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

# 11-[3-(Dimethylamino)propyl]-6,11-dihydrodibenzo[*b*,*e*]thiepin-11-ol

**Jerry P. Jasinski,[a]* Ray J. Butcher,[b] Q. N. M. Hakim Al-arique,[c] H. S. Yathirajan[c] and A.R. Ramesha[d]**

[a]Department of Chemistry, Keene State College, 229 Main Street, Keene, NH 03435-2001, USA, [b]Department of Chemistry, Howard University, 525 College Street NW, Washington, DC 20059, USA, [c]Department of Studies in Chemistry, University of Mysore, Manasagangotri, 570 006, India, and [d]RL Fine Chem, Bangalore, 560 064, India
Correspondence e-mail: jjasinski@keene.edu

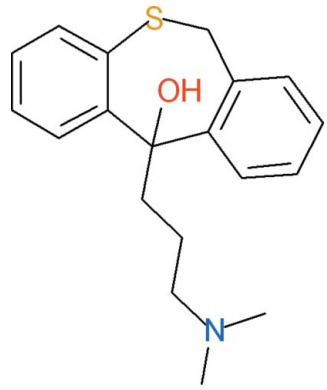
Received 6 December 2009; accepted 11 December 2009

Key indicators: single-crystal X-ray study; $T$ = 110 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.054; $wR$ factor = 0.153; data-to-parameter ratio = 16.3.

There are two independent molecules (*A* and *B*) in the asymmetric unit of the title compound, $C_{19}H_{23}NOS$. In each molecule, the seven-membered thiepine ring is bent into a slightly twisted V-shape. The dihedral angles between the mean planes of the two benzene rings fused to the thiepine ring are 75.7 (5) in molecule *A* and 73.8 (4)° in molecule *B*. In both molecules, an intramolecular O—H···N hydrogen bond occurs. In the crystal, weak intermolecular C—H···O and C—H···$\pi$-ring interactions are observed.

## Related literature

For related structures, see: Bandoli & Nicolini, (1982); Blaton *et al.* (1995); Ieawsuwan *et al.* (2006); Linden *et al.* (2004); Portalone *et al.* (2007); Roszak *et al.* (1996); Rudorf *et al.* (1999); Yoshinari & Konno, (2009); Zhang *et al.* (2008,2008*a*). For related background, see: Rudorf *et al.* (1999). For anti-depressant and anti-inflammatory properties, see: Rajsner *et al.* (1969, 1971); Rooks *et al.* (1980); Tomascovic *et al.* (2000); Truce *et al.* (1956). For pharmacological synthesis and studies, see: Ikuo *et al.* (1978); Uchida *et al.* (1979); Wyatt *et al.* (2006). For NMR, Ir and X-ray studies, see: Kolehmainen *et al.* (2007). For density functional theory (DFT), see: Becke (1988, 1993); Frisch *et al.* (2004); Hehre *et al.* (1986); Lee *et al.* (1988); Schmidt & Polik (2007).




## Experimental

### Crystal data

$C_{19}H_{23}NOS$
$M_r$ = 313.44
Monoclinic, $P2_1/n$
$a$ = 7.7215 (4) Å
$b$ = 15.3729 (10) Å
$c$ = 27.9274 (16) Å
$\beta$ = 95.401 (6)°
$V$ = 3300.3 (3) Å$^3$
$Z$ = 8
Cu $K\alpha$ radiation
$\mu$ = 1.74 mm$^{-1}$
$T$ = 110 K
0.51 × 0.42 × 0.14 mm

### Data collection

Oxford Diffraction Xcalibur diffractometer with a Ruby (Gemini Cu) detector
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
$T_{min}$ = 0.432, $T_{max}$ = 1.000
14666 measured reflections
6565 independent reflections
5490 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.029

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.153
$S$ = 1.05
6565 reflections
403 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.58 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.56 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1*A*—H1*A*···N1*A* | 0.84 | 1.86 | 2.693 (2) | 170 |
| O1*B*—H1*B*···N1*B* | 0.84 | 1.84 | 2.679 (2) | 174 |
| C4*A*—H4*AA*···O1*B* | 0.95 | 2.51 | 3.253 (2) | 135 |
| C3*A*—H3*AA*···*Cg*7$^{i}$ | 0.95 | 2.74 | 3.526 (6) | 140 |
| C17*A*—H17*A*···*Cg*1$^{ii}$ | 0.99 | 2.67 | 3.537 (7) | 147 |
| C17*A*—H17*B*···*Cg*2$^{ii}$ | 0.99 | 2.75 | 3.720 (3) | 167 |
| C17*B*—H17*C*···*Cg*8$^{iii}$ | 0.99 | 2.68 | 3.663 (6) | 170 |
| C17*B*—17D···*Cg*7$^{iii}$ | 0.99 | 2.64 | 3.538 (1) | 149 |

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x+1, y, z$; (iii) $x-1, y, z$. *Cg*1, *Cg*2, *Cg*7 and *Cg*8 are the centroids of the C1*A*—C6*A*, C8*A*—C13*A*, C1*B*–C6*B* and C8*B*—C13*B* rings, respectively.

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2007); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; 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* (Sheldrick, 2008).

QNMHA thanks the University of Mysore for use of their research facilities. RJB acknowledges the NSF MRI program (Grant No. CHE-0619278) for funds to purchase an X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2968).

## References


Bandoli, G. & Nicolini, M. (1982). *J. Chem. Crystallogr.* **12**, 425–447.
Becke, A. D. (1988). *Phys. Rev. A*, **38**, 3098–100.
Becke, A. D. (1993). *J. Chem. Phys.* **98**, 5648–5652.
Blaton, N. M., Peeters, O. M. & De Ranter, C. J. (1995). *Acta Cryst.* C**51**, 777–780.
Frisch, M. J. *et al.* (2004). *GAUSSIAN03*. Gaussian Inc., Wallingford, CT, USA.
Hehre, W.J., Random, L., Schleyer, P. R. & Pople, J.A. (1986). In *Ab Initio Molecular Orbital Theory*. New York: Wiley.
Ieawsuwan, W., Bru Roig, M. & Bolte, M. (2006). *Acta Cryst.* E**62**, o1478–o1479.
Ikuo, U., Yoshinari, S., Shizuo, M. & Suminori, U. (1978). *Chem. Pharm. Bull.* **26**, 3058–3070.
Kolehmainen, E., Laihia, K., Valkonen, A., Sievänen, E., Nissinen, M., Rudorf, W.-D., Loos, D., Perjéssy, A., Samaliková, M., Susteková, Z., Florea, S. & Wybraziec, J. (2007). *J. Mol. Struct.* **839**, 94–98.
Lee, C., Yang, W. & Parr, R. G. (1988). *Phys. Rev. B*, **37**, 785–789.
Linden, A., Furegati, M. & Rippert, A. J. (2004). *Acta Cryst.* C**60**, o223–o225.
Oxford Diffraction (2007). *CrysAlis PRO* and *CrysAlis RED*. Oxford Diffraction Ltd, Abingdon, England.
Portalone, G., Colapietro, M., Bindya, S., Ashok, M. A. & Yathirajan, H. S. (2007). *Acta Cryst.* E**63**, o746–o747.
Rajsner, M., Protiva, M. & Metysová, J. (1971). Czech. Pat. Appl. CS 143737.
Rajsner, M., Svatek, E., Seidlová, V., Adlerová, E. & Protiva, M. (1969). *Coll. Czech. Chem. Commun.* **34**, 1278.
Rooks, W. H. II, Tomolonis, A. J., Maloney, P. J., Roszkowski, A. & Wallach, M. B. (1980). *Inflamm. Res.* **10**, 266–273.
Roszak, A. W., Williams, V. E. & Lemieux, R. P. (1996). *Acta Cryst.* C**52**, 3190–3193.
Rudorf, W. D., Baumeister, U., Florea, S., Nicolae, A. & Maior, O. (1999). *Monatch. Chem.* **130**, 1475–1480.
Schmidt, J. R. & Polik, W. F. (2007). *WebMO Pro*. WebMO, LLC: Holland, MI, USA, available from http://www.webmo.net.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Tomascovic, L. L., Arneri, R. S., Brundic, A. H., Nagl, A., Mintas, M. & Sandtrom, J. (2000). *Helv. Chim. Acta*, **83**, 479–493.
Truce, W. E. & Emrick, D. D. (1956). *J. Am. Chem. Soc.* **78**, 6130–6137.
Uchida, S., Honda, F., Otsuka, M., Satoh, Y., Mori, J., Ono, T. & Hitomi, M. (1979). *Arzneimittelforschung*, **29**, 1588–1594.
Wyatt, P., Hudson, A., Charmant, J., Orpen, A. G. & Phetmung, H. (2006). *Org. Biomol. Chem.* **4**, 2218–2232.
Yoshinari, N. & Konno, T. (2009). *Acta Cryst.* E**65**, o774.
Zhang, H.-Q., Bao-Li,, Yang, G.-D. & Ma, Y.-G. (2008*a*). *Acta Cryst.* E**64**, o1304.
Zhang, H.-Q., Bao-Li,, Yang, G.-D. & Ma, Y.-G. (2008). *Acta Cryst.* E**64**, o1027.

