

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

1-(10-Bromoanthracen-9-yl)-1H-imidazole

Hon Man Lee* and Hong-Jyun Lee

National Changhua University of Education, Department of Chemistry, Changhua, 50058, Taiwan

Correspondence e-mail: leehm@cc.ncue.edu.tw

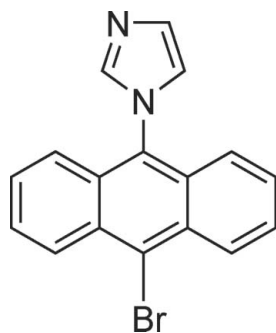
Received 27 March 2013; accepted 2 April 2013

Key indicators: single-crystal X-ray study; $T = 150$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.032; wR factor = 0.100; data-to-parameter ratio = 15.4.

In the title molecule, $\text{C}_{17}\text{H}_{11}\text{BrN}_2$, the planes of the anthracene ring system [maximum deviation from the mean plane = 0.036 (3) Å] and the imidazole ring form a dihedral angle of 85.14 (14)°. In the crystal, weak $\text{C}-\text{H}\cdots\text{N}$ and $\text{C}-\text{H}\cdots\text{Br}$ hydrogen bonds link the molecules into double chains propagating along $[01\bar{1}]$. In addition, $\pi-\pi$ stacking interactions between pairs of benzene rings are observed, with centroid-centroid distances of 3.7968 (17) and 3.8496 (16) Å.

Related literature

For the preparation of the title compound, see: Lee *et al.* (2011). For the structure of a related compound, see: Boyer *et al.* (1993).



Experimental

Crystal data

 $\text{C}_{17}\text{H}_{11}\text{BrN}_2$ $M_r = 323.19$ Triclinic, $P\bar{1}$ $a = 8.1832$ (2) Å $b = 8.8473$ (2) Å $c = 9.5814$ (2) Å $\alpha = 75.355$ (1)° $\beta = 81.624$ (1)° $\gamma = 77.134$ (1)° $V = 651.36$ (3) Å³ $Z = 2$ Mo $K\alpha$ radiation $\mu = 3.15$ mm⁻¹ $T = 150$ K $0.35 \times 0.26 \times 0.07$ mm

Data collection

Bruker SMART APEXII diffractometer

Absorption correction: multi-scan (SADABS; Sheldrick, 2003)

 $T_{\min} = 0.406$, $T_{\max} = 0.822$

6236 measured reflections

2846 independent reflections

2562 reflections with $I > 2\sigma$ $R_{\text{int}} = 0.017$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.032$ $wR(F^2) = 0.100$ $S = 1.11$

2846 reflections

185 parameters

H atoms treated by a mixture of independent and constrained refinement

 $\Delta\rho_{\text{max}} = 0.54$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.28$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C3}-\text{H3}\cdots\text{Br1}^i$	0.95	2.86	3.687 (3)	147
$\text{C3}-\text{H3}\cdots\text{N2}^{ii}$	0.95	2.58	3.393 (4)	144

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

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: DIAMOND (Brandenburg, 2006); software used to prepare material for publication: SHELXTL.

We thank the National Science Council of Taiwan for financial support of this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5602).

References

- Boyer, G., Claramunt, R. M., Elguero, J., Fathalla, M., Foces-Foces, C., Jaime, C. & Llamas-Saiz, A. L. (1993). *J. Chem. Soc. Perkin Trans. 2*, pp. 757–766.
- Brandenburg, K. (2006). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
- Bruker (2007). *APEX2* and *SAINTE*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Lee, H.-J., Cheng, P.-Y., Chen, C.-Y., Shen, J.-S., Nandi, D. & Lee, H. M. (2011). *CrystEngComm*, **13**, 4814–4816.
- Sheldrick, G. M. (2003). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

supporting information

Acta Cryst. (2013). E69, o672 [https://doi.org/10.1107/S160053681300891X]

1-(10-Bromoanthracen-9-yl)-1*H*-imidazole**Hon Man Lee and Hong-Jyun Lee****S1. Comment**

The title compound is a side-product in the preparation of 9,10-di(1*H*-imidazol-1-yl)anthracene. The latter compound is a ditopic bis(imidazole) ligand which can form intriguing coordination polymers with transition metal ions (Lee *et al.*, *et al.* 2011). The title compound however, features only one imidazole moiety. 9-(10'-Bromo-9'-anthryl)carbazole is a structure in the literature which is related to the title compound (Boyer *et al.* 1993).

