Syntheses and crystal structures of 2-(*p*-tolyl)-1*H*-perimidine hemihydrate and 1-methyl-2-(*p*-tolyl)-1*H*-perimidine

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The title compounds, 2-(4-methylphenyl)-1*H*-perimidine hemihydrate (**1**, $C_{18}H_{14}N_2 \cdot 0.5H_2O$) and 1-methyl-2-(4-methylphenyl)-1*H*-perimidine (**2**, $C_{19}H_{16}N_2$), were prepared and characterized by ^{1}H NMR and single-crystal X-ray diffraction. The organic molecule of the hemihydrate lies on a twofold rotation axis while the water molecule lies on the intersection of three twofold rotation axes (point group symmetry 222). As a consequence, the hydrogen atoms that are part of the N—H group and the water molecule as well as the CH_3 group of the *p*-tolyl ring are disordered over two positions. In compound **1**, the perimidine and the 2-aryl rings are slightly twisted while its *N*-methylated derivative **2** has a more distorted conformation because of the steric repulsion between the *N*-methyl group and the 2-aryl ring. In the crystal structures, molecules of perimidine **2** are held together only by C—H···π contacts while the parent perimidine **1** does not exhibit this type of interaction. Its crystal packing is established by intermolecular N—H···O hydrogen bonds with the solvent water molecules and additionally stabilized by π–π stacking.

1. Chemical context

Perimidines have found applications in industry as dyes and pigments because of their finely tunable optical properties (Pozharskii *et al.*, 2020). The introduction of electron-donating/withdrawing groups to the perimidine system dramatically affects its electronic structure and allows the color as well as color intensity of the perimidine to be varied. Additionally, a significant deepening of the color of perimidines can be achieved by decorating them with aromatic rings at position 2 while their optical characteristics can be modulated by varying the *N*-substituent (Sahiba & Agarwal, 2020). Recently, we have studied the effect of the *N*-substituent(s) on the structures of 2-(pyridin-2-yl)-1-*H*-perimidines (Kalle *et al.*, 2021). Herein, we report structural studies of 1-*H*-2-(*p*-tolyl)-perimidine hemihydrate (**1**) and 1-methyl-2-(*p*-tolyl)-perimidine (**2**).
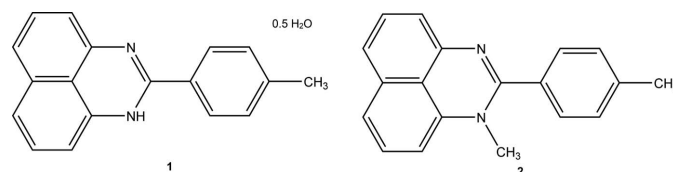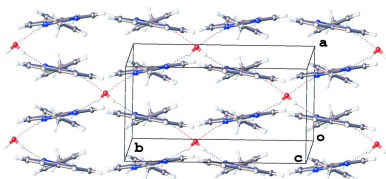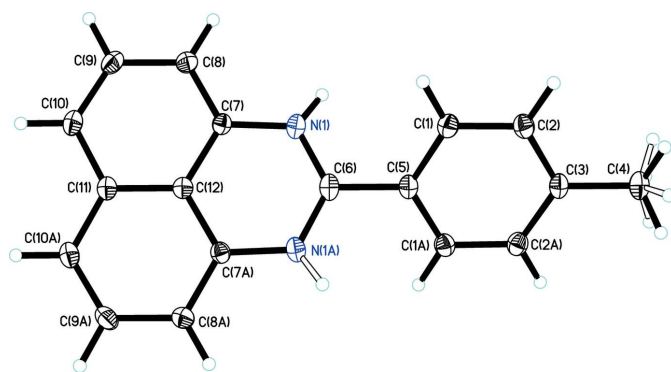
Figure 1
Molecular structure of 1-*H*-2-(*p*-tolyl)-perimidine (**1**), with displacement ellipsoids drawn at the 50% probability level. H atoms attached to N1 and N1*A* are present at half occupancy by virtue of the forced twofold symmetry. [Symmetry code: (A) $-x + \frac{5}{4}, -y + \frac{1}{4}, z$.]

2. Structural commentary

The perimidine molecule of **1** possesses *C*2 symmetry with the twofold rotation axis passing through carbon atoms C3–C6, C11 and C12 (Fig. 1). This perimidine exhibits a C6—N1 bond length of 1.3345 (12) Å, a value intermediate between the average C—N single [1.366 (13) Å] and double [1.293 (11) Å] bond lengths in perimidines according to the Cambridge Crystal Structure Database (CSD version 5.43 November 2021; Groom *et al.*, 2016). The perimidine core of **1** is flat while the *p*-tolyl ring (C1–C5) forms a dihedral angle of 34.47 (5)° with the core, which is likely an effect of the crystal packing.

The asymmetric unit of crystal **2** contains two molecules, which are *N*-methylated analogs of compound **1** (Fig. 2). Steric pressure exerted by the *N*-methyl group causes an increase of the interplanar angle between the *p*-tolyl ring and the perimidine system [53.51 (10)° for one molecule and 55.96 (9)° for the other]. Additionally, in the first molecule, the angle between the N1—C19 bond and the centroid of the perimidine plane is as large as 8.7 (2)°. while the corresponding angle in the second molecule is 6.1 (2)°.
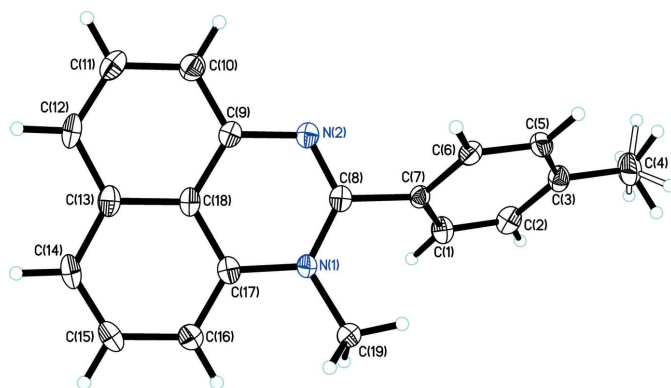
Table 1
Hydrogen-bond geometry (Å, °) for **1**.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1—H1*B*$\cdots$N1	0.89 (3)	2.13 (3)	2.9826 (10)	162 (3)
N1—H1$\cdots$O1	0.87 (3)	2.15 (3)	2.9826 (10)	160 (3)

3. Supramolecular features

Recrystallization of **1** from toluene, dichloromethane, chloroform or methanol gives crystals having an identical structure. An X-ray study of the crystals grown from hot toluene shows that compound **1** crystallizes as a hemihydrate in which the solvent molecule plays a dominant role in the crystal packing. Each water molecule, located at the intersection of three twofold rotation axes (Wyckoff position 8*a*; point group symmetry 222), arranges four 2-(*p*-tolyl)perimidines by mutual O—H$\cdots$N and N—H$\cdots$O interactions involving the O1 and N1 atoms as well as disordered hydrogen atoms H1 and H1*B* (Fig. 3, Table 1). These hydrogen-bonded associates containing the included water molecule are additionally stabilized by π–π contacts between the aromatic units [d(C1$\cdots$N1–C12$_{centroid}$) = 3.3276 (11) Å, centroid–centroid shift of 1.591 (1) Å, d(C7$\cdots$C1–C5$_{centroid}$) = 3.5950 (11) Å, centroid–centroid shift of 1.433 (1) Å]. The same interactions combine the associates into infinite stacks along the *a* axis, forming two-dimensional structural arrays. The alignment of the arrays along the *c* axis by weak van der Waals interactions between perimidine C9—H9 and C10—H10 bonds and the methyl group (C4) of the *p*-tolyl ring completes the crystal packing of **1**.

