Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# *N*,*N*-Dimethyl-4-[(*E*)-2-(3,6,7-tribromo-9-butyl-9*H*-carbazol-2-yl)ethenyl]aniline

**Sushil Kumar,[a] K. R. Justin Thomas,[a]‡ Seik Weng Ng[b,c] and Edward R. T. Tiekink[b]***

[a]Organic Materials Laboratory, Department of Chemistry, Indian Institute of Technology Roorkee, Roorkee 247 667, India, [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia, and [c]Chemistry Department, Faculty of Science, King Abdulaziz University, PO Box 80203 Jeddah, Saudi Arabia
Correspondence e-mail: edward.tiekink@gmail.com

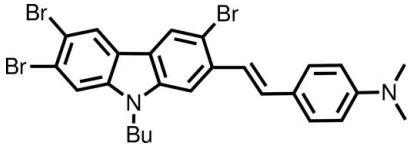
Received 28 February 2012; accepted 15 March 2012

Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.032; $wR$ factor = 0.092; data-to-parameter ratio = 17.1.

In the title molecule, $C_{26}H_{25}Br_3N_2$, a dihedral angle of 6.15 (10)° is present between the carbazole and benzene ring systems with an *E* conformation about the C=C bond [1.335 (4) Å]. The butyl group is almost perpendicular to the carbazole plane [C—N—C—C torsion angle = −98.7 (3)°]. In the crystal, supramolecular double chains along [$\overline{7}$,18,$\overline{16}$] are formed *via* C—H···Br and $\pi$–$\pi$ interactions [centroid(carbazole five-membered ring)···centroid(carbazole six-membered ring) distance = 3.6333 (13) Å].

## Related literature

For the use of carbazole derivatives in organic light-emitting diodes and photovoltaic devices, see: Thomas *et al.* (2001, 2004); Wu *et al.* (2005); Lee *et al.* (2012); Ooyama *et al.* (2011). For related structures, see: Pawluć *et al.* (2011); Zhang & Zhang (2011); Ramathilagam *et al.* (2011).




## Experimental

### *Crystal data*

$C_{26}H_{25}Br_3N_2$
$M_r$ = 605.21
Triclinic, $P\overline{1}$
$a$ = 9.7304 (3) Å
$b$ = 11.3834 (4) Å
$c$ = 11.8197 (4) Å
$\alpha$ = 114.308 (3)°
$\beta$ = 101.957 (3)°
$\gamma$ = 90.127 (3)°
$V$ = 1161.62 (7) Å$^3$
$Z$ = 2
Cu $K\alpha$ radiation
$\mu$ = 6.56 mm$^{-1}$
$T$ = 100 K
0.30 × 0.30 × 0.05 mm

### *Data collection*

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
$T_{min}$ = 0.244, $T_{max}$ = 0.735
10766 measured reflections
4827 independent reflections
4680 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.021

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.092
$S$ = 1.07
4827 reflections
282 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.18 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.81 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C26—H26*C*···Br1$^{i}$ | 0.98 | 2.91 | 3.844 (3) | 161 |

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

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

KRJT thanks the Council of Scientific and Industrial Research (CSIR), New Delhi, for financial support [grant No. 01 (2111)/07/EMR-II)]. The authors also thank the Ministry of Higher Education (Malaysia) for funding structural studies through the High-Impact Research scheme (grant No. UM.C/HIR/MOHE/SC/12).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GG2078).

## References

Agilent (2010). *CrysAlis PRO*. Agilent Technologies, Yarnton, Oxfordshire, England.
Brandenburg, K. (2006). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Lee, W., Cho, N., Kwon, J., Ko, J. & Hong, J.-I. (2012). *Chem. Asian J.* **7**, 343–350.
Ooyama, Y., Nagno, T., Inou, S., Imae, I., Komaguchi, K., Ohshita, J. & Harima, Y. (2011). *Chem. Eur. J.* **17**, 14837–14843.
Pawluć, P., Franczyk, A., Walkowiak, J., Hreczycho, G., Kubicki, M. & Marciniec, B. (2011). *Org. Lett.* **13**, 1976–1979.
Ramathilagam, C., Venkatesan, N., Rajakumar, P., Umarani, P. R. & Manivannan, V. (2011). *Acta Cryst.* E**67**, o2796.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Thomas, K. R. J., Lin, J. T., Tao, Y.-T. & Chuan, C.-H. (2004). *Chem. Mater.* **16**, 5437–5444.
Thomas, K. R. J., Lin, J. T., Tao, Y.-T. & Ko, C.-W. (2001). *J. Am. Chem. Soc.* **123**, 9404–9411.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.
Wu, F.-I., Shih, P.-I., Yuan, M.-C., Dixit, A. K., Shu, C.-F., Chung, Z.-M. & Diau, E. W.-G. (2005). *J. Mater. Chem.* **15**, 4753–4760.
Zhang, J.-Y. & Zhang, W.-Y. (2011). *Acta Cryst.* E**67**, o3307.

