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# 2,8-Dimesitylboranyl-6*H*,12*H*-5,11-methanodibenzo[*b*,*f*][1,5]diazocine

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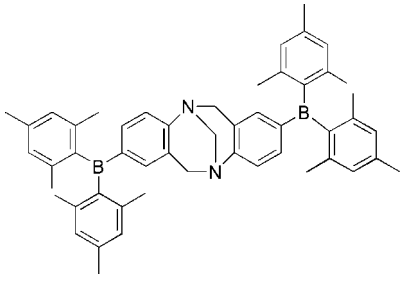
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.056; $wR$ factor = 0.172; data-to-parameter ratio = 16.8.

In the title compound, $C_{51}H_{56}B_2N_2$, a substituted Tröger's base, the dihedral angle between the two benzene rings constituting the Tröger's base framework is 104.42 (6)°. The crystal structure is stabilized by C—H$\cdots\pi$ and weak C—H$\cdots$N interactions.

## Related literature

For the original Tröger's base, see: Tröger (1887). For the chemistry of Tröger's base, see: Valík *et al.* (2005); Dolenský *et al.* (2007); Sergeyev (2009). For optoelectric applications of Tröger's base, see: Yuan *et al.* (2011); Xin *et al.* (2008); Yuan *et al.* (2007). For applications of organic boron compounds with dimesitylboryl groups in organic optoelectronics, see: Shirota & Noda (1998); Zhao *et al.* (2006); Collings *et al.* (2009); Jäkle (2010).




## Experimental

### Crystal data

$C_{51}H_{56}B_2N_2$
$M_r$ = 718.60
Triclinic, $P\overline{1}$
$a$ = 9.3565 (3) Å
$b$ = 14.0077 (6) Å
$c$ = 16.3650 (6) Å
$\alpha$ = 86.079 (3)°
$\beta$ = 83.808 (3)°
$\gamma$ = 88.377 (3)°
$V$ = 2126.87 (14) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.06 mm$^{-1}$
$T$ = 293 K
0.65 × 0.41 × 0.22 mm

### Data collection

Oxford Diffraction Xcalibur Eos Gemini CCD diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)
$T_{min}$ = 0.858, $T_{max}$ = 1.000
25278 measured reflections
8341 independent reflections
6172 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.026

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.172
$S$ = 1.02
8341 reflections
496 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.28 e Å$^{-3}$

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

*Cg*7 and *Cg*8 are the centroids of the C34–C37/C39/C40 and C43/C44/C46/C47/C49/C50 rings, respectively.

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| C14—H14*C*$\cdots$N2$^{i}$ | 0.96 | 2.64 | 3.448 (3) | 141 |
| C15—H15*A*$\cdots$*Cg*7$^{ii}$ | 0.93 | 2.94 | 3.844 (2) | 166 |
| C38—H40*B*$\cdots$*Cg*8$^{iii}$ | 0.97 | 3.00 | 3.751 (3) | 136 |

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2166).

## References

Collings, J. C., Poon, S.-Y., Droumaguet, C. L., Charlot, M., Katan, C., Pålsson, L. O., Beeby, A., Mosely, J. A., Kaiser, H. M., Kaufmann, D., Wong, W.-Y., Blanchard-Desce, M. & Marder, T. B. (2009). *Chem. Eur. J.* **15**, 198–208.
Dolenský, B., Elguero, J., Král, V., Pardo, C. & Valík, M. (2007). *Adv. Heterocycl. Chem.* **93**, 1–56.
Jäkle, F. (2010). *Chem. Rev.* **110**, 3985–4022.
Oxford Diffraction (2009). *CrysAlis PRO*, *CrysAlis CCD* and *CrysAlis RED*. Oxford Diffraction Ltd, Yarnton, England.
Sergeyev, S. (2009). *Helv. Chim. Acta*, **92**, 415–444.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Shirota, Y. & Noda, T. (1998). *J. Am. Chem. Soc.* **120**, 9714–9715.
Tröger, J. (1887). *J. Prakt. Chem.* **36**, 225–245.
Valík, M., Strongin, R. M. & Král, V. (2005). *Supramol. Chem.* **17**, 347–367.
Xin, Q., Tao, X. T., Wang, F. Z., Sun, J. L., Zou, D. C., Wang, F. J., Liu, H. J., Liu, Z. & Jiang, M. H. (2008). *Org. Electron.* **9**, 1076–1086.
Yuan, C. X., Tao, X. T., Ren, Y., Yang, J. X., Yu, W. T., Wang, L. & Jiang, M. H. (2007). *J. Phys. Chem. C*, **111**, 12811–12816.
Yuan, C. X., Xin, Q., Liu, H. J., Wang, L., Jiang, M. H. & Tao, X. T. (2011). *Sci. Chin. Chem.* **54**, 587–595.
Zhao, C. H., Wakamiya, A., Inukai, Y. & Yamaguchi, S. (2006). *J. Am. Chem. Soc.* **128**, 15934–15935.

# supplementary materials

*Acta Cryst.* (2012). E**68**, o22 [ **doi:10.1107/S1600536811051051** ]

# 2,8-Dimesitylboranyl-6*H*,12*H*-5,11-methanodibenzo[*b*,*f*][1,5]diazocine

**C.-X. Yuan**

## Comment

Tröger's base (TB) (Tröger, 1887), an old compound with more than 100 years' history, has gained current interest because of its $C_2$ symmetry, chirality, and rigid concave shape (Valík *et al.*, 2005; Dolenský *et al.*, 2007; Sergeyev *et al.*, 2009). Our previous research showed that its special lambda (Λ)-shaped configuration is disadvantageous to formation of $\pi$–$\pi$ close stacking, resulting in high solid state fluorescence in organic compounds based on TB (Yuan *et al.*, 2007; Xin *et al.*, 2008; Yuan *et al.*, 2011). In addition, organic boron compounds with dimesitylboryl groups exhibit interesting optoelectronic properties (Shirota & Noda, 1998; Zhao *et al.*,2006; Collings *et al.*, 2009; Jäkle *et al.*, 2010). In our research in searching for new optoelectronic materials based on TB, the title compound was designed and synthesized. Here, we report the synthesis and crystal structure of the title compound $C_{51}H_{56}B_2N_2$ (I).

In the racemic title compound (Fig. 1), the dihedral angle between the two benzene rings constituting the TB framework is 104.42 (6)°, which lies within the normal range for analogs of TB (Dolenský *et al.*, 2007). The packing structure of (I) (Fig. 2) shows that molecules with the same chirality point in the same direction, while molecules with different chirality point in the opposite direction. The isomers stack alternately, forming an infinite three-dimensional network by means of noncovalent intermolecular C—H···π interactions between adjacent different chirality molecules and weak C—H···N interactions between adjacent same chirality molecules (Table 1). As expected, there are no obvious intermolecular π···π interactions in the crystal structure.

## Experimental

The reaction scheme for the synthesis of the title compound is shown in Fig. 3. n-Butyllithium (1.6 *M* in hexane, 1.86 ml) was added slowly to a solution of 2,8-dibromo-6*H*,12*H*-5,11-methanodibenzo[*b*,*f*][1,5]\ diazocine (1.243 mmol, 0.472 g) in anhydrous THF (20 ml) under nitrogen at -78 °C, and followed by stirring for a further 1.5 h. Dimesitylboron fluoride (3.729 mmol, 1 g in 5 ml THF) was then added dropwise to the reaction mixture and the reaction mixture was kept at -78 °C for another 1 h, then allowed to naturally rise to room temperature overnight. Water (20 ml) was added and the mixture was extracted with $CH_2Cl_2$ three times and the organic phase was dried over anhydrous $MgSO_4$. After removing all solvents, the residue was purified by silica gel column chromatography with petroleum ether/EtOAc (10:1) as the eluent to yield the product as a white powder (0.58 g, 65%). The colorless prismatic single-crystal of compound (I) suitable for X-ray analysis was obtained by slow evaporation of its dichloromethane-petroleum ether solution.