In the crystal structure of **2** (Fig. 4), the two crystallographically independent molecules are held together by C—H$\cdots\pi$ interactions between the *p*-tolyl and perimidine systems involving the H5 atom and the centroid of the C32–C37 ring [2.8226 (13) Å, 144.85 (18)°] and the H21 atom and the centroid of the C9–C13/C18 ring [2.6199 (12) Å, 145.74 (19)°]. The resulting dimers form stacks *via* similar non-covalent bonds involving the H24 atom and the centroid of the C9–C13/C18 ring [2.8676 (12) Å, 151.1 (2)°] and the H2 atom and the

Figure 2
Molecular structure of 1-methyl-2-(*p*-tolyl)-perimidine (**2**), with displacement ellipsoids drawn at the 50% probability level.
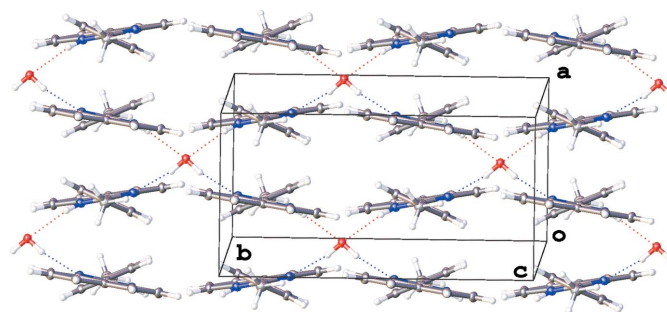

Figure 3
Hydrogen bonding and π—π stacking interactions in the crystal structure of 1-*H*-2-(*p*-tolyl)-perimidine (**1**), with displacement ellipsoids drawn at the 50% probability level. Hydrogen atoms of the minor disorder component are omitted for clarity.

centroid of the C32–C37 ring [3.1727 (13) Å, 142.3 (2)°]. The resulting layers are grafted together by weak C—H···N contacts involving the H19A and N4 atoms [d(H···N) = 2.624 (2) Å, C—H···N angle = 166.86 (18)°], forming arrays in the ab plane. The three-dimensional crystal packing is organized by the alignment of the arrays along the c axis by weak van der Waals interactions in the same manner as in the crystal of **1**. It is interesting that compound **2**, in contrast to the parent perimidine **1**, crystallizes without notable π–π interactions.

4. Database survey

A database search in the CSD (version 5.43 November 2021; Groom *et al.*, 2016) found only one crystal structure, a 2-arylperimidine hydrate in which one water molecule combines two 2-(2-methoxyphenyl)-1-*H*-perimidines by O—H···N hydrogen bonds whereas the H atom at the second nitrogen atom cannot interact with the oxygen atom of the water molecule because it participates in an intramolecular N—H···O bond with the methoxy group (PEKRIG; Foces-Foces *et al.*, 1993). A pseudo-tetrahedral pattern of hydrogen-bonded organic molecules around the included water molecule is formed by 2-amino-4-(4-pyridyl)-6-phenylamino-1,3,5-triazine, which bears many more donor and acceptor hydrogen-bonding groups than compound **1** (TETRIT; Chan *et al.*, 1996). The crystal structures of organic hydrates including N—H···O interactions have also been published [KIJPUO (Black *et al.*, 1991); FAZRED (Rosling *et al.*, 1999)].

5. Synthesis and crystallization

The title compounds were prepared as follows:

1-*H*-2-(*p*-tolyl)perimidine (**1**).

A mixture of 1,8-diaminonaphthalene (1.58 g, 0.01 mol), 4-methylbenzaldehyde (1.18 ml, 0.01 mol) and sodium meta-bisulfite (5.7 g, 0.03 mol) in ethanol (40 ml) was refluxed under Ar for 2 h. The reaction mixture was cooled, filtered and the filtrate was evaporated to dryness and washed with water. The crude solid was recrystallized from toluene and dried *in vacuo*. Yield 2.20 g (85%). Single crystals suitable for X-ray analysis were grown from hot toluene.

^{1}H NMR (DMSO-d_6, ppm, 400 MHz): δ 2.34 (*s*, 3H, CH$_3$), 6.65 (*d*, J = 7.2 Hz, 2H, H$_{naph}$), 7.04 (*d*, J = 8.0 Hz, 2H, H$_{naph}$), 7.15 (*t*, J = 7.2 Hz, 2H, H$_{naph}$), 7.30 (*d*, J = 7.2 Hz, 2H, H$_{tol}$), 7.95 (*d*, J = 8.0 Hz, 2H, H$_{tol}$). See supplementary Fig. S1.

1-Methyl-2-(*p*-tolyl)perimidine (**2**).

To a mixture of (**1**) (0.258 g, 1.0 mmol), solid KOH (0.056 g, 1.0 mmol) and anhydrous K$_2$CO$_3$ (0.138 g, 1.0 mmol) in anhydrous Ar-saturated acetonitrile methyl iodide (0.062 ml, 1.0 mmol) were added dropwise upon stirring and the resulting suspension was heated at 323 K for 1 h and then at room temperature for 1 h. The reaction mixture was evaporated to dryness and the crude product was purified by column chromatography (eluent hexane/ethyl acetate 1/1 → 1/5 *v/v*), recrystallized from a mixture of toluene/hexane and dried *in vacuo*. Yield 125 mg (46%). Single crystals suitable for
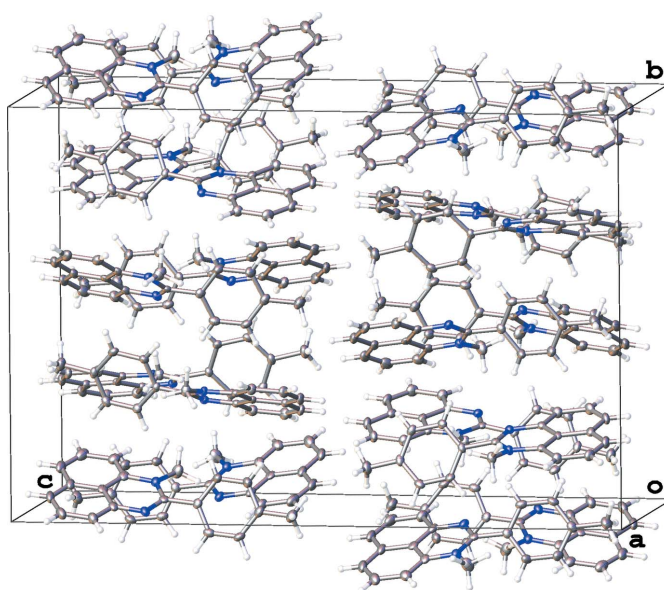
Figure 4
Fragment of the crystal packing of 1-methyl-2-(*p*-tolyl)-perimidine (**2**), with displacement ellipsoids drawn at the 50% probability level. Hydrogen atoms of the minor parts of the disordered methyl groups are omitted for clarity.