‡ Additional correspondence author: krjt8fcy@iitr.ernet.in.

# supplementary materials

*Acta Cryst.* (2012). E**68**, o1121 [doi:10.1107/S1600536812011336]

## *N*,*N*-Dimethyl-4-[(*E*)-2-(3,6,7-tribromo-9-butyl-9*H*-carbazol-2-yl)ethenyl]aniline

**Sushil Kumar, K. R. Justin Thomas, Seik Weng Ng and Edward R. T. Tiekink**

### Comment

Polysubstituted carbazole derivatives have been widely explored as functional materials for applications in organic light-emitting diodes (Thomas *et al.*, 2001; Thomas *et al.*, 2004; Wu *et al.*, 2005) and photovoltaic devices (Lee *et al.*, 2012; Ooyama *et al.*, 2011) due to their charge transporting and amorphous properties. Though the 3,6,9-trisubstituted (Thomas *et al.*, 2001; Thomas *et al.*, 2004) and 2,7,9-trisubstituted carbazole (Wu *et al.*, 2005; Lee *et al.*, 2012) compounds have been well documented in the literature, 2,3,6,7,9-pentasubstituted carbazole derivatives are relatively rare. Herein, the synthesis and crystal structure determination of the title compound, (I), are described. Several related structures are known (Pawluć *et al.*, 2011; Zhang & Zhang, 2011; Ramathilagam *et al.*, 2011).

In (I), the carbazole fused-ring system is planar with the r.m.s. deviation of the 13 fitted non-hydrogen atoms = 0.006 Å; the Br1, Br2 and Br3 atoms lie 0.058 (1), 0.062 (1) and 0.043 (1) Å out of this plane, respectively. The least-squares plane through the carbazole residue forms a dihedral angle of 6.15 (10)° with the benzene ring, indicating a small twist between the terminal ring systems. This twist is manifested in the value of the C15—C14—C17—C18 torsion angle of -11.2 (4)°. The butyl group is almost perpendicular to the carbazole plane with the C1—N1—C7—C8 torsion angle being -98.7 (3)°. Finally, the conformation about the C17═C18 bond [1.335 (4) Å] is *E*.

In the crystal packing, molecules are linked into linear supramolecular chains *via* C—H···Br interactions, Fig. 2 and Table 1. These are connected into double chains along [$\bar{7}$ 18 $\bar{1}$6] *via* *π*–*π* interactions occurring between five- and six-membered rings of the carbazole residue [centroid(N1,C1,C6,C11,C16)···centroid(C1–C6)$^{i}$ = 3.6333 (13) Å, angle between rings = 0.50 (12)° for symmetry operation *i*: 1 - *x*, 1 - *y*, -*z*]. Chains assemble into layers, with no specific interactions between them. In turn, the layers stack along (2 0 $\bar{2}$), again without specific interactions between them, Fig. 2.

### Experimental

A mixture of 2,3,6,7-tetrabromo-9-butyl-9*H*-carbazole (0.25 g, 0.47 mmol), styrene (0.29 g, 1.96 mmol), tetrabutylammonium bromide (0.32 g, 0.98 mmol), sodium acetate (1.6 g, 19.6 mmol), $Pd(OAc)_2$ (4 mg) and dimethylformamide (5 ml) was heated at 383 K for 48 h. Subsequently, it was cooled, then poured into water and extracted using ethyl acetate. On removal of solvent, a residue was obtained which on purification by column chromatography on silica gel gave an orange crystalline solid. Yield: 0.12 g, 42%. *M*.pt: 414 K. Crystals were grown from a solution of the title compound dissolved in dichloromethane/hexanes mixture (1:9 *v*/*v*).

$^{1}$H NMR (500 MHz, $CDCl_3$) *δ*: 8.20 (s, 1 H), 8.17 (s, 1 H), 7.63 (s, 1H), 7.58 (s, 1 H), 7.51 (d, J = 9.0 Hz, 2 H), 7.43 (d, J = 16 Hz, 1 H), 7.05 (d, J = 16 Hz, 1 H), 6.74 (d, J = 9 Hz, 2 H), 4.24 (t, J = 7.5 Hz, 2 H), 3.02 (s, 6 H), 1.86–1.83 (m, 2 H), 1.42–1.37 (m, 2 H), 0.97 (t, J = 7.5 Hz, 3 H); $^{13}$C NMR (125 MHz, $CDCl_3$) *δ*: 150.4, 140.7, 140.5, 136.2, 131.4, 128.1, 127.8, 127.4, 125.4, 124.6, 124.4, 124.0, 122.7, 121.6, 121.4, 115.0, 114.0, 113.5, 112.5, 112.4, 105.8, 100.0, 43.2, 40.5, 30.9, 20.6, 13.9.