$^1$H NMR (300 MHz, $CDCl_3$), δ (ppm): 1.90 (s, 24H), 2.28 (s, 12H), 4.15 (d, 2H, $J$ = 16.5 Hz), 4.37 (s, 2H), 4.64 (d, 2H, $J$ = 16.5 Hz), 6.78 (s, 8H), 7.04 (m, 4H), 7.27 (m, 2H). $^{13}$C NMR (75 MHz, $CDCl_3$), δ (ppm): 20.71, 22.80, 58.77, 66.55, 123.75, 126.58, 127.63, 135.19, 135.35, 137.94, 140.23, 141.16, 151.39.

### Refinement

All H atoms were fixed geometrically and were allowed to ride on their attached atoms, with C—H = 0.93 Å (aromatic), 0.97 ($CH_2$), and 0.96 Å ($CH_3$). The $U_{iso}$ values were constrained to be $1.5U_{eq}$(C) of the carrier atom for methyl H atoms and $1.2U_{eq}$(C) for the remaining H atoms.

### Figures

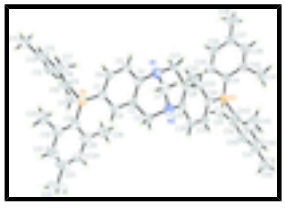


Fig. 1. The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

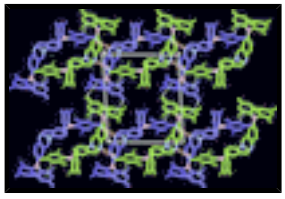


Fig. 2. Packing structure of the title compound viewed down the *a* axis, showing intermolecular C—H···π and C—H···N interactions as blue and orange dashed lines, respectively. H atoms not involved in C—H···π and C—H···N interactions have been omitted for clarity. (*S*, *S*)-(I) and (*R*, *R*)-(I) are colored as green and purple, respectively.

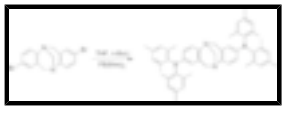


Fig. 3. Synthetic scheme for the synthesis of (I)

### 5-[bis(2,4,6-trimethylphenyl)boranyl]-13-[(2,4,5-trimethylphenyl)(2,4,6- trimethylphenyl)boranyl]-1,9-diazatetracyclo[7.7.1.$0^{2,7}$.$0^{10,15}$]heptadeca- 2,4,6,10 (15),11,13-hexaene

*Crystal data*

| | |
|---|---|
| $C_{51}H_{56}B_2N_2$ | $Z = 2$ |
| $M_r = 718.60$ | $F(000) = 772$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.122$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 9.3565$ (3) Å | Cell parameters from 8341 reflections |
| $b = 14.0077$ (6) Å | $\theta = 3.2$–$26°$ |
| $c = 16.3650$ (6) Å | $\mu = 0.06$ mm$^{-1}$ |
| $\alpha = 86.079$ (3)° | $T = 293$ K |
| $\beta = 83.808$ (3)° | Prism, colourless |
| $\gamma = 88.377$ (3)° | 0.65 × 0.41 × 0.22 mm |
| $V = 2126.87$ (14) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Oxford Diffraction Xcalibur Eos Gemini CCD diffractometer | 8341 independent reflections |
| Radiation source: fine-focus sealed tube | 6172 reflections with $I > 2\sigma(I)$ |

| | |
|---|---|
| graphite | $R_{int}$ = 0.026 |
| ω scans | $\theta_{max}$ = 26.0°, $\theta_{min}$ = 3.2° |
| Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009) | $h$ = −11→11 |
| $T_{min}$ = 0.858, $T_{max}$ = 1.000 | $k$ = −17→17 |
| 25278 measured reflections | $l$ = −20→20 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)]$ = 0.056 | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2)$ = 0.172 | H-atom parameters constrained |
| $S$ = 1.02 | $w = 1/[\sigma^2(F_o^2) + (0.0817P)^2 + 0.8104P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 8341 reflections | $(\Delta/\sigma)_{max} < 0.001$ |
| 496 parameters | $\Delta\rho_{max}$ = 0.39 e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min}$ = −0.28 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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N1 | 0.51726 (17) | 0.23628 (12) | −0.05204 (10) | 0.0431 (4) |
| N2 | 0.68504 (18) | 0.10503 (11) | −0.07519 (10) | 0.0423 (4) |
| B2 | 0.7203 (2) | 0.04164 (15) | 0.27696 (14) | 0.0393 (5) |
| B1 | 0.9474 (2) | 0.51197 (16) | −0.18209 (13) | 0.0392 (5) |
| C1 | 0.5453 (2) | 0.14646 (15) | −0.09129 (13) | 0.0506 (5) |
| H1A | 0.5426 | 0.1577 | −0.1503 | 0.061* |
| H1B | 0.4707 | 0.1016 | −0.0708 | 0.061* |
| C2 | 0.7951 (2) | 0.16395 (13) | −0.12414 (12) | 0.0429 (5) |
| H2A | 0.7995 | 0.1494 | −0.1815 | 0.052* |
| H2B | 0.8882 | 0.1483 | −0.1053 | 0.052* |
| C3 | 0.7623 (2) | 0.26997 (13) | −0.11699 (11) | 0.0364 (4) |
| C4 | 0.63185 (19) | 0.30059 (13) | −0.07553 (11) | 0.0366 (4) |