# supporting information

*Acta Cryst.* (2010). E**66**, o161–o162 [doi:10.1107/S1600536809053434]

## 11-[3-(Dimethylamino)propyl]-6,11-dihydrodibenzo[*b*,*e*]thiepin-11-ol

**Jerry P. Jasinski, Ray J. Butcher, Q. N. M. Hakim Al-arique, H. S. Yathirajan and A.R. Ramesha**

### S1. Comment

The title compound, (I), $C_{19}H_{23}NOS$, is a derivative of 6,11-dihydrodibenzo[b,e]thiepin-11-one, which is used as an intermediate for the synthesis of dosulepin, an antidepressant of the tricyclic family. The dibenzo[c,e]thiepine derivatives (Truce *et al.*, 1956) exhibit remarkable chiroptical properties (Tomascovic *et al.*, 2000). The anti-inflammatory and analgesic profile of 6,11-dihydrodibenzo[b,e]thiepin-11-one-3-acetic acid (Tiopinac) is reported (Rooks II *et al.*, 1980). Dibenzo[b,e]thiepin-5,5-dioxide derivatives are known to possess antihistaminic and antiallergenic activities (Rajsner *et al.*, 1971). In addition, by aminoalkylation of 6,11-dihydrodibenzo[b,e]thiepin-5,5-dioxide and the corresponding 11-ketone, compounds with neurotropic and psychotropic activities have been reported (Rajsner *et al.*, 1969). Also, the comparative NMR and IR spectral, X-ray structural and theoretical studies of eight 6-arylidenedibenzo[b,e]thiepin-11-one-5,5-dioxides have been reported (Kolehmainen *et al.*, 2007). A pharmacological study of [2-chloro-11-(2-dimethyl-aminoethoxy)dibenzo(b,f)thiepine] (zotepine), and a new neuroleptic drug are also reported (Uchida *et al.*, 1979). In addition, the synthesis and chemistry of enantiomerically pure 10,11-dihydrobenzo[b,f]thiepines (Wyatt *et al.*, 2006) and the synthesis and pharmacological properties of 8-chloro-10-(2-dimethylaminoethoxy) dibenzo[b,f]thiepine and related compounds have been reported (Ikuo *et al.*, 1978). In view of the importance of thiepines, this paper reports the crystal structure of the title compound, $C_{19}H_{23}NOS$, (I).

The title compound, $C_{19}H_{23}NOS$, (I), crystallizes with two independent molecules (A, Fig. 1 & B, Fig. 2) in the asymmetric unit. The seven-membered thiepine ring is bent into a slightly twisted V-shaped arrangement with sp3 hybridized atoms at C7(A & B), C14(A & B)and S1(A & B). The dihedral angles between the mean planes of the two benzene rings fused to the thiepine ring are 75.7 (5)° (A) and 73.8 (4)° (B), respectively. An intramolecular O—H···N hydrogen bond exists between the hydroxy group and the N atom from the (dimethylamino)propyl group both bonded to the C14 atom of the thiepine ring (O1A—H1A···N1A & O1B—H1B···N1; Table 1). While no classical intermolecular hydrogen bonds are present, weak C–H···O and C–H···$\pi$-ring intermolecular interactions are observed which contribute to the stability of crystal packing (Fig.3, Table 1,2).

Following a geometry optimization density functional theory calculation (Schmidt & Polik 2007) at the B3LYP 6–31-G(*d*) level (Becke, 1988, 1993; Lee *et al.* 1988; Hehre *et al.* 1986) with the Gaussian03 program package (Frisch *at al.* 2004) the angle between the mean planes of the two benzene rings changes to 73.4 (4)°, a difference of -2.32° (A) and + 0.40° (B), respectively. These results support the collective effects of the intra and intermolecular hydrogen bonding described above slightly influencing crystal packing.

### S2. Experimental

The title compound was obtained as a gift sample from *R. L*. Fine Chem, Bangalore, India. The compound was used without further purification. X-ray quality crystals (m.p. 433–435 K) of the title compound, (I), were obtained by slow evaporation from acetone solution.

### S3. Refinement

The hydroxy H atoms, H1A and H1B, were found in a difference map and refined freely. All of the C-bonded H atoms were placed in their calculated positions and then refined using the riding model with C—H = 0.95 to 0.99 Å, and with $U_{iso}$(H) = 1.18–1.50 $U_{eq}$(C). Methyl groups were allowed to rotate about their N—C bonds.

