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## Structure Reports

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## 5-Bromobenzene-1,3-dicarbonitrile

Nadine Seidel, Wilhelm Seichter and Edwin Weber\*

Institut für Organische Chemie, TU Bergakademie Freiberg, Leipziger Strasse 29, D-09596 Freiberg/Sachsen, Germany

Correspondence e-mail: edwin.weber@chemie-tu.freiberg.de

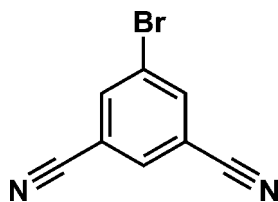
Received 25 September 2013; accepted 21 October 2013

Key indicators: single-crystal X-ray study;  $T = 173$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.031;  $wR$  factor = 0.078; data-to-parameter ratio = 21.1.

The asymmetric unit of the title compound,  $\text{C}_8\text{H}_3\text{BrN}_2$ , consists of two molecules. The crystal structure features undulating molecular sheets with the molecules linked by  $\text{C}-\text{H}\cdots\text{N}$  hydrogen bonds with one N atom acting as a bifurcated acceptor.  $\text{N}\cdots\text{Br}$  interactions also occur [ $\text{N}\cdots\text{Br} = 2.991$  (3) and  $3.099$  (3) Å]. Interlayer association is accomplished by offset face-to-face arene interactions [centroid-centroid distance =  $3.768$  (4) Å].

## Related literature

For use of aromatic nitrils in organic synthesis and for their industrial applications, see: Fabiani (1999); Ishii *et al.* (2011); Sandier & Karo (1983). For uses of aromatic nitrils in crystal engineering and the construction of metal-organic frameworks, see: Desiraju & Harlow (1989); Leonard & MacGillivray (2010); Reddy *et al.* (1993); Tiekink *et al.* (2010). For the X-ray structure of 1,3,5-tricyanobenzene, see: Reddy *et al.* (1995). For non-covalent  $\text{C}-\text{H}\cdots\text{N}$  and  $\text{N}\cdots\text{Br}$  interactions as well as arene $\cdots$ arene stacking contacts, see: Desiraju & Steiner (1999); Dance (2004); Rowland & Taylor (1996); Steiner (2002). For the preparation of the title compound, see: Doyle & Haseltine (1994).



## Experimental

## Crystal data

$\text{C}_8\text{H}_3\text{BrN}_2$   
 $M_r = 207.03$   
 Monoclinic,  $P2_1/c$   
 $a = 13.3019$  (4) Å

$b = 15.7762$  (5) Å  
 $c = 7.4265$  (2) Å  
 $\beta = 93.719$  (2)°  
 $V = 1555.19$  (8) Å<sup>3</sup>

$Z = 8$   
 Mo  $K\alpha$  radiation  
 $\mu = 5.21$  mm<sup>-1</sup>

$T = 173$  K  
 $0.45 \times 0.43 \times 0.08$  mm

## Data collection

Bruker APEXII CCD area-detector diffractometer  
 Absorption correction: multi-scan (SADABS; Bruker, 2007)  
 $T_{\min} = 0.203$ ,  $T_{\max} = 0.681$   
 16811 measured reflections  
 4198 independent reflections  
 3436 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.039$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.031$   
 $wR(F^2) = 0.078$   
 $S = 1.05$   
 4198 reflections  
 199 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.60$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.58$  e Å<sup>-3</sup>

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C4A}-\text{H4A}\cdots\text{N2}^i$	0.95	2.69	3.388 (3)	130
$\text{C4}-\text{H4}\cdots\text{N2A}^i$	0.95	2.61	3.444 (3)	147
$\text{C6A}-\text{H6A}\cdots\text{N1A}^{ii}$	0.95	2.67	3.563 (3)	157
$\text{C2}-\text{H2}\cdots\text{N1}^{iii}$	0.95	2.69	3.624 (3)	168
$\text{C2A}-\text{H2A}\cdots\text{N1}^{iii}$	0.95	2.72	3.435 (3)	133

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

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT-NT (Bruker, 2007); data reduction: SAINT-NT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 for Windows (Farrugia, 2012); software used to prepare material for publication: SHELXTL (Sheldrick, 2008).

This work was performed within the Cluster of Excellence "Structure Design of Novel High-Performance Materials via Atomic Design and Defect Engineering (ADDE)" which is supported financially by the European Union (European Regional Development Fund) and by the Ministry of Science and Art of Saxony (SMWK).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZP2009).