| | | | | |
|---|---|---|---|---|
| C5 | 0.6121 (2) | 0.39681 (14) | −0.06065 (12) | 0.0416 (4) |
| H5A | 0.5290 | 0.4170 | −0.0296 | 0.050* |
| C6 | 0.7135 (2) | 0.46231 (14) | −0.09109 (12) | 0.0417 (4) |
| H6A | 0.6975 | 0.5262 | −0.0800 | 0.050* |
| C7 | 0.8414 (2) | 0.43589 (13) | −0.13864 (11) | 0.0382 (4) |
| C8 | 0.8623 (2) | 0.33790 (13) | −0.14839 (11) | 0.0378 (4) |
| H8A | 0.9474 | 0.3173 | −0.1773 | 0.045* |
| C9 | 0.8986 (2) | 0.62122 (13) | −0.18429 (12) | 0.0389 (4) |
| C10 | 0.9727 (2) | 0.68868 (14) | −0.14580 (12) | 0.0420 (4) |
| C11 | 1.0972 (2) | 0.65917 (17) | −0.09758 (14) | 0.0556 (6) |
| H11A | 1.1338 | 0.7146 | −0.0761 | 0.083* |
| H11B | 1.1718 | 0.6299 | −0.1331 | 0.083* |
| H11C | 1.0651 | 0.6142 | −0.0529 | 0.083* |
| C12 | 0.9304 (2) | 0.78453 (14) | −0.15086 (13) | 0.0480 (5) |
| H12A | 0.9781 | 0.8276 | −0.1232 | 0.058* |
| C13 | 0.8197 (2) | 0.81844 (14) | −0.19557 (13) | 0.0470 (5) |
| C14 | 0.7811 (3) | 0.92348 (15) | −0.20363 (17) | 0.0670 (7) |
| H14A | 0.7024 | 0.9332 | −0.2366 | 0.100* |
| H14B | 0.8627 | 0.9582 | −0.2295 | 0.100* |
| H14C | 0.7537 | 0.9460 | −0.1500 | 0.100* |
| C15 | 0.7466 (2) | 0.75212 (14) | −0.23226 (13) | 0.0459 (5) |
| H15A | 0.6718 | 0.7732 | −0.2625 | 0.055* |
| C16 | 0.7802 (2) | 0.65504 (14) | −0.22575 (12) | 0.0436 (5) |
| C17 | 0.6879 (3) | 0.58954 (16) | −0.26633 (17) | 0.0622 (6) |
| H17A | 0.6139 | 0.6266 | −0.2909 | 0.093* |
| H17B | 0.6447 | 0.5433 | −0.2258 | 0.093* |
| H17C | 0.7465 | 0.5571 | −0.3081 | 0.093* |
| C18 | 1.0993 (2) | 0.48020 (13) | −0.22664 (13) | 0.0435 (5) |
| C19 | 1.1326 (3) | 0.49816 (15) | −0.31254 (14) | 0.0534 (5) |
| C20 | 1.0258 (3) | 0.5441 (2) | −0.36643 (15) | 0.0751 (8) |
| H20A | 1.0687 | 0.5500 | −0.4225 | 0.113* |
| H20B | 0.9983 | 0.6064 | −0.3484 | 0.113* |
| H20C | 0.9423 | 0.5051 | −0.3628 | 0.113* |
| C21 | 1.2663 (3) | 0.47011 (18) | −0.35033 (17) | 0.0684 (7) |
| H21A | 1.2852 | 0.4806 | −0.4071 | 0.082* |
| C22 | 1.3716 (3) | 0.42734 (19) | −0.3067 (2) | 0.0720 (8) |
| C23 | 1.5150 (3) | 0.3967 (3) | −0.3497 (3) | 0.1117 (14) |
| H23A | 1.5742 | 0.3685 | −0.3098 | 0.168* |
| H23B | 1.5617 | 0.4515 | −0.3781 | 0.168* |
| H23C | 1.5000 | 0.3507 | −0.3887 | 0.168* |
| C24 | 1.3400 (2) | 0.41133 (17) | −0.22313 (19) | 0.0662 (7) |
| H24A | 1.4104 | 0.3840 | −0.1924 | 0.079* |
| C25 | 1.2059 (2) | 0.43463 (15) | −0.18253 (15) | 0.0512 (5) |
| C26 | 1.1834 (3) | 0.4101 (2) | −0.09124 (16) | 0.0723 (7) |
| H26A | 1.2688 | 0.3794 | −0.0734 | 0.108* |
| H26B | 1.1041 | 0.3676 | −0.0790 | 0.108* |
| H26C | 1.1628 | 0.4675 | −0.0630 | 0.108* |
| C27 | 0.4894 (2) | 0.21334 (15) | 0.03740 (12) | 0.0467 (5) |
| H27A | 0.3945 | 0.1866 | 0.0500 | 0.056* |

| | | | | |
|---|---|---|---|---|
| H27B | 0.4914 | 0.2716 | 0.0661 | 0.056* |
| C28 | 0.60092 (19) | 0.14230 (13) | 0.06734 (11) | 0.0377 (4) |
| C29 | 0.69825 (19) | 0.09638 (13) | 0.01080 (11) | 0.0367 (4) |
| C30 | 0.8076 (2) | 0.03798 (13) | 0.03987 (12) | 0.0401 (4) |
| H30A | 0.8744 | 0.0089 | 0.0026 | 0.048* |
| C31 | 0.8177 (2) | 0.02289 (14) | 0.12294 (12) | 0.0413 (4) |
| H31A | 0.8926 | −0.0154 | 0.1406 | 0.050* |
| C32 | 0.7184 (2) | 0.06351 (13) | 0.18185 (11) | 0.0385 (4) |
| C33 | 0.6120 (2) | 0.12375 (14) | 0.15082 (12) | 0.0396 (4) |
| H33A | 0.5454 | 0.1528 | 0.1881 | 0.048* |
| C34 | 0.6102 (2) | 0.09831 (14) | 0.33754 (11) | 0.0406 (4) |
| C35 | 0.6192 (2) | 0.19725 (15) | 0.34510 (12) | 0.0457 (5) |
| C42 | 0.7362 (3) | 0.25709 (17) | 0.29743 (16) | 0.0668 (7) |
| H37A | 0.7231 | 0.3225 | 0.3113 | 0.100* |
| H37B | 0.7312 | 0.2534 | 0.2394 | 0.100* |
| H37C | 0.8284 | 0.2334 | 0.3113 | 0.100* |
| C36 | 0.5181 (2) | 0.24404 (17) | 0.39760 (13) | 0.0538 (5) |
| H38A | 0.5287 | 0.3088 | 0.4040 | 0.065* |
| C37 | 0.4024 (3) | 0.19763 (19) | 0.44059 (13) | 0.0588 (6) |
| C38 | 0.2895 (3) | 0.2517 (3) | 0.49355 (19) | 0.0949 (10) |
| H40A | 0.3146 | 0.3178 | 0.4918 | 0.142* |
| H40B | 0.2843 | 0.2248 | 0.5493 | 0.142* |
| H40C | 0.1978 | 0.2467 | 0.4731 | 0.142* |
| C39 | 0.3923 (2) | 0.10108 (19) | 0.43229 (14) | 0.0586 (6) |
| H41A | 0.3148 | 0.0687 | 0.4607 | 0.070* |
| C40 | 0.4933 (2) | 0.05027 (16) | 0.38313 (12) | 0.0467 (5) |
| C41 | 0.4710 (3) | −0.05449 (17) | 0.37687 (17) | 0.0651 (7) |
| H43A | 0.3867 | −0.0739 | 0.4121 | 0.098* |
| H43B | 0.5531 | −0.0903 | 0.3936 | 0.098* |
| H43C | 0.4588 | −0.0663 | 0.3210 | 0.098* |
| C43 | 0.8282 (2) | −0.03840 (14) | 0.30881 (11) | 0.0410 (4) |
| C44 | 0.8245 (2) | −0.13399 (15) | 0.28621 (12) | 0.0484 (5) |
| C45 | 0.7138 (3) | −0.16693 (17) | 0.23423 (17) | 0.0706 (7) |
| H46A | 0.7295 | −0.2337 | 0.2258 | 0.106* |
| H46B | 0.7223 | −0.1309 | 0.1819 | 0.106* |
| H46C | 0.6193 | −0.1571 | 0.2619 | 0.106* |
| C46 | 0.9208 (3) | −0.20248 (17) | 0.31466 (14) | 0.0594 (6) |
| H47A | 0.9144 | −0.2653 | 0.3005 | 0.071* |
| C47 | 1.0246 (3) | −0.1808 (2) | 0.36275 (15) | 0.0654 (7) |
| C48 | 1.1298 (4) | −0.2561 (3) | 0.3933 (2) | 0.1131 (13) |
| H49A | 1.1110 | −0.3166 | 0.3728 | 0.170* |
| H49B | 1.1186 | −0.2615 | 0.4524 | 0.170* |
| H49C | 1.2263 | −0.2378 | 0.3739 | 0.170* |
| C49 | 1.0302 (2) | −0.0873 (2) | 0.38415 (14) | 0.0614 (6) |
| H50A | 1.1013 | −0.0711 | 0.4160 | 0.074* |
| C50 | 0.9336 (2) | −0.01686 (16) | 0.35988 (12) | 0.0481 (5) |
| C51 | 0.9476 (3) | 0.08288 (19) | 0.38673 (16) | 0.0653 (7) |
| H52A | 1.0246 | 0.0838 | 0.4210 | 0.098* |
| H52B | 0.8593 | 0.1022 | 0.4172 | 0.098* |