### Refinement

Carbon-bound H-atoms were placed in calculated positions [C—H = 0.95 to 0.99 Å, $U_{iso}$(H) = 1.2 to 1.5$U_{eq}$(C)] and were included in the refinement in the riding model approximation. The maximum and minimum residual electron density peaks of 1.18 and 0.81 e Å$^{-3}$, respectively, were located 0.86 Å and 0.44 Å from the H2 and Br1 atoms, respectively.

### Computing details

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO* (Agilent, 2010); data reduction: *CrysAlis PRO* (Agilent, 2010); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

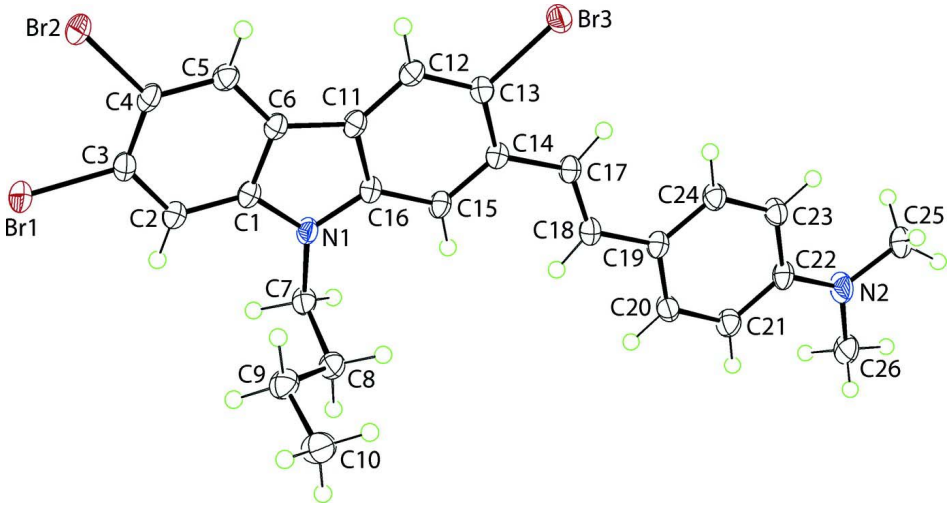



**Figure 1**

The molecular structure of (I) showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level.

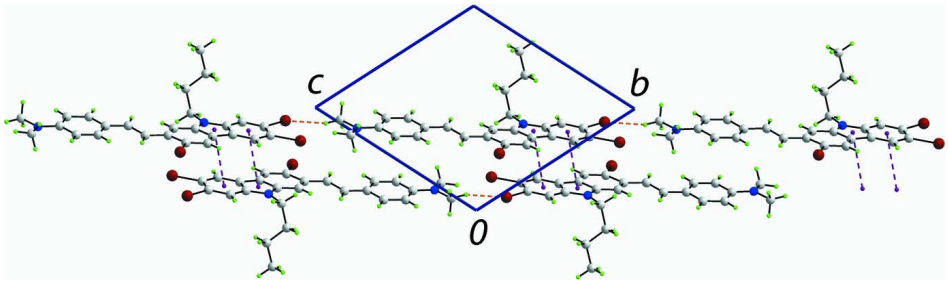



**Figure 2**

A view of the linear supramolecular chain in (I). The C—H···Br and $\pi$–$\pi$ interactions are shown as orange and purple dashed lines, respectively.