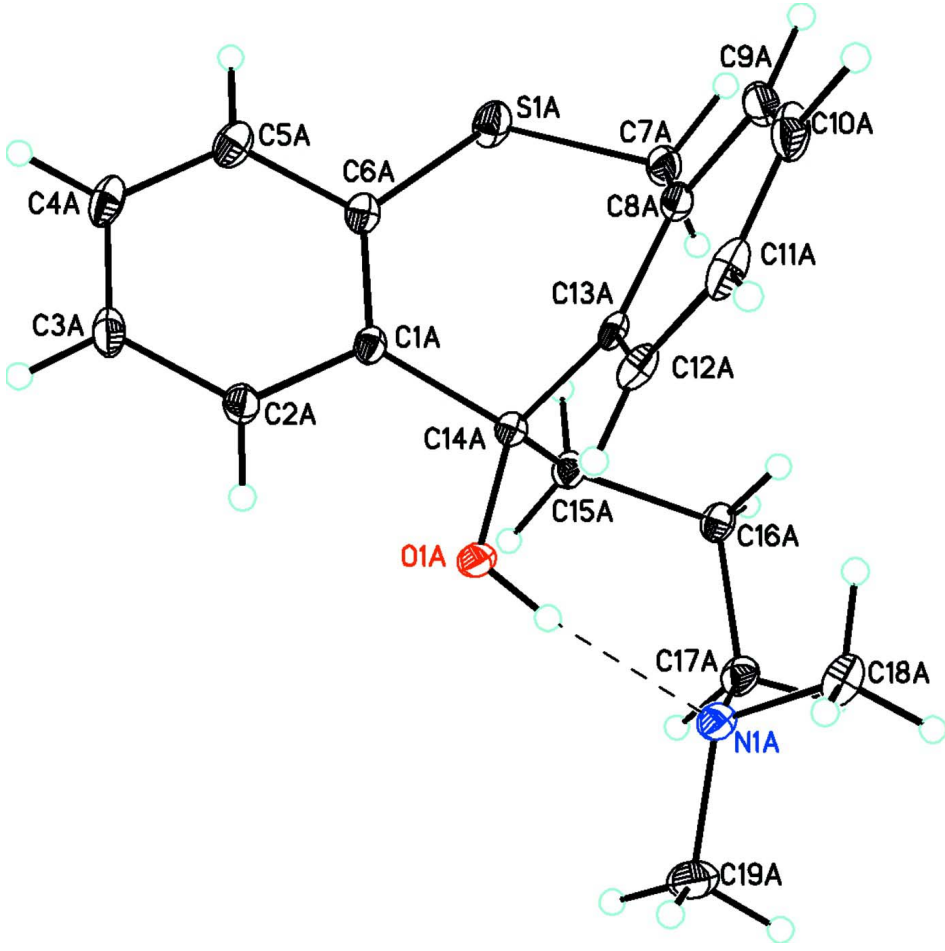



**Figure 1**

Molecular structure of molecule A in (I) showing the atom labeling scheme and 50% probability displacement ellipsoids.

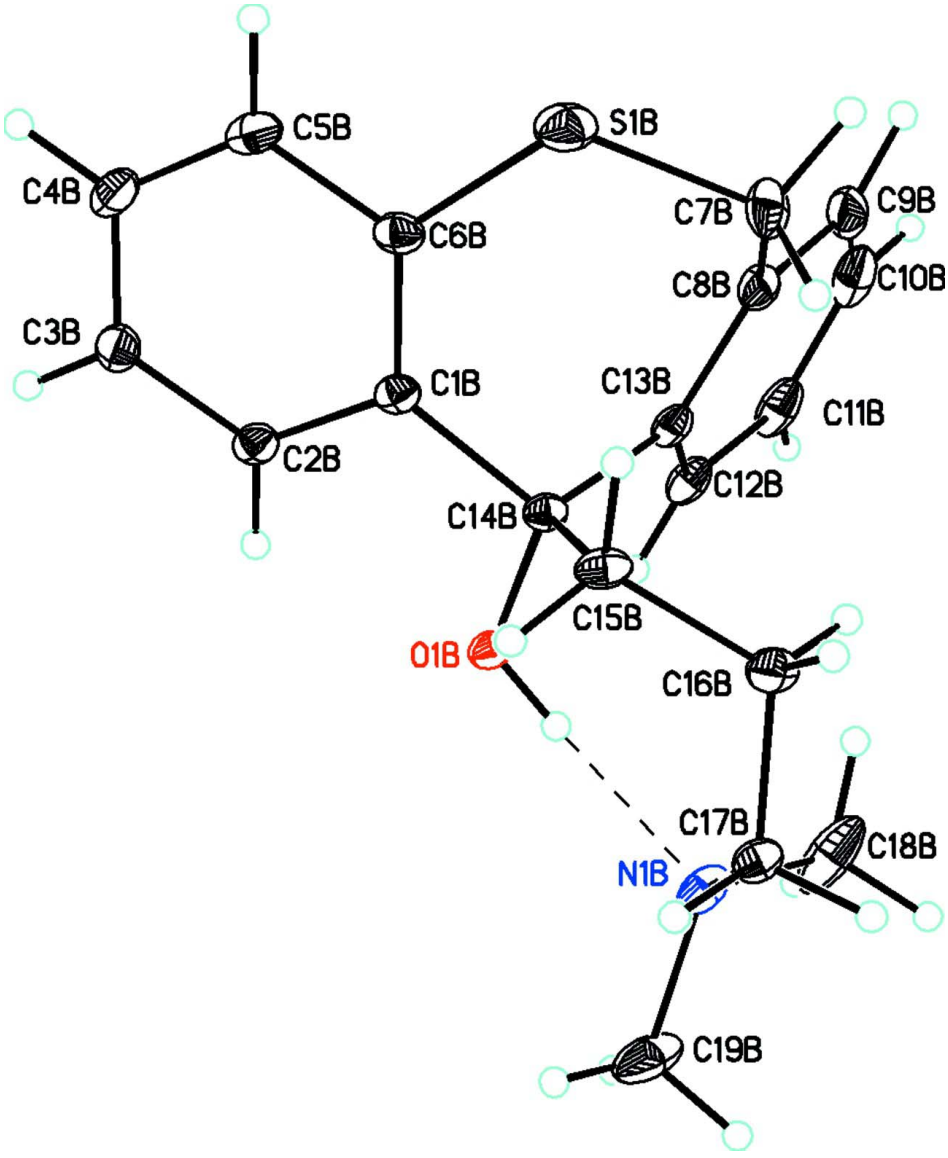



**Figure 2**

Molecular structure of molecule B in (I) showing the atom labeling scheme and 50% probability displacement ellipsoids.

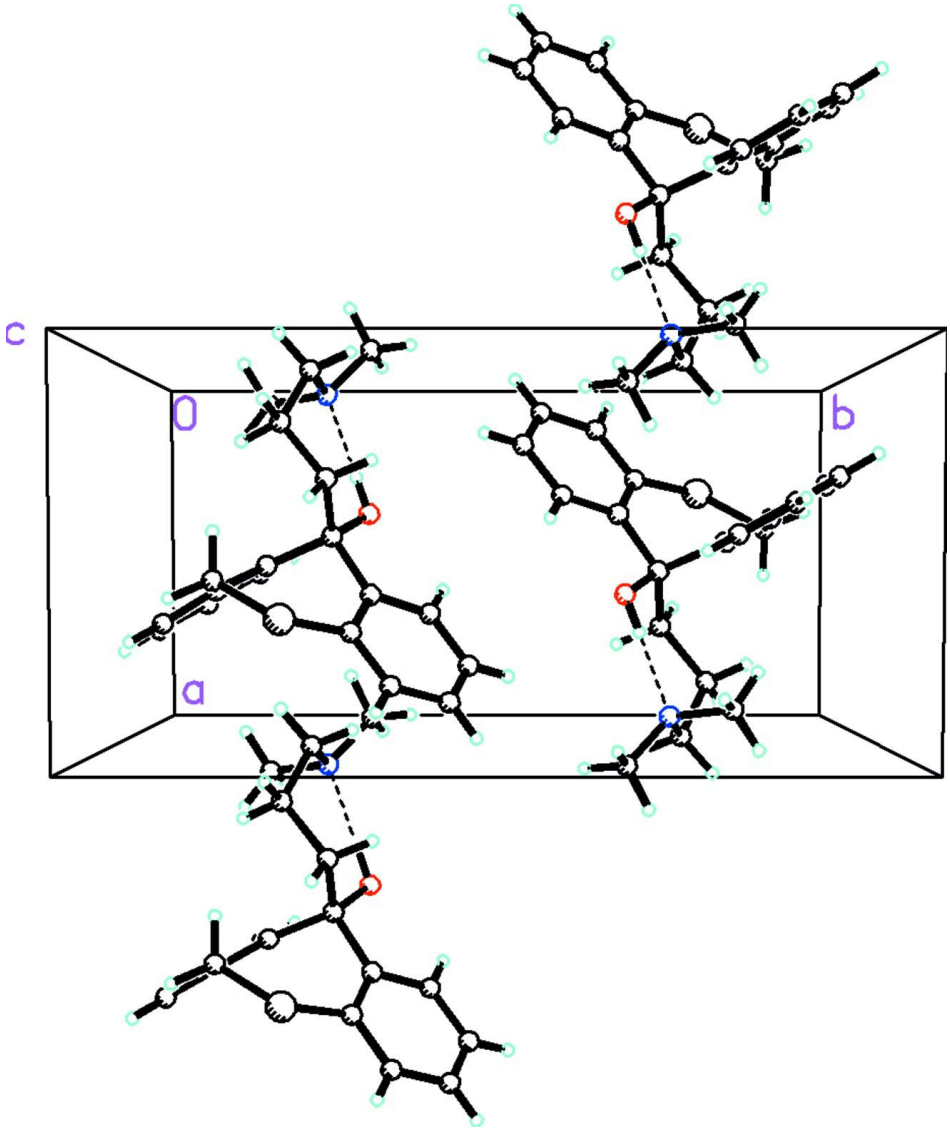



**Figure 3**

Packing diagram of (I), viewed along the *c* axis. Dashed lines indicate O—H···N intramolecular interactions in molecules A & B.