X-ray analysis were grown by slow evaporation of the solvent from a solution of the substance in toluene.

^{1}H NMR (CDCl$_3$, ppm, 400 MHz): δ 2.42(*s*, 3H, CH$_3$), 3.17 (*s*, 3H, N—CH$_3$), 6.28 (*d*, J = 7.2 Hz, 1H, H$_{naph}$), 6.94 (*d*, J = 7.3 Hz, 1H, H$_{naph}$), 7.17–7.24 (*m*, 3H, H$_{naph}$), 7.28–7.32 (*m*, 3H, H$_{naph}$ + H$_{tol}$), 7.44 (*d*, J = 7.7 Hz, 2H, H$_{tol}$). See supplementary Fig. S2.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All C—H hydrogen atoms in the structures of **1** and **2** were placed in calculated positions and refined using a riding model [C—H = 0.94–0.97 Å with U_{iso}(H) = 1.2–1.5U_{eq}(C)]. N—H and O—H hydrogen atoms (structure **1**) were located in difference electron-density maps and were refined with a fixed occupancy of 0.5. *para*-Methyl groups in both crystallographically independent molecules of **2** were found to be rotationally disordered with occupancy ratios of 0.6/0.4 and 0.7/0.3. The same group in the structure of **1** was similarly disordered with an occupancy ratio of 0.5/0.5. The SIMU instruction was used to restrain the U_{ij} components of the neighboring C6 and N1 atoms in the structure of **1**. The most disagreeable reflections with an error/s.u. of more than 10 (0 0 4 in the structure of **1**; 5 0 34 and 6 1 33 in the structure of **2**) were omitted using the OMIT instruction in *SHELXL* (Sheldrick, 2015).

Acknowledgements

Table 2
Experimental details.

	C$_{18}$H$_{14}$N$_2$·0.5H$_2$O	C$_{19}$H$_{16}$N$_2$
Crystal data		
M_r	267.32	272.34
Crystal system, space group	Orthorhombic, $Fddd$	Orthorhombic, $Pbca$
Temperature (K)	100	100
a, b, c (Å)	7.2131 (2), 13.8648 (5), 53.4532 (18)	11.6878 (4), 18.0941 (6), 26.9604 (8)
V (Å^3)	5345.8 (3)	5701.6 (3)
Z	16	16
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.08	0.08
Crystal size (mm)	0.13 × 0.1 × 0.1	0.12 × 0.09 × 0.08
Data collection		
Diffractometer	Bruker D8 Venture	Bruker D8 Venture
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.672, 0.746	0.676, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14708, 2138, 1630	53425, 5047, 3857
R_{int}	0.044	0.093
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.725	0.596
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.049, 0.140, 1.04	0.073, 0.157, 1.14
No. of reflections	2138	5047
No. of parameters	126	383
No. of restraints	6	0
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.42, −0.34	0.23, −0.29

Computer programs: *APEX3* and *SAINT* (Bruker, 2017), *SHELXS* (Sheldrick, 2008), *SHELXL* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

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Computing details

For both structures, data collection: *APEX3* (Bruker, 2017); cell refinement: *SAINT* (Bruker, 2017); data reduction: *SAINT* (Bruker, 2017); program(s) used to solve structure: *SHELXS* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

2-(4-Methylphenyl)-1*H*-perimidine hemihydrate (1)

Crystal data

$C_{18}H_{14}N_2 \cdot 0.5H_2O$	$D_x = 1.329$ Mg m^{-3}
$M_r = 267.32$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Orthorhombic, *Fddd*	Cell parameters from 4300 reflections
$a = 7.2131$ (2) Å	$\theta = 3.0–31.5°$
$b = 13.8648$ (5) Å	$\mu = 0.08$ mm^{-1}
$c = 53.4532$ (18) Å	$T = 100$ K
$V = 5345.8$ (3) Å^3	Block, orange
$Z = 16$	$0.13 \times 0.1 \times 0.1$ mm
$F(000) = 2256$	

Data collection

Bruker D8 Venture diffractometer	$T_{min} = 0.672$, $T_{max} = 0.746$
Radiation source: microfocus sealed X-ray tube, Incoatec Iμs	14708 measured reflections
	2138 independent reflections
Focusing mirrors monochromator	1630 reflections with $I > 2\sigma(I)$
Detector resolution: 10.4 pixels mm^{-1}	$R_{int} = 0.044$
ω–scan	$\theta_{max} = 31.0°$, $\theta_{min} = 3.0°$
Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015)	$h = -9 \rightarrow 10$
	$k = -20 \rightarrow 16$
	$l = -77 \rightarrow 77$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Hydrogen site location: mixed
$R[F^2 > 2\sigma(F^2)] = 0.049$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.140$	
$S = 1.04$	$w = 1/[\sigma^2(F_o^2) + (0.0761P)^2 + 4.7998P]$
2138 reflections	where $P = (F_o^2 + 2F_c^2)/3$
126 parameters	$(\Delta/\sigma)_{max} = 0.001$
6 restraints	