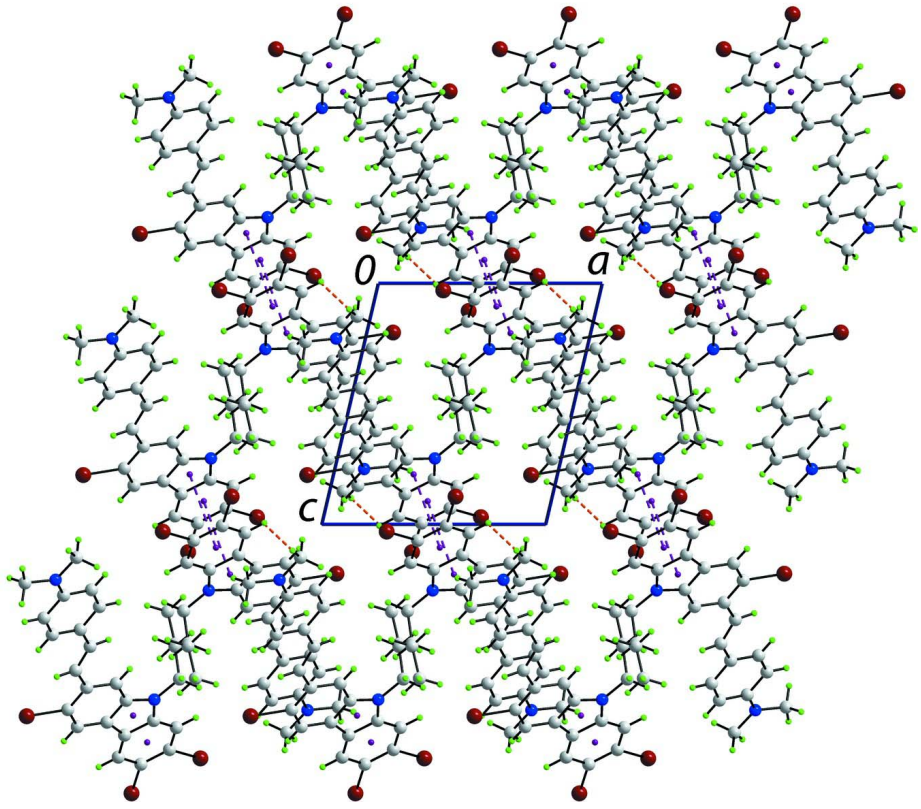



**Figure 3**

A view in projection down the *b* axis of the stacking of layers, formed by non-interacting supramolecular chains, in (I). The C—H···Br and $\pi$–$\pi$ interactions are shown as orange and purple dashed lines, respectively.

### *N*,*N*-Dimethyl-4-[(*E*)-2-(3,6,7-tribromo-9-butyl-9*H*- carbazol-2-yl)ethenyl]aniline

*Crystal data*

$C_{26}H_{25}Br_3N_2$
$M_r = 605.21$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 9.7304$ (3) Å
$b = 11.3834$ (4) Å
$c = 11.8197$ (4) Å
$\alpha = 114.308$ (3)°
$\beta = 101.957$ (3)°
$\gamma = 90.127$ (3)°
$V = 1161.62$ (7) Å$^3$
$Z = 2$
$F(000) = 600$
$D_x = 1.730$ Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 7879 reflections
$\theta = 4.2$–$76.4°$
$\mu = 6.56$ mm$^{-1}$
$T = 100$ K
Plate, orange
0.30 × 0.30 × 0.05 mm

*Data collection*

Agilent SuperNova Dual diffractometer with an Atlas detector
Radiation source: SuperNova (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.4041 pixels mm$^{-1}$
$\omega$ scan
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
$T_{min} = 0.244$, $T_{max} = 0.735$
10766 measured reflections
4827 independent reflections
4680 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$

$\theta_{max}$ = 76.6°, $\theta_{min}$ = 4.2°
$h$ = −12→12
$k$ = −14→14
$l$ = −14→10

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.092
$S$ = 1.07
4827 reflections
282 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
$w = 1/[\sigma^2(F_o^2) + (0.0613P)^2 + 0.89P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.18 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.81 e Å$^{-3}$

*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 (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Br1 | 0.29708 (3) | 0.83996 (3) | 0.02986 (2) | 0.02733 (9) |
| Br2 | 0.56802 (3) | 0.78783 (3) | −0.11524 (2) | 0.02739 (9) |
| Br3 | 1.11706 (3) | 0.35337 (3) | 0.20455 (3) | 0.02790 (9) |
| N1 | 0.5643 (2) | 0.5740 (2) | 0.27349 (19) | 0.0222 (4) |
| N2 | 1.1308 (3) | 0.0298 (3) | 0.7703 (2) | 0.0333 (5) |
| C1 | 0.5457 (2) | 0.6291 (2) | 0.1869 (2) | 0.0209 (4) |
| C2 | 0.4366 (3) | 0.6979 (2) | 0.1578 (2) | 0.0228 (5) |
| H2 | 0.3598 | 0.7132 | 0.1986 | 0.027* |
| C3 | 0.4443 (3) | 0.7433 (2) | 0.0664 (2) | 0.0226 (5) |
| C4 | 0.5569 (3) | 0.7208 (2) | 0.0055 (2) | 0.0227 (5) |
| C5 | 0.6653 (3) | 0.6523 (2) | 0.0351 (2) | 0.0232 (5) |
| H5 | 0.7418 | 0.6373 | −0.0061 | 0.028* |
| C6 | 0.6601 (2) | 0.6056 (2) | 0.1262 (2) | 0.0205 (4) |
| C7 | 0.4735 (2) | 0.5794 (2) | 0.3587 (2) | 0.0236 (5) |
| H7A | 0.4651 | 0.4940 | 0.3615 | 0.028* |
| H7B | 0.3780 | 0.5967 | 0.3240 | 0.028* |
| C8 | 0.5283 (3) | 0.6836 (2) | 0.4944 (2) | 0.0263 (5) |
| H8A | 0.4684 | 0.6752 | 0.5494 | 0.032* |
| H8B | 0.6253 | 0.6681 | 0.5274 | 0.032* |
| C9 | 0.5301 (3) | 0.8209 (3) | 0.5043 (2) | 0.0295 (5) |
| H9A | 0.4321 | 0.8398 | 0.4793 | 0.035* |
| H9B | 0.5833 | 0.8280 | 0.4441 | 0.035* |
| C10 | 0.5972 (3) | 0.9205 (3) | 0.6384 (3) | 0.0357 (6) |
| H10A | 0.5967 | 1.0074 | 0.6403 | 0.054* |