### 11-[3-(Dimethylamino)propyl]-6,11-dihydrodibenzo[*b*,*e*]thiepin- 11-ol

*Crystal data*

$C_{19}H_{23}NOS$
$M_r = 313.44$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 7.7215\ (4)$ Å
$b = 15.3729\ (10)$ Å
$c = 27.9274\ (16)$ Å
$\beta = 95.401\ (6)°$
$V = 3300.3\ (3)$ Å$^3$
$Z = 8$
$F(000) = 1344$
$D_x = 1.262$ Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 6805 reflections
$\theta = 4.3–74.0°$
$\mu = 1.74$ mm$^{-1}$
$T = 110$ K
Plate, colorless
0.51 × 0.42 × 0.14 mm

*Data collection*

Oxford Diffraction Xcalibur diffractometer with a Ruby (Gemini Cu) detector
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 10.5081 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
$T_{min}$ = 0.432, $T_{max}$ = 1.000
14666 measured reflections
6565 independent reflections
5490 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.029
$\theta_{max}$ = 74.2°, $\theta_{min}$ = 4.3°
$h$ = −9→9
$k$ = −13→19
$l$ = −17→34

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.153
$S$ = 1.05
6565 reflections
403 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
$w = 1/[\sigma^2(F_o^2) + (0.1079P)^2 + 0.6589P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.58 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.56 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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1A | 0.69626 (7) | 0.25999 (3) | 0.288172 (19) | 0.02978 (15) |
| O1A | 0.91923 (17) | 0.54941 (9) | 0.28401 (5) | 0.0240 (3) |
| H1A | 1.0075 | 0.5603 | 0.2696 | 0.029* |
| N1A | 1.2061 (2) | 0.56334 (11) | 0.23664 (6) | 0.0242 (4) |
| C1A | 0.7385 (2) | 0.44069 (13) | 0.31337 (6) | 0.0189 (4) |
| C2A | 0.6889 (2) | 0.50798 (13) | 0.34289 (6) | 0.0230 (4) |
| H2AA | 0.7418 | 0.5635 | 0.3408 | 0.028* |
| C3A | 0.5643 (3) | 0.49613 (15) | 0.37524 (7) | 0.0276 (4) |
| H3AA | 0.5350 | 0.5429 | 0.3952 | 0.033* |
| C4A | 0.4833 (3) | 0.41658 (15) | 0.37828 (7) | 0.0284 (4) |
| H4AA | 0.3984 | 0.4079 | 0.4003 | 0.034* |
| C5A | 0.5275 (3) | 0.34982 (14) | 0.34876 (7) | 0.0264 (4) |
| H5AA | 0.4697 | 0.2955 | 0.3502 | 0.032* |
| C6A | 0.6554 (2) | 0.35985 (13) | 0.31669 (6) | 0.0202 (4) |
| C7A | 0.7862 (3) | 0.28132 (13) | 0.23129 (7) | 0.0238 (4) |
| H7AA | 0.9147 | 0.2814 | 0.2370 | 0.029* |

| | | | | |
|---|---|---|---|---|
| H7AB | 0.7527 | 0.2330 | 0.2089 | 0.029* |
| C8A | 0.7295 (2) | 0.36527 (13) | 0.20746 (6) | 0.0202 (4) |
| C9A | 0.6275 (3) | 0.36079 (15) | 0.16343 (7) | 0.0280 (4) |
| H9AA | 0.5927 | 0.3055 | 0.1508 | 0.034* |
| C10A | 0.5764 (3) | 0.43455 (17) | 0.13802 (7) | 0.0331 (5) |
| H10A | 0.5075 | 0.4301 | 0.1081 | 0.040* |
| C11A | 0.6263 (3) | 0.51514 (16) | 0.15646 (7) | 0.0306 (5) |
| H11A | 0.5926 | 0.5665 | 0.1391 | 0.037* |
| C12A | 0.7258 (2) | 0.52091 (13) | 0.20050 (7) | 0.0232 (4) |
| H12A | 0.7588 | 0.5766 | 0.2129 | 0.028* |
| C13A | 0.7782 (2) | 0.44720 (12) | 0.22683 (6) | 0.0170 (4) |
| C14A | 0.8737 (2) | 0.46053 (12) | 0.27754 (6) | 0.0181 (4) |
| C15A | 1.0403 (2) | 0.40533 (13) | 0.28923 (6) | 0.0207 (4) |
| H15A | 1.1021 | 0.4278 | 0.3194 | 0.025* |
| H15B | 1.0046 | 0.3448 | 0.2955 | 0.025* |
| C16A | 1.1698 (2) | 0.40312 (13) | 0.25052 (7) | 0.0218 (4) |
| H16A | 1.2402 | 0.3494 | 0.2550 | 0.026* |
| H16B | 1.1027 | 0.3994 | 0.2186 | 0.026* |
| C17A | 1.2933 (2) | 0.48049 (13) | 0.25020 (7) | 0.0241 (4) |
| H17A | 1.3558 | 0.4868 | 0.2826 | 0.029* |
| H17B | 1.3810 | 0.4683 | 0.2274 | 0.029* |
| C18A | 1.1570 (3) | 0.56816 (15) | 0.18463 (7) | 0.0296 (5) |
| H18A | 1.0974 | 0.6234 | 0.1769 | 0.044* |
| H18B | 1.0791 | 0.5197 | 0.1748 | 0.044* |
| H18C | 1.2618 | 0.5646 | 0.1675 | 0.044* |
| C19A | 1.3169 (3) | 0.63736 (16) | 0.25201 (10) | 0.0396 (6) |
| H19A | 1.2540 | 0.6917 | 0.2442 | 0.059* |
| H19B | 1.4230 | 0.6358 | 0.2353 | 0.059* |
| H19C | 1.3477 | 0.6342 | 0.2868 | 0.059* |
| S1B | 0.66729 (7) | 0.22246 (4) | 0.627252 (18) | 0.03356 (16) |
| O1B | 0.39362 (17) | 0.32974 (9) | 0.47928 (5) | 0.0224 (3) |
| H1B | 0.2941 | 0.3119 | 0.4691 | 0.027* |
| N1B | 0.0713 (2) | 0.27183 (13) | 0.45327 (6) | 0.0272 (4) |
| C1B | 0.6076 (2) | 0.33566 (12) | 0.54588 (6) | 0.0194 (4) |
| C2B | 0.6575 (2) | 0.41167 (13) | 0.52343 (7) | 0.0225 (4) |
| H2BA | 0.5966 | 0.4284 | 0.4937 | 0.027* |
| C3B | 0.7936 (3) | 0.46361 (14) | 0.54324 (8) | 0.0269 (4) |
| H3BA | 0.8237 | 0.5154 | 0.5274 | 0.032* |
| C4B | 0.8849 (3) | 0.43913 (14) | 0.58631 (8) | 0.0296 (5) |
| H4BA | 0.9773 | 0.4743 | 0.6003 | 0.036* |
| C5B | 0.8406 (3) | 0.36365 (14) | 0.60857 (7) | 0.0279 (4) |
| H5BA | 0.9048 | 0.3467 | 0.6378 | 0.033* |
| C6B | 0.7032 (2) | 0.31114 (13) | 0.58920 (7) | 0.0227 (4) |
| C7B | 0.5684 (3) | 0.13299 (14) | 0.59244 (7) | 0.0292 (4) |
| H7BA | 0.6145 | 0.0780 | 0.6070 | 0.035* |
| H7BB | 0.4418 | 0.1340 | 0.5955 | 0.035* |
| C8B | 0.5951 (2) | 0.13126 (13) | 0.53919 (7) | 0.0249 (4) |
| C9B | 0.6839 (3) | 0.05921 (14) | 0.52276 (9) | 0.0340 (5) |