$\Delta\rho_{max} = 0.42$ e Å^{-3} $\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ $\Delta\rho_{min} = -0.34$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.8750	0.3750	0.3750	0.0216 (4)	
H1B	0.790 (4)	0.335 (2)	0.3693 (6)	0.036 (9)*	0.5
N1	0.65901 (13)	0.20824 (7)	0.35517 (2)	0.0176 (2)	
H1	0.708 (4)	0.253 (2)	0.3644 (6)	0.026 (8)*	0.5
C1	0.55996 (16)	0.20495 (8)	0.40781 (2)	0.0177 (2)	
H1A	0.508 (2)	0.2610 (11)	0.3988 (3)	0.024 (4)*	
C2	0.55826 (15)	0.20393 (8)	0.43382 (2)	0.0181 (3)	
H2	0.503 (2)	0.2585 (11)	0.4429 (3)	0.022 (3)*	
C3	0.6250	0.1250	0.44720 (3)	0.0171 (3)	
C4	0.6250	0.1250	0.47536 (3)	0.0226 (4)	
H4A	0.6649	0.1883	0.4815	0.034*	0.5
H4B	0.7105	0.0754	0.4815	0.034*	0.5
H4C	0.4996	0.1113	0.4815	0.034*	0.5
C5	0.6250	0.1250	0.39454 (3)	0.0155 (3)	
C6	0.6250	0.1250	0.36684 (3)	0.0182 (3)	
C7	0.65540 (15)	0.21186 (8)	0.32902 (2)	0.0148 (2)	
C8	0.68100 (16)	0.29750 (8)	0.31632 (2)	0.0188 (3)	
H8	0.705 (2)	0.3573 (10)	0.3255 (3)	0.022 (4)*	
C9	0.67686 (17)	0.29749 (8)	0.28998 (2)	0.0210 (3)	
H9	0.697 (2)	0.3594 (11)	0.2812 (3)	0.031 (4)*	
C10	0.65083 (16)	0.21420 (8)	0.27653 (2)	0.0193 (3)	
H10	0.654 (2)	0.2141 (10)	0.2581 (3)	0.029 (4)*	
C11	0.6250	0.1250	0.28908 (3)	0.0162 (3)	
C12	0.6250	0.1250	0.31562 (3)	0.0144 (3)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0249 (9)	0.0176 (8)	0.0222 (8)	0.000	0.000	0.000
N1	0.0173 (4)	0.0223 (5)	0.0133 (4)	−0.0015 (3)	−0.0005 (3)	0.0017 (3)
C1	0.0172 (5)	0.0200 (5)	0.0160 (5)	−0.0012 (4)	0.0005 (4)	0.0013 (4)
C2	0.0172 (5)	0.0210 (5)	0.0160 (5)	−0.0009 (4)	0.0021 (4)	−0.0015 (4)
C3	0.0153 (7)	0.0230 (8)	0.0128 (7)	−0.0030 (6)	0.000	0.000
C4	0.0244 (8)	0.0294 (9)	0.0141 (7)	0.0001 (7)	0.000	0.000
C5	0.0126 (6)	0.0209 (7)	0.0130 (7)	−0.0034 (5)	0.000	0.000
C6	0.0150 (6)	0.0261 (7)	0.0134 (6)	−0.0007 (5)	0.000	0.000
C7	0.0140 (5)	0.0167 (5)	0.0137 (5)	−0.0007 (4)	−0.0005 (4)	0.0009 (4)
C8	0.0222 (5)	0.0163 (5)	0.0179 (5)	−0.0023 (4)	−0.0002 (4)	0.0010 (4)

C9	0.0251 (6)	0.0192 (5)	0.0188 (5)	−0.0008 (4)	0.0006 (4)	0.0060 (4)
C10	0.0202 (5)	0.0238 (6)	0.0140 (5)	0.0012 (4)	0.0003 (4)	0.0025 (4)
C11	0.0143 (7)	0.0201 (7)	0.0142 (7)	0.0011 (6)	0.000	0.000
C12	0.0116 (6)	0.0167 (7)	0.0149 (7)	0.0013 (5)	0.000	0.000

Geometric parameters (Å, º)

O1—H1B	0.89 (3)	C5—C1[i]	1.3971 (14)
N1—H1	0.87 (3)	C5—C6	1.481 (2)
N1—C6	1.3345 (12)	C6—N1[i]	1.3345 (12)
N1—C7	1.3993 (14)	C7—C8	1.3801 (15)
C1—H1A	0.987 (15)	C7—C12	1.4182 (13)
C1—C2	1.3901 (15)	C8—H8	0.978 (15)
C1—C5	1.3972 (14)	C8—C9	1.4083 (16)
C2—H2	0.983 (15)	C9—H9	0.988 (16)
C2—C3	1.3932 (14)	C9—C10	1.3734 (17)
C3—C2[i]	1.3932 (14)	C10—H10	0.987 (16)
C3—C4	1.505 (2)	C10—C11	1.4192 (13)
C4—H4A	0.9800	C11—C10[i]	1.4194 (13)
C4—H4B	0.9800	C11—C12	1.419 (2)
C4—H4C	0.9800	C12—C7[i]	1.4181 (13)
C6—N1—H1	116 (2)	N1[i]—C6—N1	124.28 (14)
C6—N1—C7	119.64 (10)	N1—C6—C5	117.86 (7)
C7—N1—H1	123 (2)	N1[i]—C6—C5	117.86 (7)
C2—C1—H1A	119.4 (9)	N1—C7—C12	118.49 (10)
C2—C1—C5	120.17 (11)	C8—C7—N1	121.32 (10)
C5—C1—H1A	120.3 (9)	C8—C7—C12	120.19 (10)
C1—C2—H2	119.4 (8)	C7—C8—H8	120.5 (9)
C1—C2—C3	121.22 (11)	C7—C8—C9	119.26 (11)
C3—C2—H2	119.3 (8)	C9—C8—H8	120.2 (9)
C2[i]—C3—C2	118.23 (14)	C8—C9—H9	118.1 (9)
C2[i]—C3—C4	120.88 (7)	C10—C9—C8	121.76 (11)
C2—C3—C4	120.89 (7)	C10—C9—H9	120.2 (9)
C3—C4—H4A	109.5	C9—C10—H10	121.5 (9)
C3—C4—H4B	109.5	C9—C10—C11	120.21 (11)
C3—C4—H4C	109.5	C11—C10—H10	118.3 (9)
H4A—C4—H4B	109.5	C10—C11—C10[i]	123.58 (14)
H4A—C4—H4C	109.5	C12—C11—C10	118.21 (7)
H4B—C4—H4C	109.5	C12—C11—C10[i]	118.21 (7)
C1[i]—C5—C1	118.98 (14)	C7[i]—C12—C7	119.34 (13)
C1[i]—C5—C6	120.51 (7)	C7—C12—C11	120.33 (7)
C1—C5—C6	120.51 (7)	C7[i]—C12—C11	120.33 (7)
N1—C7—C8—C9	179.77 (10)	C7—N1—C6—N1[i]	1.69 (7)
N1—C7—C12—C7[i]	1.61 (6)	C7—N1—C6—C5	−178.31 (7)
N1—C7—C12—C11	−178.39 (6)	C7—C8—C9—C10	−1.02 (18)
C1—C2—C3—C2[i]	−0.82 (7)	C8—C7—C12—C7[i]	−178.51 (12)

C1—C2—C3—C4	179.18 (7)	C8—C7—C12—C11	1.49 (12)
C1^i—C5—C6—N1^i	34.94 (7)	C8—C9—C10—C11	0.73 (17)
C1^i—C5—C6—N1	−145.06 (7)	C9—C10—C11—C10^i	−179.34 (13)
C1—C5—C6—N1	34.94 (7)	C9—C10—C11—C12	0.66 (12)
C1—C5—C6—N1^i	−145.06 (7)	C10—C11—C12—C7	−1.75 (7)
C2—C1—C5—C1^i	−0.81 (7)	C10^i—C11—C12—C7^i	−1.75 (7)
C2—C1—C5—C6	179.20 (7)	C10^i—C11—C12—C7	178.25 (7)
C5—C1—C2—C3	1.64 (15)	C10—C11—C12—C7^i	178.25 (7)
C6—N1—C7—C8	176.84 (9)	C12—C7—C8—C9	−0.10 (16)
C6—N1—C7—C12	−3.29 (13)		

Symmetry code: (i) −x+5/4, −y+1/4, z.