The molecular structure of the title compound is shown in Fig. 1. The anthracene ring system [maximum deviation from the mean plane = 0.036 (3) Å for C11] and imidazole ring form a dihedral angle of 85.14 (14) Å. In the crystal, weak hydrogen bonds of the type C—H...N and C—H...Br link the molecules into one-dimensional double chains propagating along [0, 1, -1] (Fig. 2). Double chains are further stabilized by π - π stacking interaction between pairs of anthracene rings. The contact distances are 3.7968 (17) [Cg1...Cg1(-x, 2 - y, 1 - z)] and 3.8496 (16) Å [Cg1...Cg1(-x, 2 - y, 1 - z)]. Cg1 and Cg2 are the centroids of C12—C17 and C4/C5/C10—C12/C17, respectively.

S2. Experimental

The compound was isolated as a side-product in the preparation of 9,10-di(1*H*-imidazol-1-yl)anthracene (dia) (Lee *et al.*, 2011). Suitable crystals were obtained by slow evaporation of a methanol solution of the compound at room temperature.

S3. Refinement

The hydrogen atom upon C2 was located in a difference Fourier map and freely refined. All the other hydrogen atoms were positioned geometrically and refined as riding atoms, with C—H = 0.95 Å with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

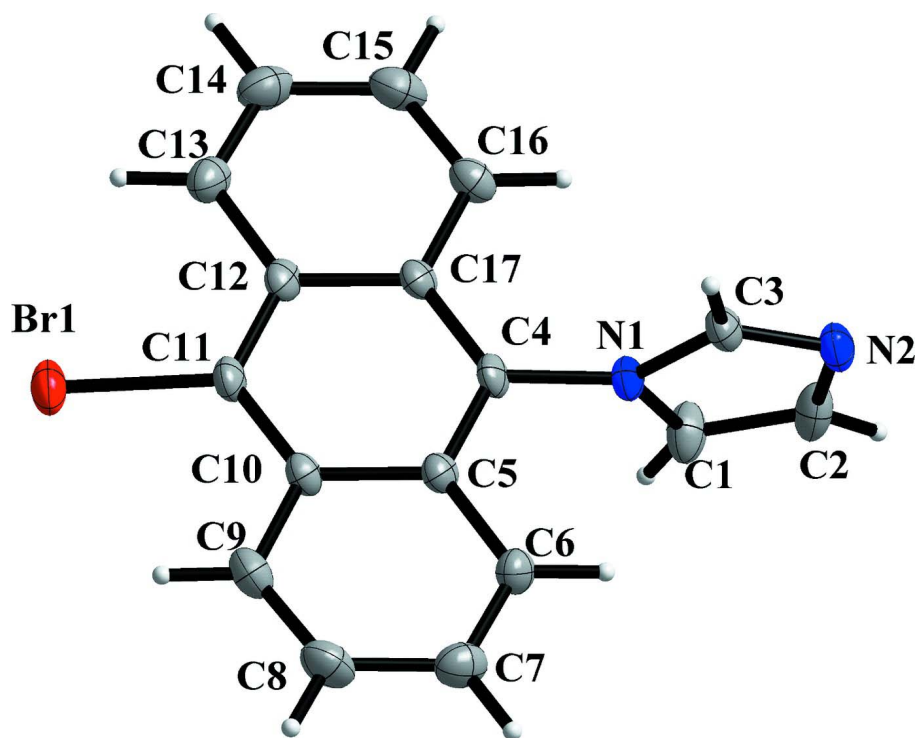


Figure 1

The molecular structure of the title compound, showing 50% probability displacement ellipsoids for the non-hydrogen atoms. The H atoms are depicted by circles of an arbitrary radius.

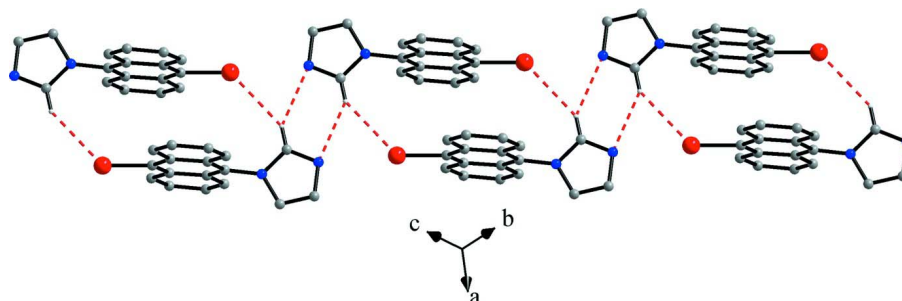


Figure 2

A view of a double chain displaying the hydrogen bonds as dashed lines. The viewing direction is along [1,1,1].