| | | | | |
|---|---|---|---|---|
| H9BA | 0.7316 | 0.0173 | 0.5453 | 0.041* |
| C10B | 0.7035 (3) | 0.04778 (15) | 0.47439 (10) | 0.0382 (6) |
| H10B | 0.7637 | −0.0015 | 0.4638 | 0.046* |
| C11B | 0.6349 (3) | 0.10843 (16) | 0.44183 (8) | 0.0341 (5) |
| H11B | 0.6440 | 0.1002 | 0.4084 | 0.041* |
| C12B | 0.5524 (2) | 0.18169 (14) | 0.45762 (7) | 0.0257 (4) |
| H12B | 0.5087 | 0.2240 | 0.4348 | 0.031* |
| C13B | 0.5316 (2) | 0.19501 (13) | 0.50640 (7) | 0.0199 (4) |
| C14B | 0.4538 (2) | 0.28306 (12) | 0.52111 (6) | 0.0187 (4) |
| C15B | 0.3036 (2) | 0.27781 (14) | 0.55385 (7) | 0.0231 (4) |
| H15C | 0.3525 | 0.2592 | 0.5863 | 0.028* |
| H15D | 0.2554 | 0.3370 | 0.5570 | 0.028* |
| C16B | 0.1534 (2) | 0.21639 (14) | 0.53708 (7) | 0.0258 (4) |
| H16C | 0.2030 | 0.1642 | 0.5227 | 0.031* |
| H16D | 0.0976 | 0.1970 | 0.5657 | 0.031* |
| C17B | 0.0125 (2) | 0.25346 (13) | 0.50080 (7) | 0.0220 (4) |
| H17C | −0.0853 | 0.2116 | 0.4968 | 0.026* |
| H17D | −0.0321 | 0.3080 | 0.5140 | 0.026* |
| C18B | 0.0944 (3) | 0.1914 (2) | 0.42672 (9) | 0.0515 (8) |
| H18D | 0.1890 | 0.1573 | 0.4433 | 0.077* |
| H18E | 0.1232 | 0.2054 | 0.3942 | 0.077* |
| H18F | −0.0136 | 0.1575 | 0.4248 | 0.077* |
| C19B | −0.0530 (3) | 0.3298 (2) | 0.42629 (9) | 0.0479 (7) |
| H19D | −0.0118 | 0.3430 | 0.3950 | 0.072* |
| H19E | −0.0635 | 0.3839 | 0.4444 | 0.072* |
| H19F | −0.1668 | 0.3012 | 0.4215 | 0.072* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1A | 0.0386 (3) | 0.0189 (2) | 0.0344 (3) | −0.0007 (2) | 0.0165 (2) | 0.00348 (19) |
| O1A | 0.0191 (7) | 0.0210 (7) | 0.0333 (7) | −0.0042 (5) | 0.0094 (5) | −0.0068 (6) |
| N1A | 0.0208 (8) | 0.0233 (8) | 0.0293 (8) | −0.0028 (6) | 0.0070 (6) | −0.0039 (7) |
| C1A | 0.0150 (8) | 0.0269 (9) | 0.0148 (8) | 0.0016 (7) | 0.0015 (6) | 0.0003 (7) |
| C2A | 0.0194 (9) | 0.0291 (10) | 0.0208 (8) | 0.0002 (7) | 0.0025 (7) | −0.0039 (8) |
| C3A | 0.0247 (10) | 0.0398 (12) | 0.0188 (8) | 0.0059 (9) | 0.0047 (7) | −0.0055 (8) |
| C4A | 0.0240 (10) | 0.0434 (12) | 0.0189 (8) | 0.0055 (9) | 0.0078 (7) | 0.0078 (8) |
| C5A | 0.0249 (10) | 0.0315 (11) | 0.0234 (9) | 0.0026 (8) | 0.0059 (7) | 0.0092 (8) |
| C6A | 0.0209 (9) | 0.0222 (9) | 0.0177 (8) | 0.0033 (7) | 0.0022 (7) | 0.0030 (7) |
| C7A | 0.0269 (10) | 0.0198 (9) | 0.0258 (9) | 0.0003 (7) | 0.0088 (7) | −0.0037 (7) |
| C8A | 0.0184 (9) | 0.0251 (10) | 0.0177 (8) | −0.0006 (7) | 0.0051 (7) | −0.0007 (7) |
| C9A | 0.0237 (10) | 0.0395 (12) | 0.0210 (9) | −0.0004 (9) | 0.0031 (7) | −0.0090 (8) |
| C10A | 0.0236 (10) | 0.0594 (15) | 0.0164 (8) | 0.0080 (10) | 0.0018 (7) | 0.0004 (9) |
| C11A | 0.0210 (10) | 0.0468 (13) | 0.0254 (9) | 0.0101 (9) | 0.0091 (7) | 0.0159 (9) |
| C12A | 0.0166 (8) | 0.0265 (10) | 0.0277 (9) | 0.0028 (7) | 0.0089 (7) | 0.0068 (8) |
| C13A | 0.0121 (8) | 0.0230 (9) | 0.0169 (8) | 0.0016 (7) | 0.0065 (6) | 0.0015 (7) |
| C14A | 0.0166 (8) | 0.0192 (9) | 0.0190 (8) | −0.0008 (7) | 0.0041 (6) | −0.0021 (7) |
| C15A | 0.0168 (8) | 0.0257 (10) | 0.0198 (8) | 0.0013 (7) | 0.0026 (6) | −0.0003 (7) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C16A | 0.0171 (9) | 0.0246 (9) | 0.0242 (9) | 0.0036 (7) | 0.0049 (7) | 0.0001 (7) |
| C17A | 0.0160 (8) | 0.0306 (10) | 0.0260 (9) | 0.0008 (8) | 0.0033 (7) | −0.0002 (8) |
| C18A | 0.0264 (10) | 0.0345 (11) | 0.0293 (10) | 0.0043 (8) | 0.0103 (8) | 0.0074 (9) |
| C19A | 0.0314 (12) | 0.0322 (12) | 0.0572 (14) | −0.0121 (10) | 0.0155 (11) | −0.0117 (11) |
| S1B | 0.0336 (3) | 0.0426 (3) | 0.0233 (3) | 0.0001 (2) | −0.00317 (19) | 0.0080 (2) |
| O1B | 0.0184 (6) | 0.0281 (7) | 0.0199 (6) | −0.0033 (5) | −0.0022 (5) | 0.0059 (5) |
| N1B | 0.0221 (8) | 0.0414 (10) | 0.0180 (7) | −0.0099 (7) | 0.0010 (6) | 0.0005 (7) |
| C1B | 0.0158 (8) | 0.0226 (9) | 0.0200 (8) | 0.0041 (7) | 0.0026 (7) | −0.0039 (7) |
| C2B | 0.0179 (9) | 0.0246 (9) | 0.0248 (9) | 0.0030 (7) | 0.0018 (7) | −0.0044 (8) |
| C3B | 0.0213 (9) | 0.0237 (9) | 0.0357 (10) | 0.0016 (8) | 0.0033 (8) | −0.0048 (8) |
| C4B | 0.0206 (9) | 0.0308 (11) | 0.0362 (11) | 0.0004 (8) | −0.0034 (8) | −0.0133 (9) |
| C5B | 0.0222 (10) | 0.0354 (11) | 0.0250 (9) | 0.0063 (8) | −0.0038 (7) | −0.0070 (8) |
| C6B | 0.0213 (9) | 0.0254 (9) | 0.0212 (8) | 0.0062 (7) | 0.0014 (7) | −0.0019 (8) |
| C7B | 0.0353 (11) | 0.0253 (10) | 0.0283 (10) | −0.0100 (9) | 0.0094 (8) | 0.0047 (8) |
| C8B | 0.0171 (9) | 0.0241 (10) | 0.0336 (10) | −0.0039 (7) | 0.0027 (7) | 0.0009 (8) |
| C9B | 0.0218 (10) | 0.0223 (10) | 0.0581 (14) | −0.0020 (8) | 0.0040 (9) | 0.0019 (10) |
| C10B | 0.0218 (10) | 0.0288 (11) | 0.0657 (16) | −0.0039 (9) | 0.0135 (10) | −0.0190 (11) |
| C11B | 0.0229 (10) | 0.0411 (12) | 0.0403 (11) | −0.0105 (9) | 0.0127 (9) | −0.0188 (10) |
| C12B | 0.0175 (9) | 0.0341 (11) | 0.0264 (9) | −0.0067 (8) | 0.0061 (7) | −0.0057 (8) |
| C13B | 0.0117 (8) | 0.0243 (9) | 0.0241 (9) | −0.0032 (7) | 0.0045 (6) | −0.0036 (7) |
| C14B | 0.0169 (9) | 0.0228 (9) | 0.0163 (8) | 0.0010 (7) | 0.0014 (6) | 0.0015 (7) |
| C15B | 0.0168 (9) | 0.0341 (10) | 0.0184 (8) | 0.0037 (8) | 0.0022 (7) | 0.0015 (8) |
| C16B | 0.0178 (9) | 0.0327 (11) | 0.0274 (9) | −0.0008 (8) | 0.0048 (7) | 0.0102 (8) |
| C17B | 0.0169 (9) | 0.0289 (10) | 0.0206 (8) | −0.0005 (7) | 0.0038 (7) | −0.0008 (7) |
| C18B | 0.0343 (13) | 0.079 (2) | 0.0434 (13) | −0.0256 (13) | 0.0172 (11) | −0.0361 (14) |
| C19B | 0.0280 (12) | 0.0747 (19) | 0.0382 (12) | −0.0149 (12) | −0.0115 (9) | 0.0277 (13) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1A—C6A | 1.7713 (19) | S1B—C6B | 1.766 (2) |
| S1A—C7A | 1.822 (2) | S1B—C7B | 1.811 (2) |
| O1A—C14A | 1.418 (2) | O1B—C14B | 1.412 (2) |
| O1A—H1A | 0.8400 | O1B—H1B | 0.8400 |
| N1A—C19A | 1.463 (3) | N1B—C18B | 1.461 (3) |
| N1A—C18A | 1.468 (3) | N1B—C19B | 1.465 (3) |
| N1A—C17A | 1.473 (3) | N1B—C17B | 1.470 (2) |
| C1A—C2A | 1.398 (3) | C1B—C2B | 1.397 (3) |
| C1A—C6A | 1.406 (3) | C1B—C6B | 1.408 (2) |
| C1A—C14A | 1.543 (2) | C1B—C14B | 1.545 (2) |
| C2A—C3A | 1.393 (3) | C2B—C3B | 1.393 (3) |
| C2A—H2AA | 0.9500 | C2B—H2BA | 0.9500 |
| C3A—C4A | 1.380 (3) | C3B—C4B | 1.388 (3) |
| C3A—H3AA | 0.9500 | C3B—H3BA | 0.9500 |
| C4A—C5A | 1.380 (3) | C4B—C5B | 1.375 (3) |
| C4A—H4AA | 0.9500 | C4B—H4BA | 0.9500 |
| C5A—C6A | 1.402 (3) | C5B—C6B | 1.401 (3) |
| C5A—H5AA | 0.9500 | C5B—H5BA | 0.9500 |
| C7A—C8A | 1.498 (3) | C7B—C8B | 1.521 (3) |