Hydrogen-bond geometry (Å, º)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O1—H1B⋯N1	0.89 (3)	2.13 (3)	2.9826 (10)	162 (3)
N1—H1⋯O1	0.87 (3)	2.15 (3)	2.9826 (10)	160 (3)

1-Methyl-2-(*p*-tolyl)-1-*H*-perimidine (2)

Crystal data

C$_{19}$H$_{16}$N$_2$
M_r = 272.34
Orthorhombic, *Pbca*
a = 11.6878 (4) Å
b = 18.0941 (6) Å
c = 26.9604 (8) Å
V = 5701.6 (3) Å^3
Z = 16
F(000) = 2304

D_x = 1.269 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7540 reflections
θ = 2.2–28.3°
μ = 0.08 mm^{-1}
T = 100 K
Block, yellow
0.12 × 0.09 × 0.08 mm

Data collection

Bruker D8 Venture
   diffractometer
Radiation source: microfocus sealed X-ray tube,
   Incoatec Iμs
Focusing mirrors monochromator
Detector resolution: 10.4 pixels mm^{-1}
ω–scan
Absorption correction: multi-scan
   (*SADABS*; Krause *et al.*, 2015)

T_{min} = 0.676, T_{max} = 0.746
53425 measured reflections
5047 independent reflections
3857 reflections with $I > 2\sigma(I)$
R_{int} = 0.093
θ_{max} = 25.1°, θ_{min} = 2.2°
h = −13→13
k = −21→21
l = −31→32

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.073
$wR(F^2)$ = 0.157
S = 1.14
5047 reflections
383 parameters
0 restraints
Primary atom site location: dual

Hydrogen site location: inferred from
   neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0485P)^2 + 7.2287P]$
   where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
N1	0.43727 (19)	0.18405 (12)	0.31230 (8)	0.0175 (5)	
N2	0.2447 (2)	0.21911 (12)	0.29690 (8)	0.0185 (5)	
C1	0.3882 (2)	0.11253 (15)	0.21059 (10)	0.0209 (6)	
H1	0.4128	0.0760	0.2335	0.025*	
C2	0.3842 (3)	0.09595 (15)	0.16034 (11)	0.0233 (7)	
H2	0.4038	0.0477	0.1493	0.028*	
C3	0.3516 (2)	0.14950 (16)	0.12585 (10)	0.0217 (7)	
C4	0.3475 (3)	0.13008 (18)	0.07119 (11)	0.0325 (8)	
H4AA	0.4255	0.1230	0.0588	0.049*	0.7
H4AB	0.3107	0.1703	0.0528	0.049*	0.7
H4AC	0.3036	0.0844	0.0667	0.049*	0.7
H4BD	0.2695	0.1372	0.0587	0.049*	0.3
H4BE	0.3702	0.0784	0.0667	0.049*	0.3
H4BF	0.4002	0.1622	0.0528	0.049*	0.3
C5	0.3240 (2)	0.21969 (16)	0.14290 (10)	0.0224 (7)	
H5	0.3035	0.2571	0.1199	0.027*	
C6	0.3261 (2)	0.23577 (15)	0.19325 (10)	0.0197 (6)	
H6	0.3066	0.2840	0.2043	0.024*	
C7	0.3567 (2)	0.18187 (15)	0.22769 (10)	0.0166 (6)	
C8	0.3451 (2)	0.19748 (14)	0.28191 (10)	0.0167 (6)	
C9	0.2275 (2)	0.22857 (14)	0.34790 (10)	0.0175 (6)	
C10	0.1229 (3)	0.25252 (16)	0.36522 (11)	0.0239 (7)	
H10	0.0632	0.2635	0.3425	0.029*	
C11	0.1044 (3)	0.26077 (16)	0.41622 (11)	0.0270 (7)	
H11	0.0322	0.2779	0.4277	0.032*	
C12	0.1890 (3)	0.24445 (16)	0.45006 (11)	0.0258 (7)	
H12	0.1742	0.2496	0.4845	0.031*	
C13	0.2973 (3)	0.22019 (15)	0.43391 (10)	0.0215 (7)	
C14	0.3895 (3)	0.20256 (16)	0.46636 (11)	0.0268 (7)	
H14	0.3798	0.2075	0.5012	0.032*	
C15	0.4915 (3)	0.17867 (16)	0.44797 (11)	0.0261 (7)	
H15	0.5510	0.1663	0.4705	0.031*	
C16	0.5117 (3)	0.17171 (16)	0.39662 (10)	0.0233 (7)	
H16	0.5840	0.1556	0.3846	0.028*	
C17	0.4243 (2)	0.18870 (14)	0.36411 (10)	0.0184 (6)	
C18	0.3162 (2)	0.21197 (14)	0.38191 (10)	0.0174 (6)	
C19	0.5531 (2)	0.17366 (16)	0.29268 (10)	0.0229 (7)	
H19A	0.5765	0.1221	0.2973	0.034*	
H19B	0.6063	0.2062	0.3104	0.034*	

H19C	0.5540	0.1857	0.2572	0.034*	
N3	0.2012 (2)	0.42161 (12)	0.21218 (8)	0.0219 (6)	
N4	0.3830 (2)	0.47987 (13)	0.20977 (8)	0.0226 (6)	
C20	0.2838 (3)	0.40519 (16)	0.32035 (10)	0.0259 (7)	
H20	0.2647	0.3582	0.3071	0.031*	
C21	0.2985 (3)	0.41308 (16)	0.37083 (11)	0.0287 (7)	
H21	0.2901	0.3711	0.3917	0.034*	
C22	0.3253 (3)	0.48092 (16)	0.39184 (11)	0.0258 (7)	
C23	0.3434 (3)	0.48919 (19)	0.44674 (11)	0.0387 (9)	
H23A	0.4250	0.4843	0.4543	0.058*	0.6
H23B	0.3005	0.4507	0.4643	0.058*	0.6
H23C	0.3164	0.5379	0.4574	0.058*	0.6
H23D	0.3890	0.5336	0.4532	0.058*	0.4
H23E	0.3838	0.4457	0.4595	0.058*	0.4
H23F	0.2691	0.4936	0.4633	0.058*	0.4
C24	0.3369 (3)	0.54109 (16)	0.36007 (11)	0.0255 (7)	
H24	0.3546	0.5883	0.3735	0.031*	
C25	0.3231 (3)	0.53364 (15)	0.30924 (11)	0.0238 (7)	
H25	0.3318	0.5756	0.2884	0.029*	
C26	0.2967 (2)	0.46554 (15)	0.28853 (10)	0.0205 (6)	
C27	0.2939 (3)	0.45635 (14)	0.23366 (10)	0.0208 (7)	
C28	0.3886 (3)	0.46785 (15)	0.15836 (11)	0.0250 (7)	
C29	0.4843 (3)	0.49011 (17)	0.13268 (11)	0.0291 (7)	
H29	0.5461	0.5130	0.1496	0.035*	
C30	0.4898 (3)	0.47866 (17)	0.08107 (12)	0.0359 (8)	
H30	0.5562	0.4935	0.0634	0.043*	
C31	0.4011 (3)	0.44640 (17)	0.05601 (11)	0.0347 (8)	
H31	0.4064	0.4400	0.0211	0.042*	
C32	0.3017 (3)	0.42245 (16)	0.08105 (11)	0.0300 (8)	
C33	0.2067 (3)	0.38821 (17)	0.05775 (12)	0.0350 (8)	
H33	0.2070	0.3814	0.0228	0.042*	
C34	0.1150 (3)	0.36494 (17)	0.08484 (12)	0.0356 (8)	
H34	0.0530	0.3414	0.0684	0.043*	
C35	0.1098 (3)	0.37489 (16)	0.13666 (11)	0.0291 (7)	
H35	0.0449	0.3586	0.1549	0.035*	
C36	0.2001 (3)	0.40848 (15)	0.16054 (11)	0.0241 (7)	
C37	0.2970 (3)	0.43318 (15)	0.13339 (11)	0.0241 (7)	
C38	0.0958 (3)	0.40401 (19)	0.23934 (12)	0.0341 (8)	
H38A	0.0888	0.3503	0.2429	0.051*	
H38B	0.0297	0.4231	0.2210	0.051*	
H38C	0.0985	0.4269	0.2723	0.051*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0187 (13)	0.0200 (12)	0.0137 (12)	0.0014 (10)	0.0004 (10)	−0.0016 (9)
N2	0.0223 (13)	0.0151 (12)	0.0180 (13)	−0.0003 (10)	0.0015 (10)	−0.0008 (9)
C1	0.0273 (17)	0.0156 (14)	0.0198 (16)	−0.0042 (12)	0.0009 (13)	0.0021 (11)