| | | | | |
|---|---|---|---|---|
| H52C | 0.9677 | 0.1262 | 0.3391 | 0.098* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0345 (8) | 0.0484 (10) | 0.0461 (9) | −0.0048 (7) | −0.0092 (7) | 0.0084 (7) |
| N2 | 0.0504 (10) | 0.0381 (8) | 0.0387 (9) | −0.0070 (7) | −0.0052 (7) | −0.0019 (7) |
| B2 | 0.0376 (11) | 0.0381 (11) | 0.0428 (12) | −0.0068 (9) | −0.0072 (9) | −0.0001 (9) |
| B1 | 0.0407 (11) | 0.0400 (11) | 0.0385 (11) | −0.0025 (9) | −0.0096 (9) | −0.0042 (9) |
| C1 | 0.0517 (12) | 0.0526 (12) | 0.0498 (12) | −0.0127 (10) | −0.0177 (10) | 0.0042 (10) |
| C2 | 0.0540 (12) | 0.0358 (10) | 0.0372 (10) | −0.0014 (9) | 0.0043 (9) | −0.0042 (8) |
| C3 | 0.0415 (10) | 0.0357 (9) | 0.0316 (9) | 0.0013 (8) | −0.0035 (8) | −0.0008 (7) |
| C4 | 0.0333 (9) | 0.0423 (10) | 0.0339 (9) | 0.0014 (8) | −0.0072 (8) | 0.0035 (8) |
| C5 | 0.0329 (9) | 0.0467 (11) | 0.0437 (11) | 0.0078 (8) | −0.0002 (8) | −0.0016 (8) |
| C6 | 0.0429 (11) | 0.0352 (10) | 0.0469 (11) | 0.0053 (8) | −0.0043 (9) | −0.0053 (8) |
| C7 | 0.0373 (10) | 0.0380 (10) | 0.0391 (10) | 0.0015 (8) | −0.0038 (8) | −0.0026 (8) |
| C8 | 0.0360 (9) | 0.0395 (10) | 0.0368 (9) | 0.0029 (8) | 0.0010 (8) | −0.0030 (8) |
| C9 | 0.0382 (10) | 0.0361 (10) | 0.0417 (10) | −0.0042 (8) | −0.0001 (8) | −0.0027 (8) |
| C10 | 0.0414 (10) | 0.0421 (11) | 0.0414 (10) | −0.0106 (8) | 0.0044 (8) | −0.0053 (8) |
| C11 | 0.0534 (13) | 0.0603 (14) | 0.0553 (13) | −0.0144 (11) | −0.0108 (11) | −0.0061 (11) |
| C12 | 0.0493 (12) | 0.0415 (11) | 0.0524 (12) | −0.0146 (9) | 0.0077 (10) | −0.0135 (9) |
| C13 | 0.0459 (11) | 0.0341 (10) | 0.0568 (12) | −0.0021 (9) | 0.0158 (10) | −0.0055 (9) |
| C14 | 0.0688 (16) | 0.0363 (11) | 0.0908 (18) | −0.0001 (11) | 0.0171 (14) | −0.0080 (11) |
| C15 | 0.0423 (11) | 0.0400 (11) | 0.0536 (12) | 0.0018 (9) | 0.0011 (9) | −0.0015 (9) |
| C16 | 0.0440 (11) | 0.0377 (10) | 0.0495 (11) | −0.0014 (8) | −0.0050 (9) | −0.0054 (8) |
| C17 | 0.0648 (15) | 0.0453 (12) | 0.0817 (17) | −0.0009 (11) | −0.0311 (13) | −0.0052 (11) |
| C18 | 0.0420 (11) | 0.0358 (10) | 0.0528 (12) | −0.0061 (8) | −0.0016 (9) | −0.0073 (9) |
| C19 | 0.0609 (13) | 0.0411 (11) | 0.0569 (13) | −0.0092 (10) | 0.0060 (11) | −0.0096 (10) |
| C20 | 0.096 (2) | 0.0772 (18) | 0.0498 (14) | 0.0014 (16) | −0.0017 (14) | −0.0002 (12) |
| C21 | 0.0740 (17) | 0.0557 (14) | 0.0716 (16) | −0.0175 (13) | 0.0236 (14) | −0.0203 (12) |
| C22 | 0.0468 (13) | 0.0620 (16) | 0.107 (2) | −0.0127 (12) | 0.0158 (15) | −0.0387 (15) |
| C23 | 0.0571 (17) | 0.113 (3) | 0.165 (4) | −0.0117 (17) | 0.032 (2) | −0.076 (3) |
| C24 | 0.0419 (12) | 0.0555 (14) | 0.105 (2) | −0.0005 (10) | −0.0108 (13) | −0.0305 (14) |
| C25 | 0.0421 (11) | 0.0432 (11) | 0.0699 (14) | −0.0015 (9) | −0.0085 (10) | −0.0120 (10) |
| C26 | 0.0622 (15) | 0.0836 (18) | 0.0741 (17) | 0.0123 (14) | −0.0258 (13) | −0.0042 (14) |
| C27 | 0.0330 (10) | 0.0547 (12) | 0.0494 (12) | 0.0028 (9) | −0.0001 (9) | 0.0106 (9) |
| C28 | 0.0308 (9) | 0.0389 (10) | 0.0419 (10) | −0.0007 (8) | −0.0010 (8) | 0.0040 (8) |
| C29 | 0.0381 (10) | 0.0337 (9) | 0.0381 (10) | −0.0077 (8) | −0.0029 (8) | −0.0009 (7) |
| C30 | 0.0376 (10) | 0.0398 (10) | 0.0421 (10) | 0.0023 (8) | 0.0017 (8) | −0.0058 (8) |
| C31 | 0.0348 (10) | 0.0403 (10) | 0.0483 (11) | 0.0048 (8) | −0.0054 (8) | −0.0015 (8) |
| C32 | 0.0361 (10) | 0.0381 (10) | 0.0407 (10) | −0.0011 (8) | −0.0033 (8) | −0.0008 (8) |
| C33 | 0.0335 (9) | 0.0427 (10) | 0.0407 (10) | 0.0020 (8) | 0.0027 (8) | −0.0002 (8) |
| C34 | 0.0387 (10) | 0.0468 (11) | 0.0357 (10) | −0.0007 (8) | −0.0046 (8) | 0.0033 (8) |
| C35 | 0.0453 (11) | 0.0470 (11) | 0.0432 (11) | 0.0001 (9) | 0.0011 (9) | −0.0014 (9) |
| C42 | 0.0692 (16) | 0.0493 (13) | 0.0771 (17) | −0.0102 (12) | 0.0163 (13) | −0.0044 (12) |
| C36 | 0.0595 (13) | 0.0572 (13) | 0.0440 (11) | 0.0090 (11) | −0.0028 (10) | −0.0070 (10) |
| C37 | 0.0519 (13) | 0.0812 (17) | 0.0397 (11) | 0.0125 (12) | 0.0050 (10) | 0.0002 (11) |
| C38 | 0.081 (2) | 0.119 (3) | 0.0756 (19) | 0.0248 (19) | 0.0261 (16) | −0.0110 (18) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C39 | 0.0442 (12) | 0.0805 (17) | 0.0471 (12) | −0.0031 (11) | 0.0042 (10) | 0.0109 (11) |
| C40 | 0.0413 (11) | 0.0562 (12) | 0.0415 (11) | −0.0036 (9) | −0.0054 (9) | 0.0071 (9) |
| C41 | 0.0548 (14) | 0.0626 (15) | 0.0768 (17) | −0.0161 (12) | −0.0074 (12) | 0.0114 (12) |
| C43 | 0.0407 (10) | 0.0475 (11) | 0.0338 (9) | −0.0001 (8) | −0.0018 (8) | 0.0008 (8) |
| C44 | 0.0559 (12) | 0.0469 (12) | 0.0404 (11) | 0.0036 (10) | −0.0001 (9) | 0.0019 (9) |
| C45 | 0.096 (2) | 0.0479 (13) | 0.0715 (16) | −0.0103 (13) | −0.0217 (15) | −0.0085 (12) |
| C46 | 0.0688 (15) | 0.0538 (13) | 0.0492 (13) | 0.0147 (11) | 0.0123 (12) | 0.0070 (10) |
| C47 | 0.0513 (13) | 0.0804 (18) | 0.0567 (14) | 0.0226 (12) | 0.0073 (11) | 0.0202 (13) |
| C48 | 0.089 (2) | 0.115 (3) | 0.127 (3) | 0.052 (2) | −0.010 (2) | 0.027 (2) |
| C49 | 0.0398 (12) | 0.0920 (19) | 0.0499 (13) | 0.0043 (12) | −0.0058 (10) | 0.0127 (12) |
| C50 | 0.0401 (11) | 0.0653 (14) | 0.0376 (10) | −0.0018 (10) | −0.0021 (9) | 0.0030 (9) |
| C51 | 0.0590 (14) | 0.0805 (17) | 0.0607 (15) | −0.0077 (13) | −0.0188 (12) | −0.0125 (13) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| N1—C4 | 1.424 (2) | C23—H23C | 0.9600 |
| N1—C1 | 1.456 (3) | C24—C25 | 1.396 (3) |
| N1—C27 | 1.474 (2) | C24—H24A | 0.9300 |
| N2—C29 | 1.422 (2) | C25—C26 | 1.504 (3) |
| N2—C1 | 1.458 (3) | C26—H26A | 0.9600 |
| N2—C2 | 1.470 (2) | C26—H26B | 0.9600 |
| B2—C32 | 1.567 (3) | C26—H26C | 0.9600 |
| B2—C43 | 1.587 (3) | C27—C28 | 1.518 (3) |
| B2—C34 | 1.586 (3) | C27—H27A | 0.9700 |
| B1—C7 | 1.558 (3) | C27—H27B | 0.9700 |
| B1—C9 | 1.584 (3) | C28—C33 | 1.388 (3) |
| B1—C18 | 1.593 (3) | C28—C29 | 1.402 (3) |
| C1—H1A | 0.9700 | C29—C30 | 1.395 (3) |
| C1—H1B | 0.9700 | C30—C31 | 1.374 (3) |
| C2—C3 | 1.518 (2) | C30—H30A | 0.9300 |
| C2—H2A | 0.9700 | C31—C32 | 1.403 (3) |
| C2—H2B | 0.9700 | C31—H31A | 0.9300 |
| C3—C8 | 1.388 (3) | C32—C33 | 1.401 (3) |
| C3—C4 | 1.402 (3) | C33—H33A | 0.9300 |
| C4—C5 | 1.390 (3) | C34—C35 | 1.405 (3) |
| C5—C6 | 1.369 (3) | C34—C40 | 1.415 (3) |
| C5—H5A | 0.9300 | C35—C36 | 1.389 (3) |
| C6—C7 | 1.410 (3) | C35—C42 | 1.512 (3) |
| C6—H6A | 0.9300 | C42—H37A | 0.9600 |
| C7—C8 | 1.398 (3) | C42—H37B | 0.9600 |
| C8—H8A | 0.9300 | C42—H37C | 0.9600 |
| C9—C10 | 1.408 (3) | C36—C37 | 1.379 (3) |
| C9—C16 | 1.415 (3) | C36—H38A | 0.9300 |
| C10—C12 | 1.389 (3) | C37—C39 | 1.375 (4) |
| C10—C11 | 1.509 (3) | C37—C38 | 1.512 (3) |
| C11—H11A | 0.9600 | C38—H40A | 0.9600 |
| C11—H11B | 0.9600 | C38—H40B | 0.9600 |
| C11—H11C | 0.9600 | C38—H40C | 0.9600 |
| C12—C13 | 1.386 (3) | C39—C40 | 1.387 (3) |