| | | | |
|---|---|---|---|
| C7A—H7AA | 0.9900 | C7B—H7BA | 0.9900 |
| C7A—H7AB | 0.9900 | C7B—H7BB | 0.9900 |
| C8A—C9A | 1.398 (3) | C8B—C13B | 1.398 (3) |
| C8A—C13A | 1.408 (3) | C8B—C9B | 1.402 (3) |
| C9A—C10A | 1.376 (3) | C9B—C10B | 1.384 (4) |
| C9A—H9AA | 0.9500 | C9B—H9BA | 0.9500 |
| C10A—C11A | 1.382 (3) | C10B—C11B | 1.373 (4) |
| C10A—H10A | 0.9500 | C10B—H10B | 0.9500 |
| C11A—C12A | 1.390 (3) | C11B—C12B | 1.386 (3) |
| C11A—H11A | 0.9500 | C11B—H11B | 0.9500 |
| C12A—C13A | 1.390 (3) | C12B—C13B | 1.402 (3) |
| C12A—H12A | 0.9500 | C12B—H12B | 0.9500 |
| C13A—C14A | 1.548 (2) | C13B—C14B | 1.552 (3) |
| C14A—C15A | 1.550 (2) | C14B—C15B | 1.545 (2) |
| C15A—C16A | 1.540 (2) | C15B—C16B | 1.534 (3) |
| C15A—H15A | 0.9900 | C15B—H15C | 0.9900 |
| C15A—H15B | 0.9900 | C15B—H15D | 0.9900 |
| C16A—C17A | 1.525 (3) | C16B—C17B | 1.525 (3) |
| C16A—H16A | 0.9900 | C16B—H16C | 0.9900 |
| C16A—H16B | 0.9900 | C16B—H16D | 0.9900 |
| C17A—H17A | 0.9900 | C17B—H17C | 0.9900 |
| C17A—H17B | 0.9900 | C17B—H17D | 0.9900 |
| C18A—H18A | 0.9800 | C18B—H18D | 0.9800 |
| C18A—H18B | 0.9800 | C18B—H18E | 0.9800 |
| C18A—H18C | 0.9800 | C18B—H18F | 0.9800 |
| C19A—H19A | 0.9800 | C19B—H19D | 0.9800 |
| C19A—H19B | 0.9800 | C19B—H19E | 0.9800 |
| C19A—H19C | 0.9800 | C19B—H19F | 0.9800 |