C2	0.0266 (17)	0.0176 (14)	0.0257 (17)	−0.0053 (13)	0.0035 (13)	−0.0053 (12)
C3	0.0216 (16)	0.0276 (16)	0.0159 (15)	−0.0070 (13)	−0.0003 (12)	−0.0027 (12)
C4	0.041 (2)	0.0383 (19)	0.0184 (17)	−0.0029 (15)	−0.0007 (14)	−0.0038 (13)
C5	0.0211 (16)	0.0264 (16)	0.0195 (16)	−0.0002 (13)	−0.0001 (12)	0.0064 (12)
C6	0.0192 (15)	0.0192 (15)	0.0207 (16)	0.0012 (12)	0.0038 (12)	−0.0001 (11)
C7	0.0160 (15)	0.0199 (14)	0.0140 (14)	−0.0024 (11)	0.0005 (11)	−0.0023 (11)
C8	0.0225 (16)	0.0095 (13)	0.0180 (15)	−0.0037 (11)	0.0016 (12)	0.0003 (10)
C9	0.0215 (16)	0.0121 (13)	0.0188 (15)	−0.0024 (11)	0.0030 (12)	−0.0007 (10)
C10	0.0232 (17)	0.0254 (16)	0.0232 (16)	−0.0003 (13)	0.0019 (13)	−0.0006 (12)
C11	0.0258 (17)	0.0288 (17)	0.0265 (17)	0.0009 (14)	0.0100 (14)	−0.0015 (13)
C12	0.0351 (19)	0.0268 (16)	0.0155 (15)	−0.0041 (14)	0.0084 (13)	−0.0047 (12)
C13	0.0302 (17)	0.0170 (14)	0.0174 (15)	−0.0040 (13)	0.0038 (13)	0.0000 (11)
C14	0.038 (2)	0.0294 (17)	0.0128 (15)	−0.0052 (15)	−0.0012 (13)	−0.0009 (12)
C15	0.0322 (18)	0.0278 (16)	0.0182 (16)	−0.0028 (14)	−0.0082 (14)	0.0014 (12)
C16	0.0228 (16)	0.0260 (16)	0.0210 (16)	0.0011 (13)	−0.0015 (13)	−0.0012 (12)
C17	0.0254 (16)	0.0123 (14)	0.0174 (15)	−0.0021 (12)	−0.0005 (12)	−0.0009 (11)
C18	0.0246 (16)	0.0131 (13)	0.0146 (14)	−0.0061 (12)	0.0023 (12)	−0.0013 (11)
C19	0.0190 (15)	0.0301 (17)	0.0196 (15)	0.0008 (12)	0.0004 (12)	−0.0015 (12)
N3	0.0266 (14)	0.0194 (12)	0.0197 (13)	0.0025 (11)	0.0023 (11)	−0.0007 (10)
N4	0.0283 (15)	0.0201 (12)	0.0195 (14)	0.0027 (11)	0.0024 (11)	0.0046 (10)
C20	0.039 (2)	0.0180 (15)	0.0203 (16)	−0.0046 (13)	0.0070 (14)	−0.0023 (12)
C21	0.042 (2)	0.0235 (16)	0.0202 (17)	−0.0018 (14)	0.0080 (14)	0.0013 (12)
C22	0.0284 (18)	0.0270 (16)	0.0219 (16)	0.0017 (13)	0.0026 (13)	−0.0063 (12)
C23	0.057 (2)	0.0337 (19)	0.0251 (18)	0.0013 (17)	−0.0003 (17)	−0.0079 (14)
C24	0.0319 (18)	0.0169 (15)	0.0276 (18)	−0.0003 (13)	0.0002 (14)	−0.0065 (12)
C25	0.0249 (17)	0.0168 (15)	0.0297 (18)	−0.0004 (12)	0.0013 (13)	0.0026 (12)
C26	0.0191 (15)	0.0223 (15)	0.0201 (16)	0.0023 (12)	0.0034 (12)	−0.0021 (12)
C27	0.0294 (17)	0.0112 (14)	0.0219 (16)	0.0050 (12)	0.0008 (13)	0.0016 (11)
C28	0.0374 (19)	0.0171 (15)	0.0205 (16)	0.0083 (13)	0.0045 (14)	0.0051 (12)
C29	0.036 (2)	0.0277 (17)	0.0234 (17)	0.0025 (14)	0.0060 (14)	0.0052 (13)
C30	0.051 (2)	0.0285 (18)	0.0279 (19)	0.0061 (16)	0.0166 (17)	0.0078 (14)
C31	0.062 (3)	0.0271 (17)	0.0153 (16)	0.0097 (17)	0.0064 (16)	0.0034 (13)
C32	0.052 (2)	0.0214 (16)	0.0167 (16)	0.0119 (15)	0.0012 (15)	0.0031 (12)
C33	0.060 (2)	0.0280 (18)	0.0176 (17)	0.0130 (17)	−0.0071 (16)	0.0014 (13)
C34	0.049 (2)	0.0280 (18)	0.0299 (19)	0.0111 (16)	−0.0146 (17)	−0.0047 (14)
C35	0.0351 (19)	0.0222 (16)	0.0299 (18)	0.0060 (14)	−0.0040 (15)	−0.0024 (13)
C36	0.0338 (18)	0.0167 (14)	0.0218 (16)	0.0103 (13)	−0.0037 (14)	0.0014 (12)
C37	0.0372 (19)	0.0134 (14)	0.0217 (16)	0.0105 (13)	−0.0004 (14)	0.0043 (11)
C38	0.0299 (19)	0.041 (2)	0.0308 (19)	−0.0058 (15)	0.0084 (15)	−0.0078 (14)