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## supporting information

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### S1. Comment

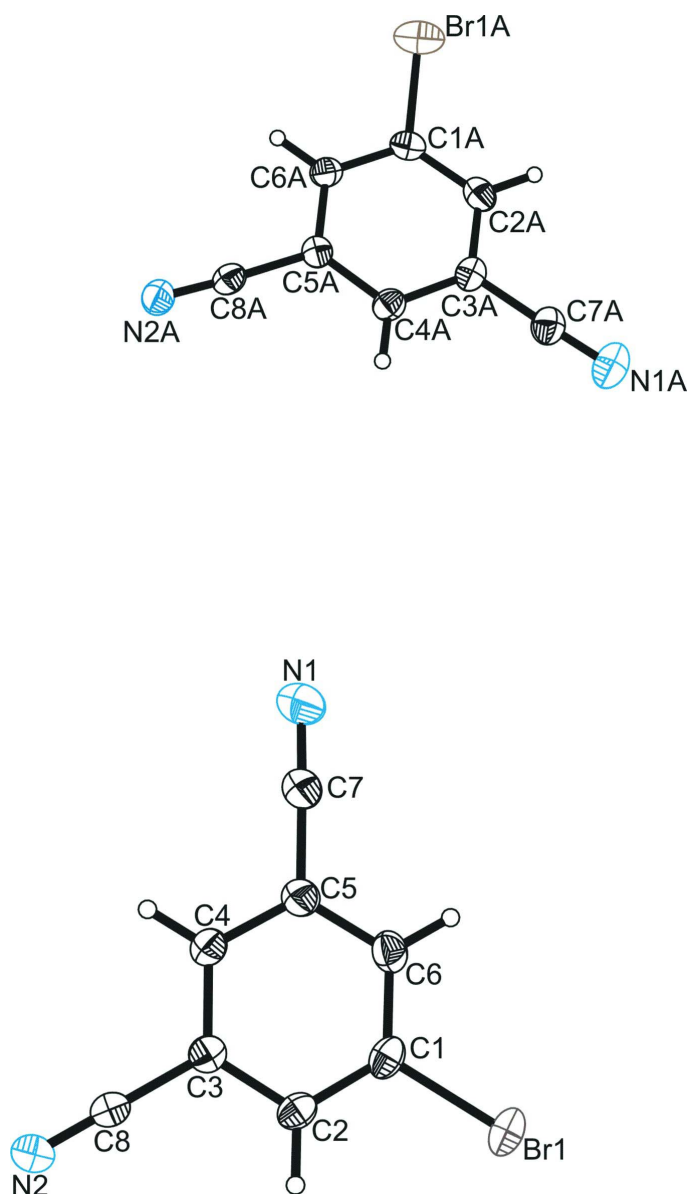
Aromatic nitriles are important intermediate compounds in organic synthesis (Ishii *et al.*, 2011). They can smoothly be converted into a great many of other functional groups, such as carboxylic acids, amidines, amines, esters and ketones (Sandier *et al.*, 1983). Furthermore, they are used as functional materials, pharmaceuticals, dyes and liquid crystals (Fabiani *et al.*, 1999). Recently, aromatic nitriles have also arisen interest for their capability of forming supramolecular interactions that turned out to good account in organic crystal engineering (Desiraju & Harlow, 1989; Reddy *et al.*, 1993; Tiekink *et al.*, 2010) or the construction of metal-organic framework structures (Leonard & MacGillivray, 2010). Relating to this latter topics, the title compound has been synthesized as a precursor and was identified by single-crystal X-ray diffraction. The compound crystallizes in the monoclinic space group  $P2_1/c$  with two molecules in the asymmetric part of the unit cell (Fig. 1). The bond distances and angles within the aromatic rings agree well with those found in the crystal structure of 1,3,5-tricyanobenzene (Reddy *et al.*, 1995). According to a tilt angle of  $12.3(1)^\circ$  between the independent molecules, the crystal structure is composed of undulated molecular layers with the molecules linked by C—H $\cdots$ N hydrogen bonds (Desiraju & Steiner, 1999) [ $d(\text{H}\cdots\text{N})$  2.61 - 2.72 Å; C—H $\cdots$ N 114 - 168°]. In this coordination structure (Figs. 2 and 3), the nitrogen N1 acts as a bifurcated acceptor (Steiner, 2002). Moreover, the interatomic distances between N2 and the bromo substituents of neighbouring molecules [2.991(2) and 3.099(2) Å], being considerably shorter than the sum of van der Waals radii of the respective atoms (3.40 Å), indicate the presence of N $\cdots$ Br interactions (Rowland & Taylor, 1996). In direction of the stacking axis of the molecular sheets, the crystal is stabilized by *offset face-to-face* arene interactions [ $C_{g_A}\cdots C_{g_A}$  = 3.768(4) Å] (Dance, 2004).