| | | | |
|---|---|---|---|
| C6A—S1A—C7A | 109.55 (9) | C6B—S1B—C7B | 110.20 (9) |
| C14A—O1A—H1A | 109.5 | C14B—O1B—H1B | 109.5 |
| C19A—N1A—C18A | 109.89 (18) | C18B—N1B—C19B | 111.0 (2) |
| C19A—N1A—C17A | 110.88 (17) | C18B—N1B—C17B | 111.00 (19) |
| C18A—N1A—C17A | 111.53 (16) | C19B—N1B—C17B | 109.77 (18) |
| C2A—C1A—C6A | 117.58 (17) | C2B—C1B—C6B | 117.73 (17) |
| C2A—C1A—C14A | 118.41 (17) | C2B—C1B—C14B | 118.00 (15) |
| C6A—C1A—C14A | 123.95 (16) | C6B—C1B—C14B | 124.27 (17) |
| C3A—C2A—C1A | 122.01 (19) | C3B—C2B—C1B | 122.07 (18) |
| C3A—C2A—H2AA | 119.0 | C3B—C2B—H2BA | 119.0 |
| C1A—C2A—H2AA | 119.0 | C1B—C2B—H2BA | 119.0 |
| C4A—C3A—C2A | 120.05 (19) | C4B—C3B—C2B | 119.4 (2) |
| C4A—C3A—H3AA | 120.0 | C4B—C3B—H3BA | 120.3 |
| C2A—C3A—H3AA | 120.0 | C2B—C3B—H3BA | 120.3 |
| C5A—C4A—C3A | 118.91 (18) | C5B—C4B—C3B | 119.56 (19) |
| C5A—C4A—H4AA | 120.5 | C5B—C4B—H4BA | 120.2 |
| C3A—C4A—H4AA | 120.5 | C3B—C4B—H4BA | 120.2 |
| C4A—C5A—C6A | 121.9 (2) | C4B—C5B—C6B | 121.55 (18) |
| C4A—C5A—H5AA | 119.0 | C4B—C5B—H5BA | 119.2 |

| | | | |
|---|---|---|---|
| C6A—C5A—H5AA | 119.0 | C6B—C5B—H5BA | 119.2 |
| C5A—C6A—C1A | 119.50 (18) | C5B—C6B—C1B | 119.62 (19) |
| C5A—C6A—S1A | 110.96 (15) | C5B—C6B—S1B | 111.62 (14) |
| C1A—C6A—S1A | 129.40 (14) | C1B—C6B—S1B | 128.64 (16) |
| C8A—C7A—S1A | 115.01 (13) | C8B—C7B—S1B | 116.69 (14) |
| C8A—C7A—H7AA | 108.5 | C8B—C7B—H7BA | 108.1 |
| S1A—C7A—H7AA | 108.5 | S1B—C7B—H7BA | 108.1 |
| C8A—C7A—H7AB | 108.5 | C8B—C7B—H7BB | 108.1 |
| S1A—C7A—H7AB | 108.5 | S1B—C7B—H7BB | 108.1 |
| H7AA—C7A—H7AB | 107.5 | H7BA—C7B—H7BB | 107.3 |
| C9A—C8A—C13A | 119.34 (18) | C13B—C8B—C9B | 119.4 (2) |
| C9A—C8A—C7A | 117.71 (18) | C13B—C8B—C7B | 123.82 (18) |
| C13A—C8A—C7A | 122.93 (16) | C9B—C8B—C7B | 116.7 (2) |
| C10A—C9A—C8A | 121.6 (2) | C10B—C9B—C8B | 121.4 (2) |
| C10A—C9A—H9AA | 119.2 | C10B—C9B—H9BA | 119.3 |
| C8A—C9A—H9AA | 119.2 | C8B—C9B—H9BA | 119.3 |
| C9A—C10A—C11A | 119.35 (18) | C11B—C10B—C9B | 119.3 (2) |
| C9A—C10A—H10A | 120.3 | C11B—C10B—H10B | 120.3 |
| C11A—C10A—H10A | 120.3 | C9B—C10B—H10B | 120.3 |
| C10A—C11A—C12A | 119.9 (2) | C10B—C11B—C12B | 120.1 (2) |
| C10A—C11A—H11A | 120.1 | C10B—C11B—H11B | 120.0 |
| C12A—C11A—H11A | 120.1 | C12B—C11B—H11B | 120.0 |
| C13A—C12A—C11A | 121.7 (2) | C11B—C12B—C13B | 121.7 (2) |
| C13A—C12A—H12A | 119.2 | C11B—C12B—H12B | 119.1 |
| C11A—C12A—H12A | 119.2 | C13B—C12B—H12B | 119.1 |
| C12A—C13A—C8A | 118.18 (17) | C8B—C13B—C12B | 117.96 (18) |
| C12A—C13A—C14A | 117.78 (17) | C8B—C13B—C14B | 123.96 (16) |
| C8A—C13A—C14A | 123.85 (16) | C12B—C13B—C14B | 117.86 (17) |
| O1A—C14A—C1A | 106.40 (14) | O1B—C14B—C1B | 106.49 (15) |
| O1A—C14A—C13A | 109.58 (15) | O1B—C14B—C15B | 108.00 (14) |
| C1A—C14A—C13A | 105.90 (14) | C1B—C14B—C15B | 110.53 (14) |
| O1A—C14A—C15A | 108.06 (14) | O1B—C14B—C13B | 109.25 (14) |
| C1A—C14A—C15A | 110.73 (14) | C1B—C14B—C13B | 105.96 (14) |
| C13A—C14A—C15A | 115.78 (14) | C15B—C14B—C13B | 116.21 (16) |
| C16A—C15A—C14A | 116.41 (15) | C16B—C15B—C14B | 116.08 (16) |
| C16A—C15A—H15A | 108.2 | C16B—C15B—H15C | 108.3 |
| C14A—C15A—H15A | 108.2 | C14B—C15B—H15C | 108.3 |
| C16A—C15A—H15B | 108.2 | C16B—C15B—H15D | 108.3 |
| C14A—C15A—H15B | 108.2 | C14B—C15B—H15D | 108.3 |
| H15A—C15A—H15B | 107.3 | H15C—C15B—H15D | 107.4 |
| C17A—C16A—C15A | 115.75 (16) | C17B—C16B—C15B | 116.37 (17) |
| C17A—C16A—H16A | 108.3 | C17B—C16B—H16C | 108.2 |
| C15A—C16A—H16A | 108.3 | C15B—C16B—H16C | 108.2 |
| C17A—C16A—H16B | 108.3 | C17B—C16B—H16D | 108.2 |
| C15A—C16A—H16B | 108.3 | C15B—C16B—H16D | 108.2 |
| H16A—C16A—H16B | 107.4 | H16C—C16B—H16D | 107.3 |
| N1A—C17A—C16A | 113.87 (15) | N1B—C17B—C16B | 114.20 (16) |
| N1A—C17A—H17A | 108.8 | N1B—C17B—H17C | 108.7 |