Geometric parameters (Å, º)

N1—C8	1.375 (3)	N3—C27	1.380 (4)
N1—C17	1.407 (3)	N3—C36	1.412 (4)
N1—C19	1.466 (4)	N3—C38	1.468 (4)
N2—C8	1.301 (4)	N4—C27	1.297 (4)
N2—C9	1.400 (3)	N4—C28	1.404 (4)
C1—H1	0.9500	C20—H20	0.9500

C1—C2	1.388 (4)	C20—C21	1.379 (4)
C1—C7	1.386 (4)	C20—C26	1.397 (4)
C2—H2	0.9500	C21—H21	0.9500
C2—C3	1.396 (4)	C21—C22	1.388 (4)
C3—C4	1.516 (4)	C22—C23	1.503 (4)
C3—C5	1.389 (4)	C22—C24	1.392 (4)
C4—H4AA	0.9800	C23—H23A	0.9800
C4—H4AB	0.9800	C23—H23B	0.9800
C4—H4AC	0.9800	C23—H23C	0.9800
C4—H4BD	0.9800	C23—H23D	0.9800
C4—H4BE	0.9800	C23—H23E	0.9800
C4—H4BF	0.9800	C23—H23F	0.9800
C5—H5	0.9500	C24—H24	0.9500
C5—C6	1.388 (4)	C24—C25	1.386 (4)
C6—H6	0.9500	C25—H25	0.9500
C6—C7	1.393 (4)	C25—C26	1.388 (4)
C7—C8	1.495 (4)	C26—C27	1.489 (4)
C9—C10	1.378 (4)	C28—C29	1.376 (4)
C9—C18	1.417 (4)	C28—C37	1.412 (4)
C10—H10	0.9500	C29—H29	0.9500
C10—C11	1.400 (4)	C29—C30	1.408 (4)
C11—H11	0.9500	C30—H30	0.9500
C11—C12	1.378 (4)	C30—C31	1.369 (5)
C12—H12	0.9500	C31—H31	0.9500
C12—C13	1.409 (4)	C31—C32	1.412 (5)
C13—C14	1.424 (4)	C32—C33	1.418 (5)
C13—C18	1.427 (4)	C32—C37	1.425 (4)
C14—H14	0.9500	C33—H33	0.9500
C14—C15	1.361 (4)	C33—C34	1.364 (5)
C15—H15	0.9500	C34—H34	0.9500
C15—C16	1.410 (4)	C34—C35	1.410 (4)
C16—H16	0.9500	C35—H35	0.9500
C16—C17	1.381 (4)	C35—C36	1.377 (4)
C17—C18	1.416 (4)	C36—C37	1.421 (4)
C19—H19A	0.9800	C38—H38A	0.9800
C19—H19B	0.9800	C38—H38B	0.9800
C19—H19C	0.9800	C38—H38C	0.9800
C8—N1—C17	119.8 (2)	C27—N3—C36	119.8 (3)
C8—N1—C19	122.1 (2)	C27—N3—C38	123.2 (2)
C17—N1—C19	117.7 (2)	C36—N3—C38	116.6 (3)
C8—N2—C9	118.1 (2)	C27—N4—C28	118.5 (3)
C2—C1—H1	119.6	C21—C20—H20	119.6
C7—C1—H1	119.6	C21—C20—C26	120.8 (3)
C7—C1—C2	120.7 (3)	C26—C20—H20	119.6
C1—C2—H2	119.7	C20—C21—H21	119.2
C1—C2—C3	120.6 (3)	C20—C21—C22	121.5 (3)
C3—C2—H2	119.7	C22—C21—H21	119.2

C2—C3—C4	119.7 (3)	C21—C22—C23	121.5 (3)
C5—C3—C2	118.5 (3)	C21—C22—C24	117.6 (3)
C5—C3—C4	121.8 (3)	C24—C22—C23	121.0 (3)
C3—C4—H4AA	109.5	C22—C23—H23A	109.5
C3—C4—H4AB	109.5	C22—C23—H23B	109.5
C3—C4—H4AC	109.5	C22—C23—H23C	109.5
C3—C4—H4BD	109.5	C22—C23—H23D	109.5
C3—C4—H4BE	109.5	C22—C23—H23E	109.5
C3—C4—H4BF	109.5	C22—C23—H23F	109.5
H4AA—C4—H4AB	109.5	H23A—C23—H23B	109.5
H4AA—C4—H4AC	109.5	H23A—C23—H23C	109.5
H4AB—C4—H4AC	109.5	H23B—C23—H23C	109.5
H4BD—C4—H4BE	109.5	H23D—C23—H23E	109.5
H4BD—C4—H4BF	109.5	H23D—C23—H23F	109.5
H4BE—C4—H4BF	109.5	H23E—C23—H23F	109.5
C3—C5—H5	119.6	C22—C24—H24	119.3
C6—C5—C3	120.7 (3)	C25—C24—C22	121.4 (3)
C6—C5—H5	119.6	C25—C24—H24	119.3
C5—C6—H6	119.7	C24—C25—H25	119.7
C5—C6—C7	120.6 (3)	C24—C25—C26	120.7 (3)
C7—C6—H6	119.7	C26—C25—H25	119.7
C1—C7—C6	118.7 (2)	C20—C26—C27	121.4 (2)
C1—C7—C8	121.3 (2)	C25—C26—C20	118.1 (3)
C6—C7—C8	119.7 (2)	C25—C26—C27	120.3 (3)
N1—C8—C7	118.6 (2)	N3—C27—C26	119.0 (3)
N2—C8—N1	125.1 (2)	N4—C27—N3	124.9 (3)
N2—C8—C7	116.2 (2)	N4—C27—C26	116.0 (3)
N2—C9—C18	120.3 (2)	N4—C28—C37	120.3 (3)
C10—C9—N2	119.9 (3)	C29—C28—N4	119.3 (3)
C10—C9—C18	119.8 (2)	C29—C28—C37	120.4 (3)
C9—C10—H10	119.9	C28—C29—H29	120.3
C9—C10—C11	120.3 (3)	C28—C29—C30	119.5 (3)
C11—C10—H10	119.9	C30—C29—H29	120.3
C10—C11—H11	119.5	C29—C30—H30	119.5
C12—C11—C10	121.1 (3)	C31—C30—C29	121.0 (3)
C12—C11—H11	119.5	C31—C30—H30	119.5
C11—C12—H12	119.8	C30—C31—H31	119.4
C11—C12—C13	120.5 (3)	C30—C31—C32	121.2 (3)
C13—C12—H12	119.8	C32—C31—H31	119.4
C12—C13—C14	124.0 (3)	C31—C32—C33	124.5 (3)
C12—C13—C18	118.4 (3)	C31—C32—C37	117.6 (3)
C14—C13—C18	117.6 (3)	C33—C32—C37	117.9 (3)
C13—C14—H14	119.7	C32—C33—H33	119.6
C15—C14—C13	120.7 (3)	C34—C33—C32	120.9 (3)
C15—C14—H14	119.7	C34—C33—H33	119.6
C14—C15—H15	118.9	C33—C34—H34	119.2
C14—C15—C16	122.2 (3)	C33—C34—C35	121.7 (3)
C16—C15—H15	118.9	C35—C34—H34	119.2