1-(10-Bromoanthracen-9-yl)-1H-imidazole

Crystal data

$C_{17}H_{11}BrN_2$

$M_r = 323.19$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 8.1832(2)\ \text{\AA}$

$b = 8.8473(2)\ \text{\AA}$

$c = 9.5814(2)\ \text{\AA}$

$\alpha = 75.355(1)^\circ$

$\beta = 81.624(1)^\circ$

$\gamma = 77.134(1)^\circ$

$V = 651.36(3)\ \text{\AA}^3$

$Z = 2$

$F(000) = 324$

$D_x = 1.648\ \text{Mg m}^{-3}$

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

Cell parameters from 2906 reflections

$\theta = 2.4\text{--}27.9^\circ$

$\mu = 3.15\ \text{mm}^{-1}$

$T = 150$ K $0.35 \times 0.26 \times 0.07$ mm
 Block, colorless

Data collection

Bruker SMART APEXII diffractometer Radiation source: fine-focus sealed tube Graphite monochromator ω scans Absorption correction: multi-scan (SADABS; Sheldrick, 2003) $T_{\min} = 0.406$, $T_{\max} = 0.822$	6236 measured reflections 2846 independent reflections 2562 reflections with $I > 2\sigma$ $R_{\text{int}} = 0.017$ $\theta_{\text{max}} = 27.0^\circ$, $\theta_{\text{min}} = 2.2^\circ$ $h = -10 \rightarrow 10$ $k = -6 \rightarrow 11$ $l = -12 \rightarrow 12$
--	---

Refinement

Refinement on F^2 Least-squares matrix: full $R[F^2 > 2\sigma(F^2)] = 0.032$ $wR(F^2) = 0.100$ $S = 1.11$ 2846 reflections 185 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 atoms treated by a mixture of independent and constrained refinement $w = 1/[\sigma^2(F_o^2) + (0.0608P)^2 + 0.4219P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\text{max}} < 0.001$ $\Delta\rho_{\text{max}} = 0.54 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\text{min}} = -0.28 \text{ e } \text{\AA}^{-3}$
--	---

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.29223 (4)	1.29770 (3)	0.32328 (3)	0.02958 (12)
C1	0.0666 (4)	0.7593 (4)	0.9486 (3)	0.0298 (6)
H1	-0.0397	0.8259	0.9291	0.036*
C2	0.0985 (4)	0.6312 (4)	1.0596 (3)	0.0294 (6)
C3	0.3352 (4)	0.6527 (3)	0.9386 (3)	0.0221 (5)
H3	0.4520	0.6345	0.9072	0.027*
C4	0.2461 (3)	0.8922 (3)	0.7399 (3)	0.0185 (5)
C5	0.2927 (3)	1.0313 (3)	0.7525 (3)	0.0182 (5)
C6	0.3187 (3)	1.0569 (3)	0.8880 (3)	0.0230 (5)
H6	0.3047	0.9771	0.9739	0.028*
C7	0.3633 (4)	1.1936 (4)	0.8968 (3)	0.0288 (6)
H7	0.3781	1.2091	0.9883	0.035*
C8	0.3875 (4)	1.3121 (3)	0.7700 (4)	0.0308 (6)