| | | | |
|---|---|---|---|
| C12—H12A | 0.9300 | C39—H41A | 0.9300 |
| C13—C15 | 1.376 (3) | C40—C41 | 1.500 (3) |
| C13—C14 | 1.505 (3) | C41—H43A | 0.9600 |
| C14—H14A | 0.9600 | C41—H43B | 0.9600 |
| C14—H14B | 0.9600 | C41—H43C | 0.9600 |
| C14—H14C | 0.9600 | C43—C50 | 1.411 (3) |
| C15—C16 | 1.387 (3) | C43—C44 | 1.416 (3) |
| C15—H15A | 0.9300 | C44—C46 | 1.389 (3) |
| C16—C17 | 1.510 (3) | C44—C45 | 1.510 (3) |
| C17—H17A | 0.9600 | C45—H46A | 0.9600 |
| C17—H17B | 0.9600 | C45—H46B | 0.9600 |
| C17—H17C | 0.9600 | C45—H46C | 0.9600 |
| C18—C25 | 1.407 (3) | C46—C47 | 1.368 (4) |
| C18—C19 | 1.413 (3) | C46—H47A | 0.9300 |
| C19—C21 | 1.393 (3) | C47—C49 | 1.381 (4) |
| C19—C20 | 1.506 (4) | C47—C48 | 1.519 (3) |
| C20—H20A | 0.9600 | C48—H49A | 0.9600 |
| C20—H20B | 0.9600 | C48—H49B | 0.9600 |
| C20—H20C | 0.9600 | C48—H49C | 0.9600 |
| C21—C22 | 1.378 (4) | C49—C50 | 1.387 (3) |
| C21—H21A | 0.9300 | C49—H50A | 0.9300 |
| C22—C24 | 1.372 (4) | C50—C51 | 1.506 (3) |
| C22—C23 | 1.512 (3) | C51—H52A | 0.9600 |
| C23—H23A | 0.9600 | C51—H52B | 0.9600 |
| C23—H23B | 0.9600 | C51—H52C | 0.9600 |
| C4—N1—C1 | 110.56 (16) | C24—C25—C18 | 120.2 (2) |
| C4—N1—C27 | 114.46 (15) | C24—C25—C26 | 117.1 (2) |
| C1—N1—C27 | 107.63 (16) | C18—C25—C26 | 122.75 (19) |
| C29—N2—C1 | 110.91 (16) | C25—C26—H26A | 109.5 |
| C29—N2—C2 | 114.56 (15) | C25—C26—H26B | 109.5 |
| C1—N2—C2 | 107.14 (15) | H26A—C26—H26B | 109.5 |
| C32—B2—C43 | 118.92 (17) | C25—C26—H26C | 109.5 |
| C32—B2—C34 | 118.46 (17) | H26A—C26—H26C | 109.5 |
| C43—B2—C34 | 122.59 (17) | H26B—C26—H26C | 109.5 |
| C7—B1—C9 | 118.77 (17) | N1—C27—C28 | 111.06 (16) |
| C7—B1—C18 | 120.67 (17) | N1—C27—H27A | 109.4 |
| C9—B1—C18 | 120.52 (17) | C28—C27—H27A | 109.4 |
| N1—C1—N2 | 111.36 (16) | N1—C27—H27B | 109.4 |
| N1—C1—H1A | 109.4 | C28—C27—H27B | 109.4 |
| N2—C1—H1A | 109.4 | H27A—C27—H27B | 108.0 |
| N1—C1—H1B | 109.4 | C33—C28—C29 | 118.57 (17) |
| N2—C1—H1B | 109.4 | C33—C28—C27 | 120.96 (17) |
| H1A—C1—H1B | 108.0 | C29—C28—C27 | 120.43 (17) |
| N2—C2—C3 | 111.47 (15) | C30—C29—C28 | 119.17 (17) |
| N2—C2—H2A | 109.3 | C30—C29—N2 | 119.18 (16) |
| C3—C2—H2A | 109.3 | C28—C29—N2 | 121.60 (17) |
| N2—C2—H2B | 109.3 | C31—C30—C29 | 120.74 (17) |
| C3—C2—H2B | 109.3 | C31—C30—H30A | 119.6 |
| H2A—C2—H2B | 108.0 | C29—C30—H30A | 119.6 |