C15—C16—H16	120.7	C34—C35—H35	120.4
C17—C16—C15	118.7 (3)	C36—C35—C34	119.1 (3)
C17—C16—H16	120.7	C36—C35—H35	120.4
N1—C17—C18	116.8 (2)	N3—C36—C37	116.6 (3)
C16—C17—N1	122.5 (3)	C35—C36—N3	122.8 (3)
C16—C17—C18	120.7 (3)	C35—C36—C37	120.6 (3)
C9—C18—C13	120.0 (3)	C28—C37—C32	120.2 (3)
C17—C18—C9	119.8 (2)	C28—C37—C36	119.9 (3)
C17—C18—C13	120.1 (3)	C36—C37—C32	119.9 (3)
N1—C19—H19A	109.5	N3—C38—H38A	109.5
N1—C19—H19B	109.5	N3—C38—H38B	109.5
N1—C19—H19C	109.5	N3—C38—H38C	109.5
H19A—C19—H19B	109.5	H38A—C38—H38B	109.5
H19A—C19—H19C	109.5	H38A—C38—H38C	109.5
H19B—C19—H19C	109.5	H38B—C38—H38C	109.5
N1—C17—C18—C9	0.5 (4)	N3—C36—C37—C28	0.9 (4)
N1—C17—C18—C13	−178.1 (2)	N3—C36—C37—C32	−179.5 (2)
N2—C9—C10—C11	178.8 (3)	N4—C28—C29—C30	−179.5 (3)
N2—C9—C18—C13	−178.6 (2)	N4—C28—C37—C32	178.7 (2)
N2—C9—C18—C17	2.7 (4)	N4—C28—C37—C36	−1.7 (4)
C1—C2—C3—C4	−179.8 (3)	C20—C21—C22—C23	−178.9 (3)
C1—C2—C3—C5	0.4 (4)	C20—C21—C22—C24	0.0 (5)
C1—C7—C8—N1	56.1 (4)	C20—C26—C27—N3	54.3 (4)
C1—C7—C8—N2	−120.2 (3)	C20—C26—C27—N4	−123.2 (3)
C2—C1—C7—C6	−3.0 (4)	C21—C20—C26—C25	−0.9 (5)
C2—C1—C7—C8	171.5 (3)	C21—C20—C26—C27	173.2 (3)
C2—C3—C5—C6	−1.5 (4)	C21—C22—C24—C25	−0.5 (5)
C3—C5—C6—C7	0.4 (4)	C22—C24—C25—C26	0.2 (5)
C4—C3—C5—C6	178.7 (3)	C23—C22—C24—C25	178.4 (3)
C5—C6—C7—C1	1.9 (4)	C24—C25—C26—C20	0.4 (4)
C5—C6—C7—C8	−172.8 (3)	C24—C25—C26—C27	−173.7 (3)
C6—C7—C8—N1	−129.4 (3)	C25—C26—C27—N3	−131.8 (3)
C6—C7—C8—N2	54.3 (4)	C25—C26—C27—N4	50.7 (4)
C7—C1—C2—C3	2.0 (4)	C26—C20—C21—C22	0.7 (5)
C8—N1—C17—C16	176.2 (2)	C27—N3—C36—C35	−179.2 (3)
C8—N1—C17—C18	−3.9 (4)	C27—N3—C36—C37	−0.5 (4)
C8—N2—C9—C10	179.0 (3)	C27—N4—C28—C29	−177.7 (3)
C8—N2—C9—C18	−2.5 (4)	C27—N4—C28—C37	2.1 (4)
C9—N2—C8—N1	−1.1 (4)	C28—N4—C27—N3	−1.8 (4)
C9—N2—C8—C7	174.9 (2)	C28—N4—C27—C26	175.5 (2)
C9—C10—C11—C12	−0.8 (4)	C28—C29—C30—C31	0.7 (5)
C10—C9—C18—C13	−0.1 (4)	C29—C28—C37—C32	−1.5 (4)
C10—C9—C18—C17	−178.8 (3)	C29—C28—C37—C36	178.1 (3)
C10—C11—C12—C13	1.1 (4)	C29—C30—C31—C32	−1.0 (5)
C11—C12—C13—C14	179.7 (3)	C30—C31—C32—C33	−179.6 (3)
C11—C12—C13—C18	−0.9 (4)	C30—C31—C32—C37	0.1 (4)
C12—C13—C14—C15	179.3 (3)	C31—C32—C33—C34	178.3 (3)

C12—C13—C18—C9	0.5 (4)	C31—C32—C37—C28	1.1 (4)
C12—C13—C18—C17	179.1 (3)	C31—C32—C37—C36	−178.5 (3)
C13—C14—C15—C16	1.3 (5)	C32—C33—C34—C35	1.0 (5)
C14—C13—C18—C9	179.9 (2)	C33—C32—C37—C28	−179.2 (3)
C14—C13—C18—C17	−1.4 (4)	C33—C32—C37—C36	1.2 (4)
C14—C15—C16—C17	−1.0 (4)	C33—C34—C35—C36	−0.5 (5)
C15—C16—C17—N1	179.3 (2)	C34—C35—C36—N3	179.0 (3)
C15—C16—C17—C18	−0.6 (4)	C34—C35—C36—C37	0.3 (4)
C16—C17—C18—C9	−179.5 (2)	C35—C36—C37—C28	179.7 (3)
C16—C17—C18—C13	1.8 (4)	C35—C36—C37—C32	−0.7 (4)
C17—N1—C8—N2	4.4 (4)	C36—N3—C27—N4	1.0 (4)
C17—N1—C8—C7	−171.5 (2)	C36—N3—C27—C26	−176.3 (2)
C18—C9—C10—C11	0.3 (4)	C37—C28—C29—C30	0.6 (4)
C18—C13—C14—C15	−0.1 (4)	C37—C32—C33—C34	−1.4 (4)
C19—N1—C8—N2	−168.0 (3)	C38—N3—C27—N4	−172.2 (3)
C19—N1—C8—C7	16.1 (4)	C38—N3—C27—C26	10.6 (4)
C19—N1—C17—C16	−11.1 (4)	C38—N3—C36—C35	−5.7 (4)
C19—N1—C17—C18	168.9 (2)	C38—N3—C36—C37	173.1 (3)