| | | | | |
|---|---|---|---|---|
| H10B | 0.6947 | 0.9029 | 0.6632 | 0.054* |
| H10C | 0.5434 | 0.9155 | 0.6980 | 0.054* |
| C11 | 0.7525 (3) | 0.5336 (2) | 0.1799 (2) | 0.0213 (4) |
| C12 | 0.8799 (3) | 0.4835 (2) | 0.1613 (2) | 0.0223 (5) |
| H12 | 0.9246 | 0.4940 | 0.1014 | 0.027* |
| C13 | 0.9406 (2) | 0.4177 (2) | 0.2322 (2) | 0.0217 (4) |
| C14 | 0.8789 (2) | 0.3989 (2) | 0.3234 (2) | 0.0207 (4) |
| C15 | 0.7510 (3) | 0.4504 (2) | 0.3406 (2) | 0.0216 (4) |
| H15 | 0.7059 | 0.4402 | 0.4004 | 0.026* |
| C16 | 0.6895 (2) | 0.5168 (2) | 0.2704 (2) | 0.0207 (4) |
| C17 | 0.9466 (2) | 0.3259 (2) | 0.3949 (2) | 0.0211 (4) |
| H17 | 1.0239 | 0.2799 | 0.3683 | 0.025* |
| C18 | 0.9070 (3) | 0.3201 (2) | 0.4942 (2) | 0.0238 (5) |
| H18 | 0.8316 | 0.3687 | 0.5218 | 0.029* |
| C19 | 0.9685 (3) | 0.2460 (2) | 0.5642 (2) | 0.0222 (5) |
| C20 | 0.9072 (3) | 0.2399 (3) | 0.6593 (2) | 0.0258 (5) |
| H20 | 0.8267 | 0.2851 | 0.6769 | 0.031* |
| C21 | 0.9600 (3) | 0.1702 (3) | 0.7288 (3) | 0.0274 (5) |
| H21 | 0.9152 | 0.1683 | 0.7923 | 0.033* |
| C22 | 1.0787 (3) | 0.1029 (2) | 0.7058 (2) | 0.0245 (5) |
| C23 | 1.1426 (3) | 0.1108 (2) | 0.6119 (2) | 0.0253 (5) |
| H23 | 1.2248 | 0.0679 | 0.5958 | 0.030* |
| C24 | 1.0881 (3) | 0.1797 (2) | 0.5433 (2) | 0.0243 (5) |
| H24 | 1.1331 | 0.1822 | 0.4801 | 0.029* |
| C25 | 1.2647 (3) | −0.0235 (3) | 0.7574 (3) | 0.0300 (5) |
| H25A | 1.3375 | 0.0461 | 0.7772 | 0.045* |
| H25B | 1.2562 | −0.0885 | 0.6698 | 0.045* |
| H25C | 1.2909 | −0.0641 | 0.8166 | 0.045* |
| C26 | 1.0606 (3) | 0.0186 (3) | 0.8627 (3) | 0.0328 (6) |
| H26A | 0.9602 | −0.0093 | 0.8233 | 0.049* |
| H26B | 1.0708 | 0.1029 | 0.9360 | 0.049* |
| H26C | 1.1033 | −0.0453 | 0.8912 | 0.049* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Br1 | 0.02941 (16) | 0.02848 (15) | 0.02854 (15) | 0.00817 (11) | 0.00398 (11) | 0.01757 (11) |
| Br2 | 0.03297 (16) | 0.03048 (15) | 0.02791 (15) | 0.00781 (11) | 0.00784 (11) | 0.02082 (12) |
| Br3 | 0.02538 (15) | 0.03522 (16) | 0.03272 (16) | 0.01107 (11) | 0.01128 (11) | 0.02151 (12) |
| N1 | 0.0211 (9) | 0.0276 (10) | 0.0239 (9) | 0.0051 (8) | 0.0045 (8) | 0.0172 (8) |
| N2 | 0.0314 (12) | 0.0441 (13) | 0.0403 (13) | 0.0144 (10) | 0.0105 (10) | 0.0322 (11) |
| C1 | 0.0224 (11) | 0.0212 (10) | 0.0206 (10) | 0.0004 (9) | 0.0019 (8) | 0.0117 (9) |
| C2 | 0.0244 (11) | 0.0240 (11) | 0.0226 (11) | 0.0030 (9) | 0.0040 (9) | 0.0130 (9) |
| C3 | 0.0235 (11) | 0.0209 (10) | 0.0229 (11) | 0.0036 (9) | 0.0010 (9) | 0.0109 (9) |
| C4 | 0.0295 (12) | 0.0206 (10) | 0.0194 (10) | 0.0024 (9) | 0.0017 (9) | 0.0117 (9) |
| C5 | 0.0274 (12) | 0.0224 (11) | 0.0224 (11) | 0.0022 (9) | 0.0060 (9) | 0.0119 (9) |
| C6 | 0.0229 (11) | 0.0194 (10) | 0.0196 (10) | 0.0016 (8) | 0.0024 (8) | 0.0097 (9) |
| C7 | 0.0200 (11) | 0.0291 (12) | 0.0287 (12) | 0.0031 (9) | 0.0068 (9) | 0.0184 (10) |
| C8 | 0.0274 (12) | 0.0322 (13) | 0.0270 (12) | 0.0070 (10) | 0.0095 (9) | 0.0184 (10) |