### S2. Experimental

The title compound was synthesized from 5-bromo-1,3-benzenedicarboxylic acid following the literature procedure (Doyle & Haseltine, 1994). Single crystals of X-ray diffraction quality were obtained as colourless plates *via* crystallization from acetone.

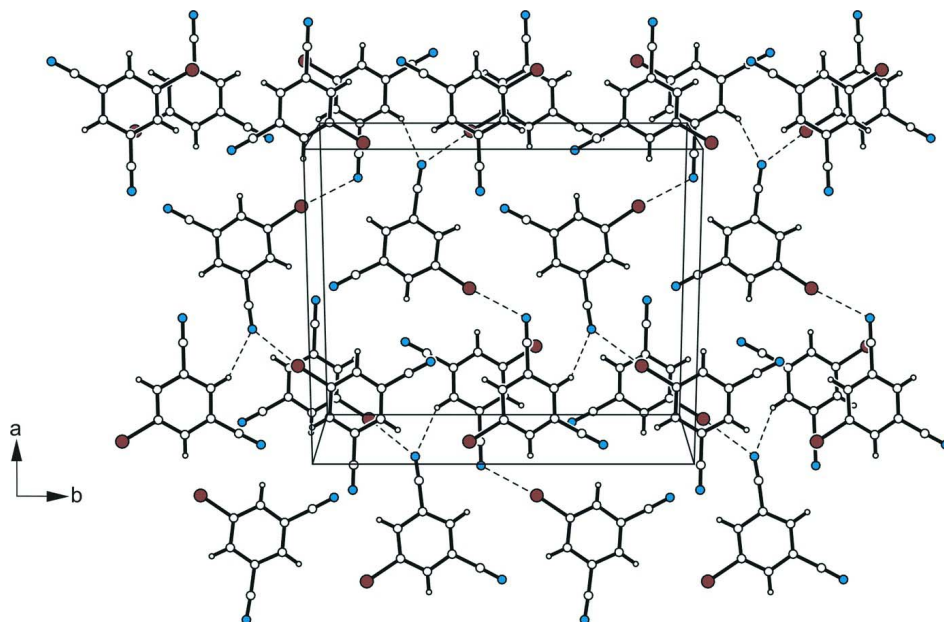
### S3. Refinement

H atoms were positioned geometrically and allowed to ride on their respective parent atoms, with C—H = 0.95 Å and  $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$  for aryl.

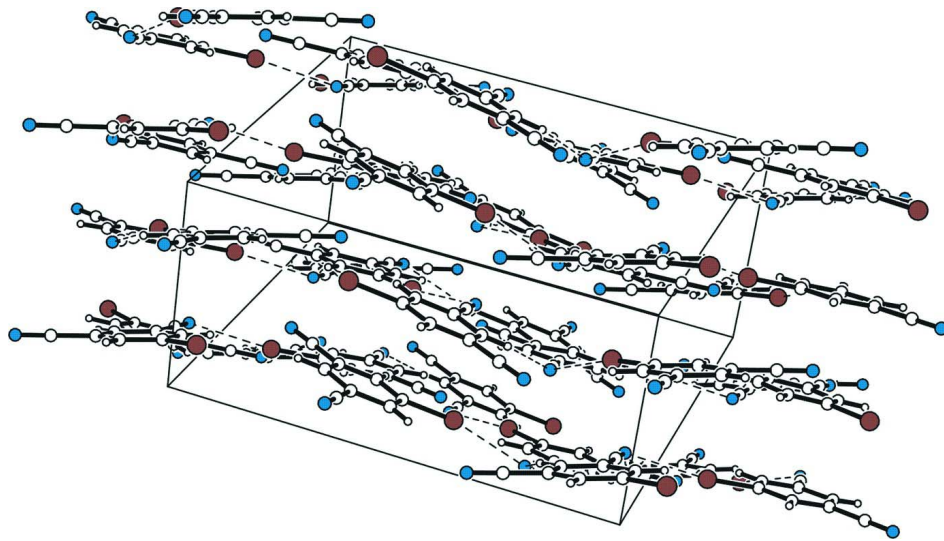


**Figure 1**

Asymmetric unit of the title compound, showing the atom numbering scheme. Displacement ellipsoids for the non-H atoms are drawn at the 50% probability level.