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|---|---|---|---|
| C8—C3—C4 | 118.87 (16) | C30—C31—C32 | 122.02 (17) |
| C8—C3—C2 | 120.89 (16) | C30—C31—H31A | 119.0 |
| C4—C3—C2 | 120.20 (17) | C32—C31—H31A | 119.0 |
| C5—C4—C3 | 118.98 (17) | C33—C32—C31 | 115.95 (17) |
| C5—C4—N1 | 119.50 (16) | C33—C32—B2 | 120.79 (17) |
| C3—C4—N1 | 121.45 (17) | C31—C32—B2 | 123.23 (17) |
| C6—C5—C4 | 120.86 (17) | C28—C33—C32 | 123.43 (17) |
| C6—C5—H5A | 119.6 | C28—C33—H33A | 118.3 |
| C4—C5—H5A | 119.6 | C32—C33—H33A | 118.3 |
| C5—C6—C7 | 122.04 (17) | C35—C34—C40 | 117.55 (18) |
| C5—C6—H6A | 119.0 | C35—C34—B2 | 122.38 (17) |
| C7—C6—H6A | 119.0 | C40—C34—B2 | 119.99 (18) |
| C8—C7—C6 | 115.80 (17) | C36—C35—C34 | 120.17 (19) |
| C8—C7—B1 | 122.30 (17) | C36—C35—C42 | 117.3 (2) |
| C6—C7—B1 | 121.79 (17) | C34—C35—C42 | 122.54 (18) |
| C3—C8—C7 | 123.14 (17) | C35—C42—H37A | 109.5 |
| C3—C8—H8A | 118.4 | C35—C42—H37B | 109.5 |
| C7—C8—H8A | 118.4 | H37A—C42—H37B | 109.5 |
| C10—C9—C16 | 117.43 (17) | C35—C42—H37C | 109.5 |
| C10—C9—B1 | 121.20 (17) | H37A—C42—H37C | 109.5 |
| C16—C9—B1 | 121.36 (16) | H37B—C42—H37C | 109.5 |
| C12—C10—C9 | 119.99 (19) | C37—C36—C35 | 122.2 (2) |
| C12—C10—C11 | 118.57 (18) | C37—C36—H38A | 118.9 |
| C9—C10—C11 | 121.44 (18) | C35—C36—H38A | 118.9 |
| C10—C11—H11A | 109.5 | C39—C37—C36 | 117.6 (2) |
| C10—C11—H11B | 109.5 | C39—C37—C38 | 121.4 (2) |
| H11A—C11—H11B | 109.5 | C36—C37—C38 | 121.0 (3) |
| C10—C11—H11C | 109.5 | C37—C38—H40A | 109.5 |
| H11A—C11—H11C | 109.5 | C37—C38—H40B | 109.5 |
| H11B—C11—H11C | 109.5 | H40A—C38—H40B | 109.5 |
| C13—C12—C10 | 122.51 (18) | C37—C38—H40C | 109.5 |
| C13—C12—H12A | 118.7 | H40A—C38—H40C | 109.5 |
| C10—C12—H12A | 118.7 | H40B—C38—H40C | 109.5 |
| C15—C13—C12 | 117.24 (18) | C37—C39—C40 | 122.4 (2) |
| C15—C13—C14 | 121.4 (2) | C37—C39—H41A | 118.8 |
| C12—C13—C14 | 121.4 (2) | C40—C39—H41A | 118.8 |
| C13—C14—H14A | 109.5 | C39—C40—C34 | 119.9 (2) |
| C13—C14—H14B | 109.5 | C39—C40—C41 | 118.3 (2) |
| H14A—C14—H14B | 109.5 | C34—C40—C41 | 121.66 (19) |
| C13—C14—H14C | 109.5 | C40—C41—H43A | 109.5 |
| H14A—C14—H14C | 109.5 | C40—C41—H43B | 109.5 |
| H14B—C14—H14C | 109.5 | H43A—C41—H43B | 109.5 |
| C13—C15—C16 | 122.4 (2) | C40—C41—H43C | 109.5 |
| C13—C15—H15A | 118.8 | H43A—C41—H43C | 109.5 |
| C16—C15—H15A | 118.8 | H43B—C41—H43C | 109.5 |
| C15—C16—C9 | 120.22 (18) | C50—C43—C44 | 117.15 (19) |
| C15—C16—C17 | 117.08 (19) | C50—C43—B2 | 121.31 (18) |
| C9—C16—C17 | 122.68 (18) | C44—C43—B2 | 121.53 (17) |
| C16—C17—H17A | 109.5 | C46—C44—C43 | 120.3 (2) |