| C9 | 0.0344 (13) | 0.0315 (13) | 0.0281 (12) | 0.0033 (10) | 0.0084 (10) | 0.0172 (11) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C10 | 0.0428 (16) | 0.0347 (14) | 0.0303 (13) | 0.0040 (12) | 0.0104 (12) | 0.0133 (11) |
| C11 | 0.0242 (11) | 0.0199 (10) | 0.0212 (11) | 0.0006 (9) | 0.0022 (9) | 0.0116 (9) |
| C12 | 0.0254 (12) | 0.0231 (11) | 0.0211 (11) | 0.0018 (9) | 0.0051 (9) | 0.0120 (9) |
| C13 | 0.0193 (11) | 0.0225 (10) | 0.0238 (11) | 0.0021 (8) | 0.0035 (9) | 0.0109 (9) |
| C14 | 0.0198 (11) | 0.0218 (11) | 0.0216 (11) | 0.0014 (8) | 0.0024 (8) | 0.0112 (9) |
| C15 | 0.0238 (11) | 0.0227 (11) | 0.0230 (11) | 0.0029 (9) | 0.0037 (9) | 0.0150 (9) |
| C16 | 0.0203 (11) | 0.0217 (10) | 0.0215 (11) | 0.0023 (8) | 0.0020 (8) | 0.0118 (9) |
| C17 | 0.0206 (10) | 0.0193 (10) | 0.0239 (11) | 0.0013 (8) | 0.0018 (8) | 0.0112 (9) |
| C18 | 0.0230 (11) | 0.0240 (11) | 0.0262 (11) | 0.0056 (9) | 0.0028 (9) | 0.0137 (9) |
| C19 | 0.0214 (11) | 0.0235 (11) | 0.0240 (11) | 0.0017 (9) | 0.0023 (9) | 0.0136 (9) |
| C20 | 0.0220 (11) | 0.0318 (12) | 0.0301 (12) | 0.0086 (9) | 0.0080 (9) | 0.0183 (10) |
| C21 | 0.0257 (12) | 0.0344 (13) | 0.0292 (12) | 0.0037 (10) | 0.0069 (10) | 0.0200 (11) |
| C22 | 0.0234 (11) | 0.0261 (11) | 0.0285 (12) | 0.0036 (9) | 0.0021 (9) | 0.0177 (10) |
| C23 | 0.0228 (11) | 0.0272 (12) | 0.0303 (12) | 0.0061 (9) | 0.0061 (9) | 0.0164 (10) |
| C24 | 0.0238 (11) | 0.0262 (12) | 0.0274 (12) | 0.0045 (9) | 0.0055 (9) | 0.0160 (10) |
| C25 | 0.0283 (13) | 0.0314 (13) | 0.0345 (13) | 0.0084 (10) | 0.0028 (10) | 0.0200 (11) |
| C26 | 0.0347 (14) | 0.0421 (15) | 0.0350 (14) | 0.0110 (12) | 0.0093 (11) | 0.0286 (12) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Br1—C3 | 1.895 (2) | C11—C12 | 1.386 (3) |
| Br2—C4 | 1.895 (2) | C11—C16 | 1.413 (3) |
| Br3—C13 | 1.906 (2) | C12—C13 | 1.388 (3) |
| N1—C16 | 1.382 (3) | C12—H12 | 0.9500 |
| N1—C1 | 1.388 (3) | C13—C14 | 1.423 (3) |
| N1—C7 | 1.455 (3) | C14—C15 | 1.394 (3) |
| N2—C22 | 1.378 (3) | C14—C17 | 1.479 (3) |
| N2—C26 | 1.447 (3) | C15—C16 | 1.389 (3) |
| N2—C25 | 1.448 (3) | C15—H15 | 0.9500 |
| C1—C2 | 1.390 (3) | C17—C18 | 1.335 (4) |
| C1—C6 | 1.415 (3) | C17—H17 | 0.9500 |
| C2—C3 | 1.390 (3) | C18—C19 | 1.458 (3) |
| C2—H2 | 0.9500 | C18—H18 | 0.9500 |
| C3—C4 | 1.401 (4) | C19—C24 | 1.398 (3) |
| C4—C5 | 1.385 (3) | C19—C20 | 1.401 (3) |
| C5—C6 | 1.393 (3) | C20—C21 | 1.390 (4) |
| C5—H5 | 0.9500 | C20—H20 | 0.9500 |
| C6—C11 | 1.442 (3) | C21—C22 | 1.399 (4) |
| C7—C8 | 1.530 (4) | C21—H21 | 0.9500 |
| C7—H7A | 0.9900 | C22—C23 | 1.412 (3) |
| C7—H7B | 0.9900 | C23—C24 | 1.379 (3) |
| C8—C9 | 1.518 (4) | C23—H23 | 0.9500 |
| C8—H8A | 0.9900 | C24—H24 | 0.9500 |
| C8—H8B | 0.9900 | C25—H25A | 0.9800 |
| C9—C10 | 1.520 (4) | C25—H25B | 0.9800 |
| C9—H9A | 0.9900 | C25—H25C | 0.9800 |
| C9—H9B | 0.9900 | C26—H26A | 0.9800 |
| C10—H10A | 0.9800 | C26—H26B | 0.9800 |
| C10—H10B | 0.9800 | C26—H26C | 0.9800 |
| C10—H10C | 0.9800 | | |