H8	0.4218	1.4055	0.7767	0.037*
C9	0.3622 (4)	1.2942 (3)	0.6381 (3)	0.0266 (6)
H9	0.3776	1.3761	0.5543	0.032*
C10	0.3129 (3)	1.1539 (3)	0.6238 (3)	0.0192 (5)
C11	0.2836 (3)	1.1299 (3)	0.4912 (3)	0.0207 (5)
C12	0.2413 (3)	0.9892 (3)	0.4780 (3)	0.0194 (5)
C13	0.2162 (4)	0.9609 (3)	0.3427 (3)	0.0269 (6)
H13	0.2307	1.0392	0.2559	0.032*
C14	0.1720 (4)	0.8240 (4)	0.3366 (3)	0.0323 (7)
H14	0.1561	0.8076	0.2457	0.039*
C15	0.1494 (4)	0.7059 (3)	0.4631 (4)	0.0313 (7)
H15	0.1166	0.6115	0.4571	0.038*
C16	0.1741 (3)	0.7257 (3)	0.5940 (3)	0.0241 (6)
H16	0.1598	0.6443	0.6784	0.029*
C17	0.2214 (3)	0.8676 (3)	0.6065 (3)	0.0188 (5)
H2	0.028 (4)	0.592 (4)	1.127 (4)	0.028 (9)*
N1	0.2190 (3)	0.7738 (3)	0.8691 (2)	0.0197 (4)
N2	0.2670 (3)	0.5647 (3)	1.0537 (3)	0.0255 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.03324 (19)	0.02543 (17)	0.02217 (17)	-0.00272 (12)	-0.00137 (11)	0.00551 (11)
C1	0.0215 (14)	0.0357 (16)	0.0255 (15)	-0.0028 (12)	-0.0044 (11)	0.0041 (12)
C2	0.0327 (16)	0.0333 (15)	0.0203 (14)	-0.0138 (13)	-0.0029 (12)	0.0037 (12)
C3	0.0235 (13)	0.0176 (12)	0.0214 (13)	0.0005 (10)	-0.0061 (10)	0.0005 (10)
C4	0.0173 (12)	0.0156 (11)	0.0184 (12)	0.0014 (9)	-0.0049 (10)	0.0016 (10)
C5	0.0164 (12)	0.0174 (12)	0.0184 (12)	0.0019 (9)	-0.0045 (9)	-0.0024 (10)
C6	0.0243 (13)	0.0233 (13)	0.0193 (13)	-0.0003 (10)	-0.0058 (10)	-0.0025 (10)
C7	0.0279 (15)	0.0314 (15)	0.0287 (15)	0.0010 (12)	-0.0091 (12)	-0.0123 (12)
C8	0.0332 (16)	0.0218 (13)	0.0402 (17)	-0.0043 (11)	-0.0097 (13)	-0.0098 (12)
C9	0.0271 (14)	0.0175 (12)	0.0323 (15)	-0.0020 (11)	-0.0061 (12)	-0.0006 (11)
C10	0.0181 (12)	0.0155 (11)	0.0212 (13)	0.0003 (9)	-0.0052 (10)	-0.0003 (10)
C11	0.0208 (13)	0.0172 (12)	0.0179 (12)	0.0023 (10)	-0.0032 (10)	0.0026 (10)
C12	0.0170 (12)	0.0190 (12)	0.0179 (12)	0.0038 (9)	-0.0046 (9)	-0.0014 (10)
C13	0.0279 (14)	0.0283 (14)	0.0204 (13)	0.0046 (11)	-0.0063 (11)	-0.0043 (11)
C14	0.0329 (16)	0.0378 (16)	0.0277 (15)	0.0034 (13)	-0.0093 (12)	-0.0154 (13)
C15	0.0310 (16)	0.0240 (14)	0.0417 (18)	0.0012 (12)	-0.0110 (13)	-0.0141 (13)
C16	0.0225 (13)	0.0191 (12)	0.0296 (15)	-0.0009 (10)	-0.0059 (11)	-0.0046 (11)
C17	0.0175 (12)	0.0156 (11)	0.0204 (13)	0.0022 (9)	-0.0050 (10)	-0.0019 (10)
N1	0.0218 (11)	0.0175 (10)	0.0170 (10)	-0.0018 (8)	-0.0044 (9)	0.0012 (8)
N2	0.0345 (13)	0.0192 (11)	0.0208 (11)	-0.0053 (9)	-0.0076 (10)	0.0017 (9)

Geometric parameters (Å, °)

