6—C5—C4	176.9 (6)
N1—C3—C2—Br1	2.2 (8)	C3—C2—C1—C6	0.8 (10)
C4—C3—C2—Br1	178.7 (4)	Br1—C2—C1—C6	−179.1 (5)
N1—C3—C4—C5	177.6 (5)	C5—C6—C1—C2	0.0 (9)
C2—C3—C4—C5	1.1 (8)	C7—C6—C1—C2	−177.1 (6)
N1—C3—C4—Br2	−4.1 (8)	C1—C6—C7—C8	97.6 (8)
C2—C3—C4—Br2	179.3 (4)	C5—C6—C7—C8	−79.4 (8)
C3—C4—C5—C6	−0.3 (9)	C9—C8—C7—C6	−179.1 (6)
Br2—C4—C5—C6	−178.6 (4)	C7—C8—C9—C10	−174.7 (7)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···N1$^{\text{i}}$	0.86	2.53	3.181 (7)	134
N1—H1*A*···Br1	0.86	2.68	3.095 (5)	111
N1—H1*B*···Br2	0.86	2.64	3.074 (5)	113

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