| | | | |
|---|---|---|---|
| C16A—C17A—H17A | 108.8 | C16B—C17B—H17C | 108.7 |
| N1A—C17A—H17B | 108.8 | N1B—C17B—H17D | 108.7 |
| C16A—C17A—H17B | 108.8 | C16B—C17B—H17D | 108.7 |
| H17A—C17A—H17B | 107.7 | H17C—C17B—H17D | 107.6 |
| N1A—C18A—H18A | 109.5 | N1B—C18B—H18D | 109.5 |
| N1A—C18A—H18B | 109.5 | N1B—C18B—H18E | 109.5 |
| H18A—C18A—H18B | 109.5 | H18D—C18B—H18E | 109.5 |
| N1A—C18A—H18C | 109.5 | N1B—C18B—H18F | 109.5 |
| H18A—C18A—H18C | 109.5 | H18D—C18B—H18F | 109.5 |
| H18B—C18A—H18C | 109.5 | H18E—C18B—H18F | 109.5 |
| N1A—C19A—H19A | 109.5 | N1B—C19B—H19D | 109.5 |
| N1A—C19A—H19B | 109.5 | N1B—C19B—H19E | 109.5 |
| H19A—C19A—H19B | 109.5 | H19D—C19B—H19E | 109.5 |
| N1A—C19A—H19C | 109.5 | N1B—C19B—H19F | 109.5 |
| H19A—C19A—H19C | 109.5 | H19D—C19B—H19F | 109.5 |
| H19B—C19A—H19C | 109.5 | H19E—C19B—H19F | 109.5 |
| | | | |
| C6A—C1A—C2A—C3A | 1.2 (3) | C6B—C1B—C2B—C3B | −1.7 (3) |
| C14A—C1A—C2A—C3A | 178.23 (17) | C14B—C1B—C2B—C3B | 179.50 (17) |
| C1A—C2A—C3A—C4A | −1.2 (3) | C1B—C2B—C3B—C4B | 0.8 (3) |
| C2A—C3A—C4A—C5A | −0.2 (3) | C2B—C3B—C4B—C5B | 0.6 (3) |
| C3A—C4A—C5A—C6A | 1.6 (3) | C3B—C4B—C5B—C6B | −1.0 (3) |
| C4A—C5A—C6A—C1A | −1.6 (3) | C4B—C5B—C6B—C1B | 0.1 (3) |
| C4A—C5A—C6A—S1A | 174.51 (16) | C4B—C5B—C6B—S1B | −176.25 (16) |
| C2A—C1A—C6A—C5A | 0.2 (3) | C2B—C1B—C6B—C5B | 1.2 (3) |
| C14A—C1A—C6A—C5A | −176.66 (16) | C14B—C1B—C6B—C5B | 179.94 (17) |
| C2A—C1A—C6A—S1A | −175.12 (14) | C2B—C1B—C6B—S1B | 176.89 (15) |
| C14A—C1A—C6A—S1A | 8.0 (3) | C14B—C1B—C6B—S1B | −4.4 (3) |
| C7A—S1A—C6A—C5A | 156.28 (14) | C7B—S1B—C6B—C5B | −153.88 (15) |
| C7A—S1A—C6A—C1A | −28.0 (2) | C7B—S1B—C6B—C1B | 30.1 (2) |
| C6A—S1A—C7A—C8A | −29.24 (17) | C6B—S1B—C7B—C8B | 22.7 (2) |
| S1A—C7A—C8A—C9A | −114.43 (17) | S1B—C7B—C8B—C13B | −63.9 (2) |
| S1A—C7A—C8A—C13A | 67.3 (2) | S1B—C7B—C8B—C9B | 118.40 (19) |
| C13A—C8A—C9A—C10A | 1.4 (3) | C13B—C8B—C9B—C10B | −2.9 (3) |
| C7A—C8A—C9A—C10A | −176.99 (18) | C7B—C8B—C9B—C10B | 174.94 (19) |
| C8A—C9A—C10A—C11A | −0.3 (3) | C8B—C9B—C10B—C11B | 0.2 (3) |
| C9A—C10A—C11A—C12A | −0.6 (3) | C9B—C10B—C11B—C12B | 2.2 (3) |
| C10A—C11A—C12A—C13A | 0.3 (3) | C10B—C11B—C12B—C13B | −1.9 (3) |
| C11A—C12A—C13A—C8A | 0.7 (3) | C9B—C8B—C13B—C12B | 3.1 (3) |
| C11A—C12A—C13A—C14A | −174.38 (16) | C7B—C8B—C13B—C12B | −174.58 (17) |
| C9A—C8A—C13A—C12A | −1.6 (3) | C9B—C8B—C13B—C14B | −171.44 (17) |
| C7A—C8A—C13A—C12A | 176.71 (17) | C7B—C8B—C13B—C14B | 10.9 (3) |
| C9A—C8A—C13A—C14A | 173.24 (17) | C11B—C12B—C13B—C8B | −0.7 (3) |
| C7A—C8A—C13A—C14A | −8.5 (3) | C11B—C12B—C13B—C14B | 174.11 (17) |
| C2A—C1A—C14A—O1A | 0.3 (2) | C2B—C1B—C14B—O1B | −1.8 (2) |
| C6A—C1A—C14A—O1A | 177.21 (16) | C6B—C1B—C14B—O1B | 179.50 (16) |
| C2A—C1A—C14A—C13A | −116.21 (17) | C2B—C1B—C14B—C15B | −118.81 (18) |
| C6A—C1A—C14A—C13A | 60.7 (2) | C6B—C1B—C14B—C15B | 62.4 (2) |

| | | | |
|---|---|---|---|
| C2A—C1A—C14A—C15A | 117.54 (18) | C2B—C1B—C14B—C13B | 114.50 (18) |
| C6A—C1A—C14A—C15A | −65.6 (2) | C6B—C1B—C14B—C13B | −64.2 (2) |
| C12A—C13A—C14A—O1A | −11.1 (2) | C8B—C13B—C14B—O1B | −176.78 (16) |
| C8A—C13A—C14A—O1A | 174.06 (15) | C12B—C13B—C14B—O1B | 8.7 (2) |
| C12A—C13A—C14A—C1A | 103.27 (18) | C8B—C13B—C14B—C1B | 68.8 (2) |
| C8A—C13A—C14A—C1A | −71.5 (2) | C12B—C13B—C14B—C1B | −105.66 (18) |
| C12A—C13A—C14A—C15A | −133.61 (17) | C8B—C13B—C14B—C15B | −54.3 (2) |
| C8A—C13A—C14A—C15A | 51.6 (2) | C12B—C13B—C14B—C15B | 131.16 (17) |
| O1A—C14A—C15A—C16A | −76.66 (19) | O1B—C14B—C15B—C16B | 72.5 (2) |
| C1A—C14A—C15A—C16A | 167.18 (15) | C1B—C14B—C15B—C16B | −171.34 (16) |
| C13A—C14A—C15A—C16A | 46.6 (2) | C13B—C14B—C15B—C16B | −50.6 (2) |
| C14A—C15A—C16A—C17A | 81.9 (2) | C14B—C15B—C16B—C17B | −84.3 (2) |
| C19A—N1A—C17A—C16A | 161.24 (17) | C18B—N1B—C17B—C16B | 73.7 (2) |
| C18A—N1A—C17A—C16A | −75.9 (2) | C19B—N1B—C17B—C16B | −163.21 (19) |
| C15A—C16A—C17A—N1A | −66.7 (2) | C15B—C16B—C17B—N1B | 67.5 (2) |

*Hydrogen-bond geometry (Å, º)*

Cg1, Cg2, Cg7 and Cg8 are the centroids of the C1A—C6A, C8A—C13A, C1B–C6B and C8B—C13B rings, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1*A*—H1*A*···N1*A* | 0.84 | 1.86 | 2.693 (2) | 170 |
| O1*B*—H1*B*···N1*B* | 0.84 | 1.84 | 2.679 (2) | 174 |
| C4*A*—H4*AA*···O1*B* | 0.95 | 2.51 | 3.253 (2) | 135 |
| C3*A*—H3*AA*···*Cg*7$^{i}$ | 0.95 | 2.74 | 3.526 (6) | 140 |
| C17*A*—H17*A*···*Cg*1$^{ii}$ | 0.99 | 2.67 | 3.537 (7) | 147 |
| C17*A*—H17*B*···*Cg*2$^{ii}$ | 0.99 | 2.75 | 3.720 (3) | 167 |
| C17*B*—H17*C*···*Cg*8$^{iii}$ | 0.99 | 2.68 | 3.663 (6) | 170 |
| C17*B*—17D···*Cg*7$^{iii}$ | 0.99 | 2.64 | 3.538 (1) | 149 |

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