| | | | |
|---|---|---|---|
| C16—N1—C1 | 108.3 (2) | C11—C12—C13 | 118.5 (2) |
| C16—N1—C7 | 124.7 (2) | C11—C12—H12 | 120.7 |
| C1—N1—C7 | 126.9 (2) | C13—C12—H12 | 120.7 |
| C22—N2—C26 | 120.0 (2) | C12—C13—C14 | 123.4 (2) |
| C22—N2—C25 | 120.1 (2) | C12—C13—Br3 | 116.64 (18) |
| C26—N2—C25 | 119.5 (2) | C14—C13—Br3 | 119.95 (18) |
| C2—C1—N1 | 129.2 (2) | C15—C14—C13 | 117.0 (2) |
| C2—C1—C6 | 121.6 (2) | C15—C14—C17 | 121.7 (2) |
| N1—C1—C6 | 109.1 (2) | C13—C14—C17 | 121.3 (2) |
| C1—C2—C3 | 117.4 (2) | C14—C15—C16 | 120.1 (2) |
| C1—C2—H2 | 121.3 | C14—C15—H15 | 119.9 |
| C3—C2—H2 | 121.3 | C16—C15—H15 | 119.9 |
| C2—C3—C4 | 121.7 (2) | N1—C16—C15 | 128.7 (2) |
| C2—C3—Br1 | 117.04 (19) | N1—C16—C11 | 109.5 (2) |
| C4—C3—Br1 | 121.27 (18) | C15—C16—C11 | 121.8 (2) |
| C5—C4—C3 | 120.7 (2) | C18—C17—C14 | 124.7 (2) |
| C5—C4—Br2 | 118.33 (19) | C18—C17—H17 | 117.7 |
| C3—C4—Br2 | 120.98 (18) | C14—C17—H17 | 117.7 |
| C4—C5—C6 | 118.8 (2) | C17—C18—C19 | 126.1 (2) |
| C4—C5—H5 | 120.6 | C17—C18—H18 | 117.0 |
| C6—C5—H5 | 120.6 | C19—C18—H18 | 117.0 |
| C5—C6—C1 | 119.8 (2) | C24—C19—C20 | 116.7 (2) |
| C5—C6—C11 | 133.5 (2) | C24—C19—C18 | 123.8 (2) |
| C1—C6—C11 | 106.6 (2) | C20—C19—C18 | 119.5 (2) |
| N1—C7—C8 | 112.9 (2) | C21—C20—C19 | 122.3 (2) |
| N1—C7—H7A | 109.0 | C21—C20—H20 | 118.8 |
| C8—C7—H7A | 109.0 | C19—C20—H20 | 118.8 |
| N1—C7—H7B | 109.0 | C20—C21—C22 | 120.4 (2) |
| C8—C7—H7B | 109.0 | C20—C21—H21 | 119.8 |
| H7A—C7—H7B | 107.8 | C22—C21—H21 | 119.8 |
| C9—C8—C7 | 114.0 (2) | N2—C22—C21 | 121.7 (2) |
| C9—C8—H8A | 108.8 | N2—C22—C23 | 120.8 (2) |
| C7—C8—H8A | 108.8 | C21—C22—C23 | 117.5 (2) |
| C9—C8—H8B | 108.8 | C24—C23—C22 | 121.3 (2) |
| C7—C8—H8B | 108.8 | C24—C23—H23 | 119.4 |
| H8A—C8—H8B | 107.7 | C22—C23—H23 | 119.4 |
| C8—C9—C10 | 112.2 (2) | C23—C24—C19 | 121.7 (2) |
| C8—C9—H9A | 109.2 | C23—C24—H24 | 119.1 |
| C10—C9—H9A | 109.2 | C19—C24—H24 | 119.1 |
| C8—C9—H9B | 109.2 | N2—C25—H25A | 109.5 |
| C10—C9—H9B | 109.2 | N2—C25—H25B | 109.5 |
| H9A—C9—H9B | 107.9 | H25A—C25—H25B | 109.5 |
| C9—C10—H10A | 109.5 | N2—C25—H25C | 109.5 |
| C9—C10—H10B | 109.5 | H25A—C25—H25C | 109.5 |
| H10A—C10—H10B | 109.5 | H25B—C25—H25C | 109.5 |
| C9—C10—H10C | 109.5 | N2—C26—H26A | 109.5 |
| H10A—C10—H10C | 109.5 | N2—C26—H26B | 109.5 |
| H10B—C10—H10C | 109.5 | H26A—C26—H26B | 109.5 |