**Figure 2**

Packing structure viewed along the  $c$ -axis. Relevant intermolecular interactions are indicated as broken lines.

**Figure 3**

A view along the  $b$ -axis showing the intermolecular contacts as broken lines.

### 5-Bromobenzene-1,3-dicarbonitrile

#### Crystal data

$C_8H_3BrN_2$

$M_r = 207.03$

Monoclinic,  $P2_1/c$

Hall symbol:  $-P\ 2_1/c$

$a = 13.3019(4)\ \text{\AA}$

$b = 15.7762(5)\ \text{\AA}$

$c = 7.4265(2)\ \text{\AA}$

$\beta = 93.719(2)^\circ$

$V = 1555.19(8)\ \text{\AA}^3$

$Z = 8$

$F(000) = 800$

$D_x = 1.768\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 7273 reflections

$\theta = 2.6\text{--}29.1^\circ$   
 $\mu = 5.21 \text{ mm}^{-1}$   
 $T = 173 \text{ K}$

Plate, colourless  
 $0.45 \times 0.43 \times 0.08 \text{ mm}$

*Data collection*

Bruker APEXII CCD area-detector  
 diffractometer  
 Radiation source: fine-focus sealed tube  
 Graphite monochromator  
 phi and  $\omega$  scans  
 Absorption correction: multi-scan  
 (SADABS; Bruker, 2007)  
 $T_{\min} = 0.203$ ,  $T_{\max} = 0.681$

16811 measured reflections  
 4198 independent reflections  
 3436 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.039$   
 $\theta_{\text{max}} = 29.2^\circ$ ,  $\theta_{\text{min}} = 1.5^\circ$   
 $h = -18 \rightarrow 18$   
 $k = -21 \rightarrow 21$   
 $l = -8 \rightarrow 10$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.031$   
 $wR(F^2) = 0.078$   
 $S = 1.05$   
 4198 reflections  
 199 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0289P)^2 + 1.0903P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.60 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.58 \text{ e } \text{\AA}^{-3}$

*Special details*

**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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	-0.117304 (18)	0.402498 (14)	0.12147 (3)	0.03315 (8)
N1	-0.15740 (18)	0.79184 (15)	0.2893 (4)	0.0560 (7)
N2	0.27771 (15)	0.56650 (13)	0.4706 (3)	0.0366 (5)
C1	-0.05428 (17)	0.50150 (13)	0.2166 (3)	0.0265 (4)
C2	0.04561 (16)	0.49766 (13)	0.2815 (3)	0.0251 (4)
H2	0.0823	0.4461	0.2787	0.030*
C3	0.09102 (17)	0.57163 (13)	0.3513 (3)	0.0243 (4)
C4	0.03878 (16)	0.64751 (13)	0.3566 (3)	0.0266 (4)
H4	0.0703	0.6971	0.4059	0.032*
C5	-0.06113 (17)	0.64919 (14)	0.2879 (3)	0.0288 (4)
C6	-0.10855 (17)	0.57649 (14)	0.2169 (3)	0.0292 (4)
H6	-0.1766	0.5784	0.1697	0.035*
C7	-0.11580 (18)	0.72847 (15)	0.2884 (4)	0.0377 (6)