Br1—C11	1.898 (3)	C7—H7	0.9500
C1—C2	1.350 (4)	C8—C9	1.362 (4)
C1—N1	1.377 (4)	C8—H8	0.9500

C1—H1	0.9500	C9—C10	1.431 (4)
C2—N2	1.372 (4)	C9—H9	0.9500
C2—H2	0.86 (4)	C10—C11	1.401 (4)
C3—N2	1.309 (4)	C11—C12	1.403 (4)
C3—N1	1.366 (3)	C12—C17	1.432 (4)
C3—H3	0.9500	C12—C13	1.432 (4)
C4—C17	1.400 (4)	C13—C14	1.356 (4)
C4—C5	1.404 (4)	C13—H13	0.9500
C4—N1	1.431 (3)	C14—C15	1.405 (5)
C5—C6	1.426 (4)	C14—H14	0.9500
C5—C10	1.438 (4)	C15—C16	1.358 (4)
C6—C7	1.364 (4)	C15—H15	0.9500
C6—H6	0.9500	C16—C17	1.430 (4)
C7—C8	1.411 (5)	C16—H16	0.9500
C2—C1—N1	106.2 (3)	C11—C10—C9	123.4 (2)
C2—C1—H1	126.9	C5—C10—C9	118.1 (2)
N1—C1—H1	126.9	C10—C11—C12	122.8 (2)
C1—C2—N2	110.7 (3)	C10—C11—Br1	118.82 (19)
C1—C2—H2	128 (2)	C12—C11—Br1	118.3 (2)
N2—C2—H2	121 (2)	C11—C12—C17	118.4 (2)
N2—C3—N1	112.1 (2)	C11—C12—C13	123.5 (2)
N2—C3—H3	123.9	C17—C12—C13	118.1 (2)
N1—C3—H3	123.9	C14—C13—C12	121.0 (3)
C17—C4—C5	122.4 (2)	C14—C13—H13	119.5
C17—C4—N1	119.2 (2)	C12—C13—H13	119.5
C5—C4—N1	118.4 (2)	C13—C14—C15	120.8 (3)
C4—C5—C6	122.7 (2)	C13—C14—H14	119.6
C4—C5—C10	118.7 (2)	C15—C14—H14	119.6
C6—C5—C10	118.6 (2)	C16—C15—C14	120.5 (3)
C7—C6—C5	121.3 (3)	C16—C15—H15	119.7
C7—C6—H6	119.4	C14—C15—H15	119.7
C5—C6—H6	119.4	C15—C16—C17	120.9 (3)
C6—C7—C8	120.1 (3)	C15—C16—H16	119.6
C6—C7—H7	120.0	C17—C16—H16	119.6
C8—C7—H7	120.0	C4—C17—C16	122.3 (2)
C9—C8—C7	120.9 (3)	C4—C17—C12	119.1 (2)
C9—C8—H8	119.5	C16—C17—C12	118.6 (2)
C7—C8—H8	119.5	C3—N1—C1	105.9 (2)
C8—C9—C10	121.0 (3)	C3—N1—C4	128.0 (2)
C8—C9—H9	119.5	C1—N1—C4	126.1 (2)
C10—C9—H9	119.5	C3—N2—C2	105.1 (2)
C11—C10—C5	118.5 (2)		
N1—C1—C2—N2	0.4 (4)	C17—C12—C13—C14	1.2 (4)
C17—C4—C5—C6	-179.8 (2)	C12—C13—C14—C15	0.0 (4)
N1—C4—C5—C6	1.9 (4)	C13—C14—C15—C16	-1.0 (5)
C17—C4—C5—C10	1.1 (4)	C14—C15—C16—C17	0.8 (4)

N1—C4—C5—C10	-177.3 (2)	C5—C4—C17—C16	180.0 (2)
C4—C5—C6—C7	-179.8 (3)	N1—C4—C17—C16	-1.7 (4)
C10—C5—C6—C7	-0.6 (4)	C5—C4—C17—C12	-1.1 (4)
C5—C6—C7—C8	-1.1 (4)	N1—C4—C17—C12	177.2 (2)
C6—C7—C8—C9	1.9 (5)	C15—C16—C17—C4	179.4 (3)
C7—C8—C9—C10	-0.9 (4)	C15—C16—C17—C12	0.4 (4)
C4—C5—C10—C11	0.6 (4)	C11—C12—C17—C4	-0.5 (4)
C6—C5—C10—C11	-178.6 (2)	C13—C12—C17—C4	179.7 (2)
C4—C5—C10—C9	-179.3 (2)	C11—C12—C17—C16	178.5 (2)
C6—C5—C10—C9	1.5 (4)	C13—C12—C17—C16	-1.3 (4)
C8—C9—C10—C11	179.4 (3)	N2—C3—N1—C1	0.3 (3)
C8—C9—C10—C5	-0.8 (4)	N2—C3—N1—C4	-179.4 (2)
C5—C10—C11—C12	-2.2 (4)	C2—C1—N1—C3	-0.4 (3)
C9—C10—C11—C12	177.6 (3)	C2—C1—N1—C4	179.2 (3)
C5—C10—C11—Br1	175.01 (18)	C17—C4—N1—C3	95.3 (3)
C9—C10—C11—Br1	-5.1 (4)	C5—C4—N1—C3	-86.3 (3)
C10—C11—C12—C17	2.2 (4)	C17—C4—N1—C1	-84.3 (3)
Br1—C11—C12—C17	-175.05 (18)	C5—C4—N1—C1	94.1 (3)
C10—C11—C12—C13	-178.0 (2)	N1—C3—N2—C2	0.0 (3)
Br1—C11—C12—C13	4.8 (4)	C1—C2—N2—C3	-0.3 (4)
C11—C12—C13—C14	-178.7 (3)		

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C3—H3 \cdots Br1 ⁱ	0.95	2.86	3.687 (3)	147
C3—H3 \cdots N2 ⁱⁱ	0.95	2.58	3.393 (4)	144

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