| | | | |
|---|---|---|---|
| C12—C11—C16 | 119.2 (2) | N2—C26—H26C | 109.5 |
| C12—C11—C6 | 134.4 (2) | H26A—C26—H26C | 109.5 |
| C16—C11—C6 | 106.4 (2) | H26B—C26—H26C | 109.5 |
| | | | |
| C16—N1—C1—C2 | −179.3 (2) | C12—C13—C14—C17 | 178.9 (2) |
| C7—N1—C1—C2 | −2.2 (4) | Br3—C13—C14—C17 | −2.1 (3) |
| C16—N1—C1—C6 | 0.7 (3) | C13—C14—C15—C16 | −0.1 (3) |
| C7—N1—C1—C6 | 177.8 (2) | C17—C14—C15—C16 | −179.1 (2) |
| N1—C1—C2—C3 | 179.8 (2) | C1—N1—C16—C15 | 180.0 (2) |
| C6—C1—C2—C3 | −0.2 (4) | C7—N1—C16—C15 | 2.7 (4) |
| C1—C2—C3—C4 | 0.2 (4) | C1—N1—C16—C11 | −0.6 (3) |
| C1—C2—C3—Br1 | −178.73 (17) | C7—N1—C16—C11 | −177.9 (2) |
| C2—C3—C4—C5 | −0.2 (4) | C14—C15—C16—N1 | 179.8 (2) |
| Br1—C3—C4—C5 | 178.67 (18) | C14—C15—C16—C11 | 0.4 (4) |
| C2—C3—C4—Br2 | −178.20 (19) | C12—C11—C16—N1 | 180.0 (2) |
| Br1—C3—C4—Br2 | 0.6 (3) | C6—C11—C16—N1 | 0.4 (3) |
| C3—C4—C5—C6 | 0.2 (4) | C12—C11—C16—C15 | −0.6 (3) |
| Br2—C4—C5—C6 | 178.27 (18) | C6—C11—C16—C15 | 179.8 (2) |
| C4—C5—C6—C1 | −0.2 (4) | C15—C14—C17—C18 | −11.2 (4) |
| C4—C5—C6—C11 | −179.3 (2) | C13—C14—C17—C18 | 169.8 (2) |
| C2—C1—C6—C5 | 0.2 (4) | C14—C17—C18—C19 | 178.0 (2) |
| N1—C1—C6—C5 | −179.8 (2) | C17—C18—C19—C24 | 6.3 (4) |
| C2—C1—C6—C11 | 179.5 (2) | C17—C18—C19—C20 | −174.2 (2) |
| N1—C1—C6—C11 | −0.4 (3) | C24—C19—C20—C21 | −1.0 (4) |
| C16—N1—C7—C8 | 78.0 (3) | C18—C19—C20—C21 | 179.5 (2) |
| C1—N1—C7—C8 | −98.7 (3) | C19—C20—C21—C22 | 0.2 (4) |
| N1—C7—C8—C9 | 65.2 (3) | C26—N2—C22—C21 | 1.4 (4) |
| C7—C8—C9—C10 | −175.0 (2) | C25—N2—C22—C21 | −171.3 (2) |
| C5—C6—C11—C12 | −0.2 (5) | C26—N2—C22—C23 | −177.6 (3) |
| C1—C6—C11—C12 | −179.5 (3) | C25—N2—C22—C23 | 9.7 (4) |
| C5—C6—C11—C16 | 179.3 (3) | C20—C21—C22—N2 | −178.0 (3) |
| C1—C6—C11—C16 | 0.0 (3) | C20—C21—C22—C23 | 1.1 (4) |
| C16—C11—C12—C13 | 0.4 (3) | N2—C22—C23—C24 | 177.5 (3) |
| C6—C11—C12—C13 | 179.8 (2) | C21—C22—C23—C24 | −1.6 (4) |
| C11—C12—C13—C14 | 0.0 (4) | C22—C23—C24—C19 | 0.8 (4) |
| C11—C12—C13—Br3 | −179.05 (17) | C20—C19—C24—C23 | 0.6 (4) |
| C12—C13—C14—C15 | −0.2 (4) | C18—C19—C24—C23 | 180.0 (2) |
| Br3—C13—C14—C15 | 178.85 (17) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C26—H26*C*···Br1$^{i}$ | 0.98 | 2.91 | 3.844 (3) | 161 |

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