C8	0.19580 (17)	0.56869 (13)	0.4179 (3)	0.0272 (4)
Br1A	0.370700 (19)	0.099566 (15)	0.08217 (4)	0.03739 (8)
N1A	0.37898 (18)	0.49595 (14)	0.0782 (3)	0.0460 (6)
N2A	0.78226 (14)	0.24025 (12)	0.3862 (3)	0.0319 (4)
C1A	0.44634 (16)	0.19863 (13)	0.1352 (3)	0.0264 (4)
C2A	0.40402 (17)	0.27736 (14)	0.1025 (3)	0.0277 (4)
H2A	0.3364	0.2823	0.0543	0.033*
C3A	0.46205 (16)	0.34971 (13)	0.1413 (3)	0.0257 (4)
C4A	0.56122 (16)	0.34354 (13)	0.2127 (3)	0.0252 (4)
H4A	0.6006	0.3929	0.2381	0.030*
C5A	0.60110 (15)	0.26273 (13)	0.2458 (3)	0.0233 (4)
C6A	0.54470 (16)	0.18963 (12)	0.2074 (3)	0.0247 (4)
H6A	0.5729	0.1350	0.2300	0.030*
C7A	0.41674 (18)	0.43201 (15)	0.1068 (3)	0.0317 (5)
C8A	0.70312 (17)	0.25181 (12)	0.3230 (3)	0.0262 (4)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Br1	0.03797 (14)	0.02912 (13)	0.03247 (13)	−0.01325 (9)	0.00308 (10)	−0.00301 (8)
N1	0.0359 (12)	0.0372 (12)	0.095 (2)	0.0070 (10)	0.0032 (13)	0.0007 (13)
N2	0.0309 (10)	0.0297 (10)	0.0483 (13)	0.0062 (8)	−0.0035 (9)	−0.0032 (9)
C1	0.0320 (11)	0.0244 (10)	0.0234 (10)	−0.0081 (8)	0.0047 (8)	0.0003 (7)
C2	0.0310 (11)	0.0209 (9)	0.0236 (10)	−0.0016 (8)	0.0042 (8)	0.0012 (7)
C3	0.0262 (10)	0.0238 (9)	0.0229 (10)	−0.0008 (8)	0.0029 (8)	0.0012 (7)
C4	0.0270 (11)	0.0223 (10)	0.0304 (11)	−0.0021 (8)	0.0023 (9)	−0.0009 (8)
C5	0.0253 (11)	0.0262 (10)	0.0350 (12)	0.0005 (8)	0.0039 (9)	0.0013 (8)
C6	0.0226 (10)	0.0322 (11)	0.0328 (11)	−0.0035 (9)	0.0026 (9)	0.0022 (9)
C7	0.0263 (12)	0.0314 (12)	0.0554 (16)	0.0004 (10)	0.0024 (11)	0.0001 (11)
C8	0.0297 (11)	0.0200 (9)	0.0319 (11)	0.0014 (8)	0.0016 (9)	−0.0015 (8)
Br1A	0.03607 (14)	0.03308 (13)	0.04293 (15)	−0.01449 (9)	0.00186 (10)	−0.00027 (9)
N1A	0.0482 (14)	0.0387 (12)	0.0506 (14)	0.0124 (10)	−0.0004 (11)	0.0062 (10)
N2A	0.0297 (10)	0.0259 (9)	0.0394 (11)	0.0012 (8)	−0.0039 (9)	0.0011 (8)
C1A	0.0275 (11)	0.0265 (10)	0.0256 (10)	−0.0053 (8)	0.0053 (8)	−0.0007 (8)
C2A	0.0222 (10)	0.0366 (12)	0.0244 (10)	−0.0015 (9)	0.0022 (8)	0.0013 (8)
C3A	0.0280 (11)	0.0254 (10)	0.0237 (10)	0.0039 (8)	0.0018 (8)	0.0007 (8)
C4A	0.0289 (11)	0.0226 (10)	0.0240 (10)	0.0000 (8)	0.0005 (8)	−0.0009 (8)
C5A	0.0233 (10)	0.0253 (10)	0.0212 (10)	0.0006 (8)	0.0017 (8)	−0.0001 (7)
C6A	0.0268 (10)	0.0218 (9)	0.0262 (10)	−0.0004 (8)	0.0056 (8)	0.0004 (7)
C7A	0.0316 (12)	0.0330 (12)	0.0302 (11)	0.0032 (10)	0.0003 (9)	0.0018 (9)
C8A	0.0308 (11)	0.0194 (9)	0.0282 (11)	0.0002 (8)	0.0013 (9)	0.0004 (7)

*Geometric parameters (Å, °)*

Br1—C1	1.888 (2)	Br1A—C1A	1.886 (2)
N1—C7	1.143 (3)	N1A—C7A	1.141 (3)
N2—C8	1.134 (3)	N2A—C8A	1.139 (3)
C1—C2	1.385 (3)	C1A—C2A	1.379 (3)