| | | | |
|---|---|---|---|
| C16—C17—H17B | 109.5 | C46—C44—C45 | 117.3 (2) |
| H17A—C17—H17B | 109.5 | C43—C44—C45 | 122.30 (19) |
| C16—C17—H17C | 109.5 | C44—C45—H46A | 109.5 |
| H17A—C17—H17C | 109.5 | C44—C45—H46B | 109.5 |
| H17B—C17—H17C | 109.5 | H46A—C45—H46B | 109.5 |
| C25—C18—C19 | 117.46 (19) | C44—C45—H46C | 109.5 |
| C25—C18—B1 | 121.76 (18) | H46A—C45—H46C | 109.5 |
| C19—C18—B1 | 120.78 (19) | H46B—C45—H46C | 109.5 |
| C21—C19—C18 | 119.9 (2) | C47—C46—C44 | 122.3 (2) |
| C21—C19—C20 | 117.8 (2) | C47—C46—H47A | 118.9 |
| C18—C19—C20 | 122.2 (2) | C44—C46—H47A | 118.9 |
| C19—C20—H20A | 109.5 | C46—C47—C49 | 117.8 (2) |
| C19—C20—H20B | 109.5 | C46—C47—C48 | 121.9 (3) |
| H20A—C20—H20B | 109.5 | C49—C47—C48 | 120.3 (3) |
| C19—C20—H20C | 109.5 | C47—C48—H49A | 109.5 |
| H20A—C20—H20C | 109.5 | C47—C48—H49B | 109.5 |
| H20B—C20—H20C | 109.5 | H49A—C48—H49B | 109.5 |
| C22—C21—C19 | 122.5 (2) | C47—C48—H49C | 109.5 |
| C22—C21—H21A | 118.8 | H49A—C48—H49C | 109.5 |
| C19—C21—H21A | 118.8 | H49B—C48—H49C | 109.5 |
| C24—C22—C21 | 117.5 (2) | C47—C49—C50 | 122.4 (2) |
| C24—C22—C23 | 121.3 (3) | C47—C49—H50A | 118.8 |
| C21—C22—C23 | 121.1 (3) | C50—C49—H50A | 118.8 |
| C22—C23—H23A | 109.5 | C49—C50—C43 | 120.1 (2) |
| C22—C23—H23B | 109.5 | C49—C50—C51 | 118.5 (2) |
| H23A—C23—H23B | 109.5 | C43—C50—C51 | 121.33 (19) |
| C22—C23—H23C | 109.5 | C50—C51—H52A | 109.5 |
| H23A—C23—H23C | 109.5 | C50—C51—H52B | 109.5 |
| H23B—C23—H23C | 109.5 | H52A—C51—H52B | 109.5 |
| C22—C24—C25 | 122.4 (2) | C50—C51—H52C | 109.5 |
| C22—C24—H24A | 118.8 | H52A—C51—H52C | 109.5 |
| C25—C24—H24A | 118.8 | H52B—C51—H52C | 109.5 |
| C4—N1—C1—N2 | 53.9 (2) | C19—C18—C25—C26 | −179.0 (2) |
| C27—N1—C1—N2 | −71.8 (2) | B1—C18—C25—C26 | 1.8 (3) |
| C29—N2—C1—N1 | 53.3 (2) | C4—N1—C27—C28 | −76.7 (2) |
| C2—N2—C1—N1 | −72.4 (2) | C1—N1—C27—C28 | 46.6 (2) |
| C29—N2—C2—C3 | −78.0 (2) | N1—C27—C28—C33 | 168.09 (17) |
| C1—N2—C2—C3 | 45.4 (2) | N1—C27—C28—C29 | −9.7 (3) |
| N2—C2—C3—C8 | 170.59 (16) | C33—C28—C29—C30 | −3.5 (3) |
| N2—C2—C3—C4 | −7.0 (2) | C27—C28—C29—C30 | 174.35 (17) |
| C8—C3—C4—C5 | −5.8 (3) | C33—C28—C29—N2 | 174.10 (16) |
| C2—C3—C4—C5 | 171.83 (17) | C27—C28—C29—N2 | −8.0 (3) |
| C8—C3—C4—N1 | 171.16 (16) | C1—N2—C29—C30 | 164.55 (17) |
| C2—C3—C4—N1 | −11.2 (3) | C2—N2—C29—C30 | −74.0 (2) |
| C1—N1—C4—C5 | 165.27 (17) | C1—N2—C29—C28 | −13.1 (2) |
| C27—N1—C4—C5 | −73.0 (2) | C2—N2—C29—C28 | 108.4 (2) |
| C1—N1—C4—C3 | −11.6 (2) | C28—C29—C30—C31 | 2.1 (3) |
| C27—N1—C4—C3 | 110.09 (19) | N2—C29—C30—C31 | −175.63 (17) |
| C3—C4—C5—C6 | 4.8 (3) | C29—C30—C31—C32 | 1.1 (3) |

| | | | |
|---|---|---|---|
| N1—C4—C5—C6 | −172.19 (17) | C30—C31—C32—C33 | −2.7 (3) |
| C4—C5—C6—C7 | 0.1 (3) | C30—C31—C32—B2 | 175.32 (18) |
| C5—C6—C7—C8 | −3.9 (3) | C43—B2—C32—C33 | 171.14 (17) |
| C5—C6—C7—B1 | 172.35 (18) | C34—B2—C32—C33 | −6.9 (3) |
| C9—B1—C7—C8 | 166.36 (17) | C43—B2—C32—C31 | −6.8 (3) |
| C18—B1—C7—C8 | −11.2 (3) | C34—B2—C32—C31 | 175.19 (17) |
| C9—B1—C7—C6 | −9.6 (3) | C29—C28—C33—C32 | 2.0 (3) |
| C18—B1—C7—C6 | 172.85 (17) | C27—C28—C33—C32 | −175.89 (18) |
| C4—C3—C8—C7 | 2.0 (3) | C31—C32—C33—C28 | 1.1 (3) |
| C2—C3—C8—C7 | −175.62 (18) | B2—C32—C33—C28 | −176.96 (17) |
| C6—C7—C8—C3 | 2.8 (3) | C32—B2—C34—C35 | −67.2 (2) |
| B1—C7—C8—C3 | −173.40 (17) | C43—B2—C34—C35 | 114.8 (2) |
| C7—B1—C9—C10 | 117.5 (2) | C32—B2—C34—C40 | 109.4 (2) |
| C18—B1—C9—C10 | −64.9 (3) | C43—B2—C34—C40 | −68.6 (2) |
| C7—B1—C9—C16 | −63.2 (3) | C40—C34—C35—C36 | 1.8 (3) |
| C18—B1—C9—C16 | 114.3 (2) | B2—C34—C35—C36 | 178.43 (19) |
| C16—C9—C10—C12 | −1.3 (3) | C40—C34—C35—C42 | −177.9 (2) |
| B1—C9—C10—C12 | 178.00 (18) | B2—C34—C35—C42 | −1.3 (3) |
| C16—C9—C10—C11 | 177.87 (18) | C34—C35—C36—C37 | −3.3 (3) |
| B1—C9—C10—C11 | −2.8 (3) | C42—C35—C36—C37 | 176.4 (2) |
| C9—C10—C12—C13 | −2.6 (3) | C35—C36—C37—C39 | 2.3 (3) |
| C11—C10—C12—C13 | 178.26 (19) | C35—C36—C37—C38 | −176.5 (2) |
| C10—C12—C13—C15 | 3.3 (3) | C36—C37—C39—C40 | 0.2 (3) |
| C10—C12—C13—C14 | −176.79 (19) | C38—C37—C39—C40 | 179.0 (2) |
| C12—C13—C15—C16 | −0.1 (3) | C37—C39—C40—C34 | −1.6 (3) |
| C14—C13—C15—C16 | 180.0 (2) | C37—C39—C40—C41 | −178.8 (2) |
| C13—C15—C16—C9 | −3.7 (3) | C35—C34—C40—C39 | 0.6 (3) |
| C13—C15—C16—C17 | 177.8 (2) | B2—C34—C40—C39 | −176.12 (19) |
| C10—C9—C16—C15 | 4.3 (3) | C35—C34—C40—C41 | 177.68 (19) |
| B1—C9—C16—C15 | −174.97 (18) | B2—C34—C40—C41 | 1.0 (3) |
| C10—C9—C16—C17 | −177.3 (2) | C32—B2—C43—C50 | 120.6 (2) |
| B1—C9—C16—C17 | 3.4 (3) | C34—B2—C43—C50 | −61.4 (3) |
| C7—B1—C18—C25 | −64.2 (3) | C32—B2—C43—C44 | −58.3 (3) |
| C9—B1—C18—C25 | 118.3 (2) | C34—B2—C43—C44 | 119.6 (2) |
| C7—B1—C18—C19 | 116.6 (2) | C50—C43—C44—C46 | 0.7 (3) |
| C9—B1—C18—C19 | −60.9 (3) | B2—C43—C44—C46 | 179.66 (19) |
| C25—C18—C19—C21 | 0.6 (3) | C50—C43—C44—C45 | 177.9 (2) |
| B1—C18—C19—C21 | 179.77 (19) | B2—C43—C44—C45 | −3.1 (3) |
| C25—C18—C19—C20 | 178.3 (2) | C43—C44—C46—C47 | −2.1 (3) |
| B1—C18—C19—C20 | −2.5 (3) | C45—C44—C46—C47 | −179.4 (2) |
| C18—C19—C21—C22 | −2.0 (3) | C44—C46—C47—C49 | 1.1 (3) |
| C20—C19—C21—C22 | −179.9 (2) | C44—C46—C47—C48 | −179.7 (2) |
| C19—C21—C22—C24 | 1.0 (4) | C46—C47—C49—C50 | 1.2 (3) |
| C19—C21—C22—C23 | 179.3 (2) | C48—C47—C49—C50 | −177.9 (2) |
| C21—C22—C24—C25 | 1.5 (3) | C47—C49—C50—C43 | −2.6 (3) |
| C23—C22—C24—C25 | −176.7 (2) | C47—C49—C50—C51 | 179.6 (2) |
| C22—C24—C25—C18 | −3.0 (3) | C44—C43—C50—C49 | 1.6 (3) |
| C22—C24—C25—C26 | 177.8 (2) | B2—C43—C50—C49 | −177.44 (19) |
| C19—C18—C25—C24 | 1.8 (3) | C44—C43—C50—C51 | 179.37 (19) |

| | | | |
|---|---|---|---|
| B1—C18—C25—C24 | −177.36 (19) | B2—C43—C50—C51 | 0.4 (3) |

*Hydrogen-bond geometry (Å, °)*

Cg7 and Cg8 are the centroids of the C34–C37/C39/C40 and C43/C44/C46/C47/C49/C50 rings, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C14—H14C···N2$^{i}$ | 0.96 | 2.64 | 3.448 (3) | 141. |
| C15—H15A···Cg7$^{ii}$ | 0.93 | 2.94 | 3.844 (2) | 166. |
| C38—H40B···Cg8$^{iii}$ | 0.97 | 3.00 | 3.751 (3) | 136. |

Symmetry codes: (i) *x*, *y*+1, *z*; (ii) −*x*+1, −*y*+1, −*z*; (iii) −*x*+1, −*y*, −*z*+1.

**Fig. 1**

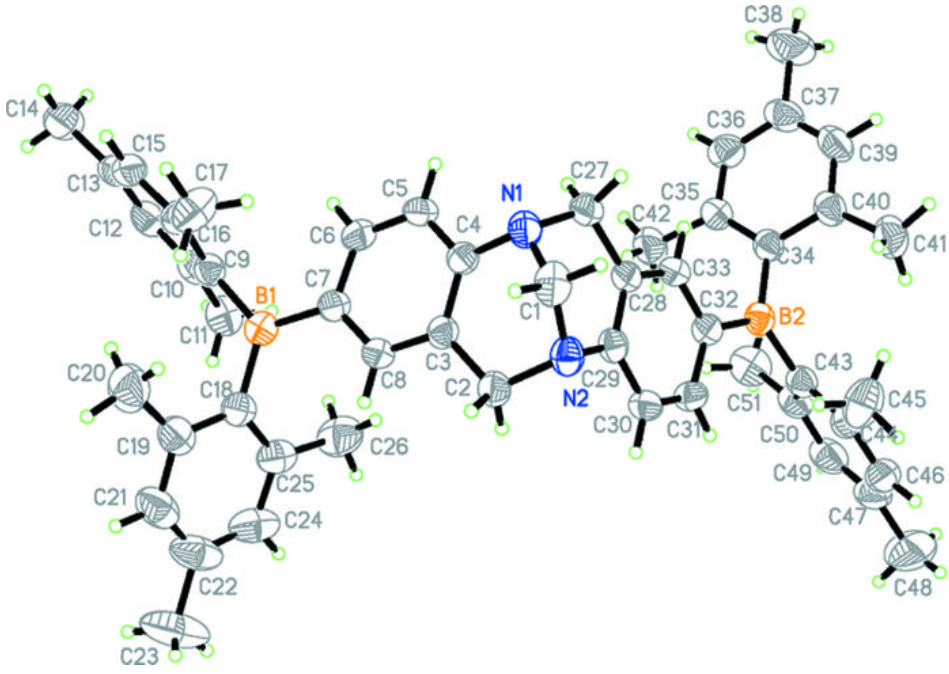
C38
C37
C36
C39
C14
C15
C13
C17
C12
C16
C9
C10
C11
B1
C5
C6
C4
N1
C27
C35
C42
C40
C41
C34
C33
C28
C32
B2
C7
C1
C3
C2
C8
N2
C29
C30
C31
C43
C45
C51
C50
C44
C49
C46
C47
C48
C20
C18
C19
C26
C25
C21
C24
C22
C23

**Fig. 2**

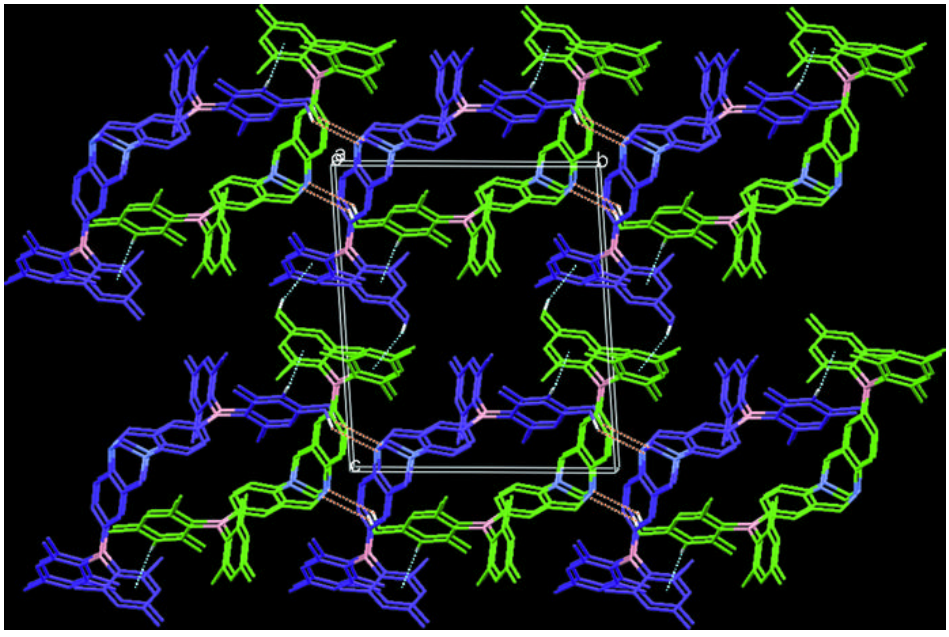

**Fig. 3**