C1—C6	1.386 (3)	C1A—C6A	1.389 (3)
C2—C3	1.398 (3)	C2A—C3A	1.397 (3)
C2—H2	0.9500	C2A—H2A	0.9500
C3—C4	1.386 (3)	C3A—C4A	1.393 (3)
C3—C8	1.449 (3)	C3A—C7A	1.447 (3)
C4—C5	1.393 (3)	C4A—C5A	1.397 (3)
C4—H4	0.9500	C4A—H4A	0.9500
C5—C6	1.396 (3)	C5A—C6A	1.395 (3)
C5—C7	1.447 (3)	C5A—C8A	1.449 (3)
C6—H6	0.9500	C6A—H6A	0.9500
C2—C1—C6	121.65 (19)	C2A—C1A—C6A	121.60 (19)
C2—C1—Br1	119.13 (16)	C2A—C1A—Br1A	120.23 (16)
C6—C1—Br1	119.21 (17)	C6A—C1A—Br1A	118.18 (15)
C1—C2—C3	118.31 (19)	C1A—C2A—C3A	119.1 (2)
C1—C2—H2	120.8	C1A—C2A—H2A	120.5
C3—C2—H2	120.8	C3A—C2A—H2A	120.5
C4—C3—C2	121.7 (2)	C4A—C3A—C2A	121.22 (19)
C4—C3—C8	119.39 (19)	C4A—C3A—C7A	120.2 (2)
C2—C3—C8	118.86 (19)	C2A—C3A—C7A	118.6 (2)
C3—C4—C5	118.3 (2)	C3A—C4A—C5A	118.05 (19)
C3—C4—H4	120.8	C3A—C4A—H4A	121.0
C5—C4—H4	120.8	C5A—C4A—H4A	121.0
C4—C5—C6	121.3 (2)	C6A—C5A—C4A	121.71 (19)
C4—C5—C7	118.9 (2)	C6A—C5A—C8A	117.39 (18)
C6—C5—C7	119.8 (2)	C4A—C5A—C8A	120.90 (18)
C1—C6—C5	118.6 (2)	C1A—C6A—C5A	118.36 (19)
C1—C6—H6	120.7	C1A—C6A—H6A	120.8
C5—C6—H6	120.7	C5A—C6A—H6A	120.8
N1—C7—C5	178.8 (3)	N1A—C7A—C3A	178.4 (3)
N2—C8—C3	179.7 (3)	N2A—C8A—C5A	177.3 (2)
C6—C1—C2—C3	1.1 (3)	C6A—C1A—C2A—C3A	0.7 (3)
Br1—C1—C2—C3	179.95 (15)	Br1A—C1A—C2A—C3A	-179.35 (16)
C1—C2—C3—C4	0.0 (3)	C1A—C2A—C3A—C4A	-0.2 (3)
C1—C2—C3—C8	-179.33 (19)	C1A—C2A—C3A—C7A	-179.9 (2)
C2—C3—C4—C5	-0.8 (3)	C2A—C3A—C4A—C5A	-0.5 (3)
C8—C3—C4—C5	178.5 (2)	C7A—C3A—C4A—C5A	179.2 (2)
C3—C4—C5—C6	0.7 (3)	C3A—C4A—C5A—C6A	0.7 (3)
C3—C4—C5—C7	-178.5 (2)	C3A—C4A—C5A—C8A	-178.87 (19)
C2—C1—C6—C5	-1.3 (3)	C2A—C1A—C6A—C5A	-0.4 (3)
Br1—C1—C6—C5	179.87 (17)	Br1A—C1A—C6A—C5A	179.62 (15)
C4—C5—C6—C1	0.4 (3)	C4A—C5A—C6A—C1A	-0.3 (3)
C7—C5—C6—C1	179.5 (2)	C8A—C5A—C6A—C1A	179.29 (19)



*Hydrogen-bond geometry (Å, °)*

<i>D—H···A</i>	<i>D—H</i>	<i>H···A</i>	<i>D···A</i>	<i>D—H···A</i>
C4A—H4A···N2 <sup>i</sup>	0.95	2.69	3.388 (3)	130
C4—H4···N2A <sup>i</sup>	0.95	2.61	3.444 (3)	147
C6A—H6A···N1A <sup>ii</sup>	0.95	2.67	3.563 (3)	157
C2—H2···N1 <sup>iii</sup>	0.95	2.69	3.624 (3)	168
C2A—H2A···N1 <sup>iii</sup>	0.95	2.72	3.435 (3)	133

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